Advanced Quantum Theory A (notes)

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Contents

Chapter 1

Quantum states and quantum dynamics

1.1 The quantum formalism

1.1.1 States

In classical mechanics the state of a system at a given time is defined by list of values of the various coordinates q_i and momenta p_i. In quantum theory (henceforth QT) the state is a vector, typically denoted $|\psi\rangle$, which resides in an abstract complex linear vector space, Hibert space $\mathcal{H}$. More precisely, $|\psi\rangle$ and $c|\psi\rangle$ with c a complex number represent the same quantum state. We say that a quantum state is a ray in $\mathcal{H}$. Each physical system has its own $\mathcal{H}$. Like any vector space, $\mathcal{H}$ always contains a unique zero vector $|0\rangle$. The state $0 \cdot |\psi\rangle$ is $|0\rangle$ (the null or zero state). The well known wave functions of the elementary quantum course are particular aspects of the corresponding $|\psi\rangle$.

That $\mathcal{H}$ is a linear space means that combinations of the form

$$\alpha_1|\psi_1\rangle + \alpha_2|\psi_2\rangle + \alpha_3|\psi_3\rangle + \cdots , \tag{1.1}$$

with the α_j complex constants, belong to $\mathcal{H}$ and are also legal quantum states. As in *any* linear vector space, each vector or state in $\mathcal{H}$ can be written exactly as a linear superposition of basis vectors: $|\psi\rangle = \sum \alpha_n |b_n\rangle$.

Some physical systems like the spin of a particle have a finite Hilbert space, namely one having a finite number of basis vectors $|b_n\rangle$. This number is the dimension of $\mathcal{H}$. Others, like the center of mass of a multiparticle system, have an infinite $\mathcal{H}$ whose basis always contains an infinite number of basis vectors. These last can be chosen as a discrete set or a continuous one.

The state of type $|\psi\rangle$ is said to be a *ket* state. As customary in the subject of vector spaces, each vector $|\psi\rangle \in \mathcal{H}$ can be assigned a dual or *adjoint* state which resides in the dual Hilbert space.[1] This type of state is called a *bra* state, denoted $\langle\psi|$. We should think of the bra $\langle\phi|$ as obtained from $|\phi\rangle$ by a special kind of conjugation called *taking the adjoint*. Thus $|\phi\rangle^\dagger = \langle\phi|$. With bras and kets the definition of a *scalar product*s of two states $|\psi\rangle$ and $|\phi\rangle$ is possible. This is, in general, a complex number, denoted $\langle\phi|\psi\rangle$, which is linear in its second argument and antilinear in its first, that is

$$\langle\phi|\big(\alpha_1|\psi_1\rangle + \alpha_2|\psi_2\rangle\big)\rangle = \alpha_1\langle\phi|\psi_1\rangle + \alpha_2\langle\phi|\psi_2\rangle \tag{1.2}$$

$$\langle\big(\alpha_1|\phi_1\rangle + \alpha_2|\phi_2\rangle\big)|\psi\rangle = \alpha_1^*\langle\phi_1|\psi\rangle + \alpha_2^*\langle\phi_2|\psi\rangle \tag{1.3}$$

For this to be consistent we must have

$$\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^* \tag{1.4}$$

It is fruitful to regard the scalar product as the product of a bra with a ket.

Note that the scalar product of any state with the null state vanishes. Whenever $\langle\psi|\phi\rangle = 0$ while neither $|\psi\rangle$ nor $|\phi\rangle$ are null, we say the two states are *orthogonal*. Of course one can consider the self-scalar product $\langle\psi|\psi\rangle$. Obviously this is real, but it is postulated to also be strictly positive unless the state in question is null, in which case the scalar product vanishes. $\langle\psi|\psi\rangle$ is said to be norm of $|\psi\rangle$.

1.1.2 Operators

One needs to define operators in Hilbert space, designated as $\hat{O}, \hat{A}$, etc. An operator maps a particular state to another state in $\mathcal{H}$. In quantum theory we only need linear or antilinear operators, that is,

$$\hat{O}\big(\alpha_1|\psi_1\rangle + \alpha_2|\psi_2\rangle\big) = \alpha_1\hat{O}|\psi_1\rangle + \alpha_2\hat{O}|\psi_2\rangle \qquad \text{(linear)} \tag{1.5}$$

$$\hat{O}\big(\alpha_1|\psi_1\rangle + \alpha_2|\psi_2\rangle\big) = \alpha_1^*\hat{O}|\psi_1\rangle + \alpha_2^*\hat{O}|\psi_2\rangle \qquad \text{(antilinear)} \tag{1.6}$$

[1] first discussed by the leading German mathematician David Hilbert (1862-1943).

There is a trivial operator, $\hat{I}$, which leaves *all* states unchanged: $\hat{I}|\phi\rangle = |\phi\rangle$.

What is $(\hat{A}|\phi\rangle)^\dagger$? Obviously it must be a bra. It is customary to denote it by $\langle\phi|\hat{A}^\dagger$ where $\hat{A}^\dagger$ is an operator related in a particular way to $\hat{A}$ which always acts on bras from the right. Roughly $\hat{A}^\dagger$ is the conjugate of $\hat{A}$, but it is more properly called the Hermitian conjugate[2] of $\hat{A}$ or the adjoint of $\hat{A}$. Suppose we replace $|\psi\rangle$ in equation (1.4) by $\hat{A}|\psi\rangle$. Then we have the useful identity

$$\langle\phi|\hat{A}|\psi\rangle = \langle\psi|\hat{A}^\dagger|\phi\rangle^* \tag{1.7}$$

Objects such as these are called matrix elements of $\hat{A}$, and will be explored further later on.

Special importance attaches to the *Hermitian operators*, those which obey

$$\hat{O}^\dagger = \hat{O} \tag{1.8}$$

In QT one requires measurable quantities such as position or angular momentum of a particle, energy of a collection of particles, etc. to be represented by Hermitian operators. The reason is that in QT the average of measurements in state $|\psi\rangle$ of a quantity represented by $\hat{O}$ is $\langle\psi|\hat{O}|\psi\rangle$. If $\hat{O}$ is Hermitian then by Eq. (1.7) its average is always real (what would we do with complex average momentum?).

Every operator has *eigenvectors* or *eigenstates*, states which are essentially unchanged under the operators action. For example, $\hat{O}|a\rangle = \lambda|a\rangle$ where λ is a possibly complex number. Here $|a\rangle$ is an eigenvector of $\hat{O}$ and λ is its *eigenvalue*. There are usually several eigenvectors (eigenvalues), and their number can be infinite if $\hat{O}$ operates in an infinite Hilbert space. It is possible for two or more eigenvectors to have a common eigenvalue, in which case they are said to be *degenerate*.

It is well known that any Hermitian operator $\hat{A}$ has only real eigenvalues, and the eigenvectors with distinct eigenvalues must all be mutually orthogonal to one another:

$$\hat{A}|a_j\rangle = \lambda_j|a_j\rangle; \qquad \langle a_i|a_j\rangle = 0 \ \text{ if and only if } \ \lambda_i \neq \lambda_j \tag{1.9}$$

The quantum doctrine holds that if $\hat{A}$ represents a physical quantity, then any ideal (errorless) measurement of that quantity can only yield an eigenvalue

[2]named in memory of the French mathematician Charles Hermite (1822-1901)

of $\hat{A}$. Since only real quantities are measured, this is another reason for representing measurable quantities only by Hermitian operators.

But *Hermiticity*[2] (being Hermitian) is not sufficient to make an operator $\hat{A}$ suitable to represent a measurable quantity. It is also necessary that all of $\hat{A}$'s eigenvectors constitute a complete set, that is that they can be used as a basis of the Hilbert space in which $\hat{A}$ acts. This makes it possible to express the action of $\hat{A}$ exclusively in terms of its eigenvectors and eigenvalues. For example, given a generic state $|\psi\rangle$ in $\mathcal{H}$ we expand it as $|\psi\rangle = \sum_j \alpha_j |a_j\rangle$. Then obviously

$$\hat{A}|\psi\rangle = \sum_j \alpha_j \lambda_j |a_j\rangle \tag{1.10}$$

An Hermitian operator whose eigenvectors constitute a complete set is said to be an *observable*.

Degenerate eigenvectors of an Hermitian operator are not automatically mutually orthogonal. But then one can use *Hilbert-Schmidt orthogonalization* to construct an equal number of linear combinations of them all sharing of course, the same eigenvalue, but being mutually orthogonal. Unless otherwise specified, we assume that all eigenvectors of an Hermitian operator are mutually orthogonal. Thus an observable supplies an *orthogonal basis* for $\mathcal{H}$.

Exercises:

1. Prove that $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger$, and hence that the product of two Hermitian operators is itself Hermitian only if the operators commute.

2. By exploiting Hermitian conjugation prove that any two nondegenerate eigenvectors of an Hermitian operator are orthogonal, but that this is not necessarily true for non-Hermitian operators or for degenerate eigenvectors of Hermitian operators.

Example: Spin

We know that an electron (or any lepton or quark) has a *dichotomic* degree of freedom called *spin*. Dichotomic means there are two possible values to it, namely $+\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$. Thus we can take the generic state of spin to be

$$|\zeta\rangle = \begin{pmatrix} a \\ b \end{pmatrix} \tag{1.11}$$

with a and b complex, each indicating probability amplitude for the respective spin value. $\mathcal{H}$ is the collection of all such "vectors". It is customary to restrict discussion to those normalized according to $|a|^2+|b|^2 = 1$. The vectorial spin operator $\boldsymbol{s}$ is $\frac{1}{2}\hbar$ times the triplet of Pauli[3] matrices $\boldsymbol{\sigma}$, where

$$\boldsymbol{\sigma} = \{\sigma_1, \sigma_2, \sigma_3\}; \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_2 = \begin{pmatrix} 0 & -\imath \\ \imath & 0 \end{pmatrix}; \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.12}$$

Focus on the third (or z) component of spin. Evidently the normalized eigenvectors of $\frac{1}{2}\hbar\sigma_3$ are

$$|\uparrow\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{and} \qquad |\downarrow\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{1.13}$$

with eigenvalues $\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$, respectively. These eigenvectors are a complete set because they can be used as a basis for $\mathcal{H}$: we can write the generic spin state (1.11) as $a|\uparrow\rangle + b|\downarrow\rangle$. It can be seen that $\mathcal{H}$ for one-particle's spin is of dimension 2.

There are other bases; for example the two vectors

$$|\rightarrow\rangle \equiv \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \text{and} \qquad |\leftarrow\rangle \equiv \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{1.14}$$

are normalized eigenvectors of $\frac{1}{2}\hbar\sigma_1$ (x component of spin) with eigenvalues $\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$, respectively. A similar statement applies for σ_2 or for the spin in direction $\boldsymbol{n}$, $\frac{1}{2}\hbar\boldsymbol{n}\cdot\boldsymbol{\sigma}$. This corresponds to the wisdom that an ideal

[3]Wolfgang Pauli (1900-1958) was an Austrian Swiss physicist of Jewish origin, one of the founders of quantum mechanics (exclusion principle) and quantum field theory, and a Nobel laureate.

measurement of the spin of an electron in any particular direction can only give of $\frac{1}{2}\hbar$ or $\frac{1}{2}\hbar$.

Notice that $|\leftarrow\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle + \frac{1}{\sqrt{2}}|\downarrow\rangle$ while $|\rightarrow\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\rangle$. This is an example of the general rule that any normalized basis of $\mathcal{H}$ can be expressed as a particular kind of linear transformation, a *unitary* one, of any other normalized basis. We shall define and see other uses of unitary transformations in Sec. 1.2.4

1.1.3 Projectors and completeness

The construction $|\phi\rangle\langle\psi|$ can be regarded as an operator. When applied to the state $|\chi\rangle$ it is defined to give the state $|\phi\rangle$ multiplied by the complex number $\langle\psi|\chi\rangle$. In fact, one of the advantages of the Dirac formalism/notation[4] is that this rule is obvious:

$$(|\phi\rangle\langle\psi|)\,|\chi\rangle = |\phi\rangle\,\langle\psi|\chi\rangle \tag{1.15}$$

Mostly this notation is used with $|\psi\rangle$ and $|\phi\rangle$ identical. For example, if the observable $\hat{A}$ has the eigenstates $|a_1\rangle, |a_2\rangle, \cdots$, it is useful to construct $\hat{P}_1 \equiv |a_1\rangle\langle a_1|, \hat{P}_2 \equiv |a_2\rangle\langle a_2|, \cdots$ which are called *projectors*. Obviously $\hat{P}_i|a_j\rangle = \delta_{ij}|a_j\rangle$, so when $\hat{P}_j$ is applied to a generic state $|\psi\rangle$, the result is the state $|a_j\rangle$ up to the factor $\langle a_j|\psi\rangle$. The projector P_j has projected the state $|\psi\rangle$ into the eigenstate $|a_j\rangle$ just as we can project an arbitrary vector onto one of the coordinate axes. The $\langle a_j|\psi\rangle$ is the analogue of the direction cosine of the vector with respect to (w.r.t.) that axes, and is referred to as the amplitude to find $|a_j\rangle$ in $|\psi\rangle$.

As an example, the projector onto the state with x component of spin $-\frac{1}{2}\hbar$ is

$$P_{\leftarrow} = |\leftarrow\rangle\langle\leftarrow| = \frac{1}{2}\begin{pmatrix}1\\-1\end{pmatrix}\begin{pmatrix}1 & -1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & -1\\-1 & 1\end{pmatrix} \tag{1.16}$$

(we do not put a ˆ over $P_{\leftarrow}$; it is not customary to label matrices as operators though they sometimes are). This example shows that hermitian operators

[4] named after Nobel Laureate Paul Adrien Maurice Dirac (1902-1984), greatest of British physicists of the 20th century. He formulated the relativistic wave equation for the electron, predicted antiparticles, constructed the compact quantum formalism, and contributed to quantum field theory.

can be represented by square matrices. Note that the trace of the matrix is unity; this is a general rule for projectors.

Returning to our generic observable $\hat{A}$ we can consider applying the sum of *all* its distinct projectors on state $|\psi\rangle$:

$$\sum_j \hat{P}_j |\psi\rangle = \sum_j |a_j\rangle \langle a_j|\psi\rangle \tag{1.17}$$

Because $\hat{A}$ is an observable, the set of $|a_j\rangle$ must be complete. Thus every base vector of the Hilbert space appears in the above sum, and is multiplied by the appropriate "direction cosine"; this means the sum is just $|\psi\rangle$ broken up along the various "axes" in Hibert space. Since $|\psi\rangle$ was arbitrary it must thus be true that

$$\sum_j \hat{P}_j = \hat{I}. \tag{1.18}$$

This result is called the "decomposition of the identity". It is true only if the set of states used to build the projectors is complete; thus it is evidently true for any observable.

We can also use projectors to define a function of any observable $\hat{A}$. Denote again its various eigenstates $|a_1\rangle, |a_2\rangle, \cdots$ with eigenvalues $a_1, a_2, \cdots$. We understand that because of degeneracy not all a_j may be distinct. Now built the corresponding projectors $\hat{P}_1, \hat{P}_2, \cdots$ and define, for any function $f(x)$,

$$f(\hat{A}) \equiv \sum_j f(a_j)\hat{P}_j. \tag{1.19}$$

This is a reasonable definition since for any i, $f(\hat{A})|a_i\rangle = f(a_i)\hat{P}_i|a_i\rangle = f(a_i)|a_i\rangle$ assuming that we have normalized all the eigenstates to unity:

$$\langle a_i|a_k\rangle = \delta_{ik}. \tag{1.20}$$

Of course finding out all eigenvectors and eigenvalues can be an enormous task, so when this is not feasible another definition is possible, provided $f(x)$ is analytic. We may then expand f:

$$f(x) = \sum_n f^{[n]}(0)x^n/n! \tag{1.21}$$

Since the notion of a power of $\hat{A}$ is clear, we may define

$$f(\hat{A}) \equiv \sum_n f^{[n]}(0)\hat{A}^n/n! \tag{1.22}$$

If f is singular at $x = 0$ we may try expanding at a different point. We shall often use these definition of function of an operator.

Exercises:

1. Prove that any projector $\hat{P}_j$ is Hermitian. In addition prove that if the $\hat{P}_j$ are associated with distinct eigenstates of an Hermitan operator, then $\hat{P}_i\hat{P}_j = \delta_{ij}$.

2. Prove that according to both definitions given above $f(\hat{A})$ is an observable if $\hat{A}$ is.

Projectors are also useful in discussing the theory of quantum measurements. We have mentioned that when an observable $\hat{O}$ is subject to an ideal measurement, the result can only be one of its eigenvalues. But which one? And if the state one started with was $|\psi\rangle$, what is the state after the measurement? Suppose the eigenvalue λ is n-fold degenerate, which means that eigenvectors $|N\rangle, |N+1\rangle, \cdots |N+n\rangle$ all share this eigenvalue. The corresponding projectors are $\hat{P}_N, \hat{P}_{N+1}, \cdots \hat{P}_{N+n}$. Then the probability that eigenvalue λ is the outcome of the measurement is equal to

$$\text{Prob}(\hat{A} = \lambda) = \langle\psi| \sum_{j=N}^{N+n} P_j|\psi\rangle. \tag{1.23}$$

In addition, if λ was the outcome, measurement "collapses" the initial state according to

$$|\psi\rangle \to \sum_{j=N}^{N+n} P_j|\psi\rangle. \tag{1.24}$$

As a special case, if the eigenvalue in $|N\rangle$ is non-degenerate, then the probability that λ_N will turn up when we measure $\hat{A}$ in state $|\psi\rangle$ is equal, by

virtue of Eq. (1.4), to $|\langle N|\psi\rangle|^2$, namely the absolute square of the amplitude that $|N\rangle$ is found in $|\psi\rangle$. Additionally, in the aftermath of the measurement the state will be $\langle N|\psi\rangle\ |N\rangle$. This last has still to be normalized.

1.2 Continuous spectrum

1.2.1 Configuration space

We have discussed eigenvalues and eigenvectors as if the former form a discrete set, whether finite or infinite. However, there are observables and other oprerators of use in QT whose *spectrum* or set of eigenvalues is a continuum, e.g., the coordinates of a particle. Here we shall use this example to illustrate the changes required of the formalism to deal with a continuous spectrum.

We may say that if the x coordinate is represented by the Hermitian operator $\hat{x}$, then we have

$$\hat{x}|x\rangle = x|x\rangle \tag{1.25}$$

The eigenvector, which describes a particle precisely at x, is thus labeled with real numbers, not integers as before. It is a matter of experience that the spectrum of $\hat{x}$ is the whole real line: $x \in (-\infty, +\infty)$ (a non-countable infinity of eigenvalues). We shall thus assume that the set of $|x\rangle$ is complete. Likewise experience tells us that the x eigenvalues are non-degenerate. It is still true that $\langle x_1|x_2\rangle = 0$, but we cannot write the analog of condition (1.20) because the norm of a continuum state diverges. Instead we opt for *continuum normalization* in terms of the Dirac delta function:

$$\langle x_1|x_2\rangle = \delta(x_1 - x_2). \tag{1.26}$$

Together with this come slight variations on our previous notation. Thus

$$P_x = |x\rangle\langle x| \tag{1.27}$$

$$\hat{I} = \int_{-\infty}^{\infty} |x\rangle\langle x|\ dx \tag{1.28}$$

All the rest of the discussion is unchanged.

Of course we know that there are additional coordinates y and z. With them come the additional observables $\hat{y}$ and $\hat{z}$. We may now speak about

joint eigevector for all coordinates $|x\rangle \otimes |y\rangle \otimes |z\rangle$. The $\otimes$ here represents a tensor product of the Hilbert space of $\hat{x}$. that of $\hat{y}$, etc. A particular ket like in this product space, $|x\rangle \otimes |y\rangle \otimes |z\rangle$, is constructed by taking one member of $\mathcal{H}(x)$, one from $\mathcal{H}(y)$, etc. and grouping them together. The factor $|x\rangle$ in this product is "seen" only by $\hat{x}$, etc. so that instead of $\hat{x}$ we should write $\hat{x} \otimes \hat{I}_y \otimes \hat{I}_z$, except we shall not be that pedantic. We may thus use the notation $|\boldsymbol{r}\rangle = |x\rangle \otimes |y\rangle \otimes |z\rangle$. Then

$$\langle \boldsymbol{r}|\boldsymbol{r}'\rangle = \delta(\boldsymbol{r}-\boldsymbol{r}') \equiv \delta(x-x')\delta(y-y')\delta(z-z') \quad (1.29)$$

$$\hat{P}_{\boldsymbol{r}} = |\boldsymbol{r}\rangle\langle\boldsymbol{r}| \quad (1.30)$$

$$\hat{I} = \int |\boldsymbol{r}\rangle\langle\boldsymbol{r}|\ d^3r \equiv \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |x\rangle\langle x| \otimes |y\rangle\langle y| \otimes |z\rangle\langle z|\, dx\, dy\, dz \quad (1.31)$$

The above "factorization" of coordinates is allowed because experience shows that x, y and z are not only independent coordinates but the x, y and z of a particle can be measured independently without any "interference" among them. Thus if we operate with $\hat{x}\hat{y}$ (more pedantly $\hat{x} \otimes \hat{y}$) on a state $|\boldsymbol{r}\rangle$ we must get $xy|\boldsymbol{r}\rangle$, and if we apply rather $\hat{y}\hat{x}$ we get $yx|\boldsymbol{r}\rangle$ which is the same. Thus $(\hat{x}\hat{y} - \hat{y}\hat{x})|\boldsymbol{r}\rangle = 0$. And since $|\boldsymbol{r}\rangle$ is a (triply) complete set, this means that

$$[\hat{x}, \hat{y}] \equiv \hat{x}\hat{y} - \hat{y}\hat{x} = 0, \quad \text{etc.} \quad (1.32)$$

In words, the *commutators* of $\hat{x}$ with $\hat{y}$, etc. vanish. This may seem trivial, but it is important because not every pair of observable in QT commute, and when they do not, rather odd things happen which have been verified experimentally.

Let us now operate with the decomposition of the identity, Eq. (1.31), on an arbitrary particle state $|\psi\rangle$ in $\mathcal{H}$:

$$|\psi\rangle = \hat{I}|\psi\rangle = \int |\boldsymbol{r}\rangle\, \langle\boldsymbol{r}|\psi\rangle\ d^3r \quad (1.33)$$

Obviously $|\psi\rangle$ is broken up along all "axes" $|\boldsymbol{r}\rangle$ in configuration space. The quantity $\langle\boldsymbol{r}|\psi\rangle$, which is also denoted $\psi(\boldsymbol{r})$, is the amplitude with which a particular position $\boldsymbol{r}$ appears in the particles' state $|\psi\rangle$. It is the usual wave function of elementary quantum mechanics. It is customary to say that it is the *position representation* of state $|\psi\rangle$.

Two familiar results for wave functions may be recovered by sandwiching $\hat{I}$ in the form (1.31) between two states:

$$\langle\psi|\phi\rangle = \langle\psi|\hat{I}|\phi\rangle = \int \langle\psi|\boldsymbol{r}\rangle\langle\boldsymbol{r}|\phi\rangle\, d^3r = \int \psi(\boldsymbol{r})^*\,\phi(\boldsymbol{r})\, d^3r, \tag{1.34}$$

$$\langle\psi|\psi\rangle = \langle\psi|\hat{I}|\psi\rangle = \int \langle\psi|\boldsymbol{r}\rangle\langle\boldsymbol{r}|\psi\rangle\, d^3r = \int \psi(\boldsymbol{r})^*\,\psi(\boldsymbol{r})\, d^3r \tag{1.35}$$

Thus the scalar product and the norm defined between abstract states coincides with those calculated with wave functions using the old algorithms. This makes it clear that there is an exact correspondence between QT in the Dirac formalism and elementary quantum mechanics. We shall always normalize states of system (as opposed to eigenvectors of observables with continuous spectrum) according to $\langle\psi|\psi\rangle = 1$ in order to agree with elementary quantum mechanics.

1.2.2 Momentum space

In classical mechanics momentum is canonically conjugate to coordinate, i.e.

$$\{x, p_x\}_P = \{y, p_y\}_P = \{z, p_z\}_P = 1 \tag{1.36}$$

$$\{x, p_y\}_P = \{x, p_z\}_P = \{z, p_y\}_P = \cdots = 0 \tag{1.37}$$

with $\{\quad,\quad\}_P$ denoting the Poisson bracket. In QT all these quantities will be Hermitian operators: $\hat{p}_x, \hat{p}_y, \hat{p}_z, \hat{\boldsymbol{p}}$.

Experience teaches that each momentum component can take on any real value, and that there is no degeneracy. Thus $\hat{\boldsymbol{p}}$ must have a continuous (triple) spectrum, just like $\hat{\boldsymbol{r}}$. Obviously $\hat{\boldsymbol{p}}$ will have the eigenvectors $|\boldsymbol{p}\rangle$ obeying

$$\hat{\boldsymbol{p}}|\boldsymbol{p}\rangle = \boldsymbol{p}|\boldsymbol{p}\rangle; \qquad |\boldsymbol{p}\rangle \equiv |p_x\rangle \otimes |p_y\rangle \otimes |p_z\rangle. \tag{1.38}$$

They evidently form a complete set which makes $\hat{\boldsymbol{p}}$ an observable too.

The following relations about momentum are true, in analogy with what

was said about coordinates:

$$\begin{aligned} \langle \boldsymbol{p}_1 | \boldsymbol{p}_2 \rangle &= \delta(\boldsymbol{p}_1 - \boldsymbol{p}_2) && (1.39) \\ \hat{P}_{\boldsymbol{p}} &= |\boldsymbol{p}\rangle\langle\boldsymbol{p}| && (1.40) \\ \hat{I} &= \int |\boldsymbol{p}\rangle\langle\boldsymbol{p}| \; d^3p && (1.41) \\ [\hat{p}_x, \hat{p}_y] &= 0, \quad \text{etc.} && (1.42) \\ |\psi\rangle &= \int |\boldsymbol{p}\rangle \, \langle\boldsymbol{p}|\psi\rangle \; d^3p && (1.43) \end{aligned}$$

as well as

$$\langle\psi|\psi\rangle = \langle\psi|\hat{I}|\psi\rangle = \int \langle\psi|\boldsymbol{p}\rangle\langle\boldsymbol{p}|\psi\rangle \, d^3p = \int \psi(\boldsymbol{p})^* \, \psi(\boldsymbol{p}) \, d^3p \qquad (1.44)$$

The quantity $\langle\boldsymbol{p}|\psi\rangle$, which is also denoted $\psi(\boldsymbol{p})$, is the amplitude with which a particular momentum $\boldsymbol{p}$ appears in the state $|\psi\rangle$. $\psi(\boldsymbol{p})$ is the *momentum representation* of state $|\psi\rangle$. One can write the scalar products between and norms of states in terms of $\psi(\boldsymbol{p})$ alone in analogy with Eqs. (1.34) and (1.35).

Now using the decomposition of the identity, once in form (1.31) and once in form (1.41) we get

$$|\boldsymbol{p}\rangle = \hat{I}|\boldsymbol{p}\rangle = \int |\boldsymbol{r}\rangle\langle\boldsymbol{r}|\boldsymbol{p}\rangle \qquad (1.45)$$

$$|\boldsymbol{r}\rangle = \hat{I}|\boldsymbol{r}\rangle = \int |\boldsymbol{p}\rangle\langle\boldsymbol{p}|\boldsymbol{r}\rangle \qquad (1.46)$$

One can thus transform from position basis $\{|\boldsymbol{r}\rangle\}$ to momentum basis $\{|\boldsymbol{p}\rangle\}$ by a linear transformation with coefficients $\langle\boldsymbol{r}|\boldsymbol{p}\rangle$ or their complex conjugates $\langle\boldsymbol{p}|\boldsymbol{r}\rangle$. Said differently one can transform $\psi(\boldsymbol{r})$ to $\psi(\boldsymbol{p})$ or viceversa, e.g.

$$\psi(\boldsymbol{p}) = \langle\boldsymbol{p}|\psi\rangle = \langle\boldsymbol{p}|\hat{I}|\psi\rangle = \int \langle\boldsymbol{p}|\boldsymbol{r}\rangle\langle\boldsymbol{r}|\psi\rangle \, d^3r = \int \langle\boldsymbol{p}|\boldsymbol{r}\rangle\psi(\boldsymbol{r})d^3r \qquad (1.47)$$

using the same coefficients (to be calculated in Sec. 1.2.4).

Think of the $\langle\boldsymbol{p}|\boldsymbol{r}\rangle$ as components of an infinite matrix $\mathcal{U}$ with continuous (triple) indeces $\boldsymbol{p}$ and $\boldsymbol{r}$. The transposed matrix is $\langle\boldsymbol{r}|\boldsymbol{p}\rangle$. Simlarly, think of $\langle\boldsymbol{p}|\psi\rangle$ and $\langle\boldsymbol{r}|\psi\rangle$ as continuous column vectors $\Psi_{\boldsymbol{p}}$ and $\Psi_{\boldsymbol{r}}$. Then Eq. (1.47)

can be written as $\Psi_{\boldsymbol{p}} = \mathcal{U}\Psi_{\boldsymbol{r}}$. Now take the Hermitian conjugate (the conjugate of the transpose, denoted also by a †) of this equation (recall that transposing switches the indeces of the matrix), to get

$$\Psi^\dagger_{\boldsymbol{p}} = (\mathcal{U}\,\Psi_{\boldsymbol{r}})^\dagger = \Psi^\dagger_{\boldsymbol{r}}\,\mathcal{U}^\dagger \tag{1.48}$$

Thus

$$1 = \int \psi(\boldsymbol{p})^*\psi(\boldsymbol{p})\,d^3p = \Psi^\dagger_{\boldsymbol{p}}\,\Psi_{\boldsymbol{p}} = \Psi^\dagger_{\boldsymbol{r}}\,\mathcal{U}^\dagger\,\mathcal{U}\,\Psi_{\boldsymbol{r}} \tag{1.49}$$

where we are applying the unit normalization convention and relying on Eq. (1.44). Of course we now must have by equation(1.35) that $\Psi^\dagger_{\boldsymbol{r}}\,\Psi_{\boldsymbol{r}} = 1$, all this for arbitrary $|\psi\rangle$. Thus

$$\mathcal{U}^\dagger\,\mathcal{U} = \mathcal{I} \tag{1.50}$$

where $\mathcal{I}$ is the *unit matrix* with appropriate indeces. A matrix with property (1.50) is said to be a *unitary matrix*. We can see that such a matrix must be involved in every transformation between two bases in Hilbert space. And because of the property (1.50) such transformations always preserve the norms of the vectors involved.

1.2.3 Position-momentum incompatibility

Dirac gave a fundamental rule for transferring information from classical to quantum mechanics. For two classical quantities $A(q,p)$ and $B(q,p)$ we obtain the quantum theory by replacing them by suitable observables, and requiring that the commutator of these be $\imath\hbar$ times the Poisson bracket of the classical quantities suitably expressed as an observable. Thus

$$\{A(q,p), B(q,p)\}_P = C(q,p) \Longrightarrow \left[\hat{A}, \hat{B}\right] = \imath\hbar\hat{C} \tag{1.51}$$

In particular, if $A = x$ and $B = p_x$ or p_y we obtain in light of Eq. (1.36) that

$$[\hat{x}, \hat{p}_x] = \imath\hbar; \qquad [\hat{x}, \hat{p}_y] = 0; \qquad [\hat{y}, \hat{p}_x] = 0; \quad \cdots \tag{1.52}$$

The first equation here says a coordinate and its conjugate momentum do not commute (coordinate and another coordinate'ss conjugate momentum do commute).

This is a momentous constraint—one of the key points of QT. We saw that it is possible to speak of joint eigenstates of $\hat{x}$ and $\hat{y}$, namely $|x, y\rangle \equiv |x\rangle \otimes |y\rangle$. If there were a $|x, p_x\rangle$ we could operate on it with the first of Eqs. (1.52) to get

$$[\hat{x}, \hat{p}_x]\,|x, p_x\rangle = (xp_x - p_x x)|x, p_x\rangle = 0 = \imath\hbar|x, p_x\rangle \tag{1.53}$$

which is nonsense! This means there is no such thing as $|x, p_x\rangle$: it is impossible to know the position and conjugate momentum in the same directions of the same particle under the same circumstances. The scale of this prohibition (which is totally absent in classical mechanics) is measured by $\hbar$, the quantum of action. However, nothing prevents us from knowing at once both x and p_y of the same particle since $\hat{x}$ commutes with $\hat{p}_y$.

The Heisenberg uncertainty principle[5] follows from $[\hat{x}, \hat{p}_x] = \imath\hbar$. More generally, if we have the commutator of Eq. (1.51) then Robertson's[6] theorem tells us that if we define the uncertainty ΔO of an operator $\hat{O}$ in a state $|\psi\rangle$ as the root mean square of it about its mean,

$$\Delta O \equiv \left(\langle\psi|\hat{O}^2|\psi\rangle - (\langle\psi|\hat{O}|\psi\rangle)^2\right)^{1/2}, \tag{1.54}$$

then in light of the notation (1.51)

$$\Delta A \Delta B \geq \tfrac{1}{2}|\langle\psi|\hat{C}|\psi\rangle\,. \tag{1.55}$$

A special case is Heisenberg's uncertainty principle

$$\Delta x \Delta p_x \geq \tfrac{1}{2}\hbar\,, \tag{1.56}$$

where the r.h.s. is the same for all states.

[5] devised by Werner Karl Heisenberg (1901-1976), a German physicist who contributed not only to quantum theory, and quantum field theory, but to nuclear physics, solid state physics and the theory of turbulent flow. His role in the failed German nuclear bomb project during the Nazi regime made him an unwelcome person in many circles after the war.

[6] Howard Percy Robertson (1903-1961) was an American physicist who made contributions to quantum theory and theoretical cosmology (the FRW metric), and codiscovered the Poynting-Robertson effect.

1.2.4 Observables as differential operators

The commutators (1.52) allow us to represent the observable $\hat{\boldsymbol{p}}$ as a differential operator in position space. Obviously the wave function or position representation of $\hat{p}_x|\psi\rangle$ is

$$\langle x|\hat{p}_x|\psi\rangle = \int_{-\infty}^{\infty}\langle x|\hat{p}_x|x'\rangle\,\langle x'|\psi\rangle\,dx' = \int_{-\infty}^{\infty}\langle x|\hat{p}_x|x'\rangle\,\psi(x')\,dx'. \tag{1.57}$$

Let us calculate $\langle x|\hat{p}_x|x'\rangle$, called the *matrix element* of $\hat{p}_x$ in position representation. To this end we form the corresponding matrix element of the first Eq. (1.52):

$$\begin{aligned} \langle x|\hat{x}\,\hat{p}_x|x'\rangle - \langle x|\hat{p}_x\,\hat{x}|x'\rangle &= \langle x'|\hat{p}_x\,\hat{x}|x\rangle^* - \langle x|\hat{p}_x\,\hat{x}|x'\rangle \\ = x\langle x'|\hat{p}_x|x\rangle^* - x'\langle x|\hat{p}_x\,|x'\rangle &= (x-x')\langle x|\hat{p}_x\,|x'\rangle = \imath\hbar\delta(x-x'). \end{aligned} \tag{1.58}$$

This yields

$$\langle x|\hat{p}_x\,|x'\rangle = \imath\hbar\frac{\delta(x-x')}{x-x'} = -\imath\hbar\delta'(x-x'). \tag{1.59}$$

We now substitute the result (1.59) in (1.57) and perform an integration by parts to take the derivative off the delta function:

$$\langle x|\hat{p}_x|\psi\rangle = \frac{\hbar}{\imath}\frac{d\psi(x)}{dx} \tag{1.60}$$

Accordingly we say that in position representation $\hat{p}_x$ and $\hat{\boldsymbol{p}}$ take the form of the differential operators $(\hbar/\imath)d/dx$ and $(\hbar/\imath)\boldsymbol{\nabla}$, respectively.

Exercises:

1. Justify the manipulations in Eq. (1.58).
2. Prove the identity involving delta functions that is used in (1.59).
3. Prove that in momentum representation $\hat{\boldsymbol{r}}$ takes the form $\imath\hbar\boldsymbol{\nabla}_{\boldsymbol{p}}$.

Let us now calculate $\langle \boldsymbol{r}|\boldsymbol{p}\rangle$; this can be interpreted as the usual wave function of a particle with momentum exactly equal to $\boldsymbol{p}$. Therefore

$$\frac{\hbar}{\imath}\boldsymbol{\nabla}\langle \boldsymbol{r}|\boldsymbol{p}\rangle = \boldsymbol{p}\langle \boldsymbol{r}|\boldsymbol{p}\rangle. \tag{1.61}$$

which we integrate to get

$$\langle \boldsymbol{r}|\boldsymbol{p}\rangle = Ne^{\imath \boldsymbol{p}\cdot\boldsymbol{r}/\hbar} \tag{1.62}$$

where N is an undetermined complex constant. Then using Eqs. (1.29) and (1.31) we have

$$\delta(\boldsymbol{r}-\boldsymbol{r}') = \int \langle \boldsymbol{r}|\boldsymbol{p}\rangle\langle \boldsymbol{p}|\boldsymbol{r}'\rangle\, d^3p = |N|^2 \int e^{\imath(\boldsymbol{p}\cdot\boldsymbol{r}-\boldsymbol{p}\cdot\boldsymbol{r}')/\hbar}\, d^3p\,. \tag{1.63}$$

However, the integral on the r.h.s. is known to be $(2\pi\hbar)^3\delta(\boldsymbol{r}-\boldsymbol{r}')$ (the Fourier representation of the delta function), so that $|N|^2 = (2\pi)^{-3}$. Thus

$$\langle \boldsymbol{r}|\boldsymbol{p}\rangle = (2\pi\hbar)^{-3/2}e^{\imath \boldsymbol{p}\cdot\boldsymbol{r}}\,, \tag{1.64}$$

where we have chosen the phase of N to be zero, this choice having no measurable consequences. If we look back at Eq. (1.47), we see that the transformation of the state from position to momentum representations is done by taking the Fourier transform.

We mentioned earlier the notion of matrix element. Matrix elements are crucial in the computation of transition probabilities for all quantum systems. For any operator $\hat{O}$ (not necessarily an observable), and any states $|\psi\rangle$ and $|\phi\rangle$, we define the matrix element as $\langle\phi|\hat{O}|\psi\rangle$. Of special importance are matrix elements in the position and momentum representations,

$$\langle \boldsymbol{r}|\hat{O}|\boldsymbol{r}'\rangle \qquad \text{and} \qquad \langle \boldsymbol{p}|\hat{O}|\boldsymbol{p}'\rangle, \tag{1.65}$$

respectively. The collection of quantities of each kind carries the same information as the operator $\hat{O}$ by itself. In fact, the two types of matrix elements are related. For suppose that in $\langle \boldsymbol{r}|\hat{O}|\boldsymbol{r}'\rangle$ we insert $\hat{I}$ on either side of the operator, which action causes no changes. Then

$$\langle \boldsymbol{r}|\hat{O}|\boldsymbol{r}'\rangle = \int \langle \boldsymbol{r}|\boldsymbol{p}\rangle\langle \boldsymbol{p}|\hat{O}|\boldsymbol{p}'\rangle\langle \boldsymbol{p}'|\boldsymbol{r}\rangle\; d^3p\; d^3p' \tag{1.66}$$

$$= (2\pi)^{-3}\int \langle \boldsymbol{p}|\hat{O}|\boldsymbol{p}'\rangle\; e^{\imath(\boldsymbol{p}\cdot\boldsymbol{r}-\boldsymbol{p}'\cdot\boldsymbol{r}')}\, d^3p\; d^3p' \tag{1.67}$$

so that one transforms from matrix element in position representation to those in momentum representation by a double Fourier transform. Recalling the $\mathcal{U}$ matrix of Eqs. (1.48) and (1.49), and denoting the matrices whose elements are shown in Eq. (1.65) by $\mathcal{O}_{\boldsymbol{r}}$ and $\mathcal{O}_{\boldsymbol{p}}$, respectively, we may write the last relation as $\mathcal{O}_{\boldsymbol{r}} = \mathcal{U}^\dagger \mathcal{O}_{\boldsymbol{p}} \mathcal{U}$. Thus transformation of the matrix representing an operator from one representation to another is also carried out with help of a unitary matrix. This is actually a special case of a unitary transformation, a notion we now elaborates.

1.2.5 Unitary operators and unitary groups

QT has need of more operators than just the observables. One needs operators to perform certain changes, e.g. symmetry operations, evolution in time of systems, etc. Among the types of additional operators that play a role in QT are the unitary and antiunitary ones.

Recall that the operator $\hat{O}^{-1}$ is called the inverse of $\hat{O}$ if $\hat{O}^{-1}\hat{O} = \hat{I}$ and $\hat{O}\hat{O}^{-1} = \hat{I}$.

$\hat{U}$ is a *unitary operator* if it is linear and $\hat{U}^\dagger = \hat{U}^{-1}$. If $\hat{U}$ is antilinear and $\hat{U}^\dagger = U^{-1}$, then $\hat{U}$ is an *antiunitary operator*. These operators are not observables; they play other roles in QT. Unitary and antiunitary operators also have eigenvalues (complex in general) and eigenvectors. The eigenvalues have unit moduli (they look like $e^{\imath\phi}$ with ϕ real).

Just as there are operations in classical physics, such as rotations, which are carried out by orthogonal matrices, so there are unitary operations in QT. Under the unitary operation connected with the operator $\hat{U}$, all states change according to $|\psi\rangle \to \hat{U}|\psi\rangle$ and all operators $\hat{O}$ change according to $\hat{O} \to \hat{U}\hat{O}\hat{U}^\dagger$. We shall talk about antiunitary operations when we come to the topic of time-reversal symmetry.

There is a significant connection between unitary and Hermitian operators. Every unitary operator $\hat{U}$ can be written as $\exp(\imath\hat{A})$ where $\hat{A}^\dagger = \hat{A}$. This turns out to be a very significant property.

Often a collection of unitary operators forms a *group*. Since the product of two unitary operators is unitary, and products of operators are associative, the collection will constitute a group if it contains the identity operator $\hat{I}$, if

every member operator has an inverse (both left and right) in the collection, and if the product of any two operators is included in the collection. We can label the separate operators of the group by a parameter, e.g. $\hat{U}_\xi$. This ξ can have finite range, be discrete with infinite range, or continuous; thus there are finite groups, discrete infinite groups and continuous groups.

An example of a *finite unitary group* is the *inversion group* with elements $\{\hat{P}, \hat{I}\}$ where $\hat{P}$ inverts $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{p}}$ into $-\hat{\boldsymbol{r}}$ and $-\hat{\boldsymbol{p}}$, and is its own inverse. The group of translations on a lattice is an example of a *discrete unitary infinite group*. The *translation group* with elements $\hat{T}_{\boldsymbol{\rho}}$ we shall study in Sec. 1.2.6 is an example of a *unitary continuous group* (with three parameters).

An important class of continuous groups is made up of the *Lie groups*.[7] A group is a Lie group if all its elements can parametrized by a continuous parameter (or several parameters), and if the generic element can be differentiated w.r.t. it (them). The "space" spanned by the parameter or parameters is called the group manifold. It is a custom to take the origin of the manifold, say $\xi = 0$, to correspond to the identity element $\hat{I}$. Thus for a Lie group one can obtain a formula for the typical element of the group near the identity as follows. We call

$$\hat{G} \equiv -\frac{\hbar}{\imath}\left(\frac{\partial \hat{U}_\xi}{\partial \xi}\right)_{\xi=0} \tag{1.68}$$

the *generator* of the group corresponding to parameter ξ. (A mathematician would drop the factor $\hbar/\imath$.) Then we have the Taylor series.[8]

$$\hat{U}_\xi = \hat{I} - (\imath/\hbar)\xi\hat{G} + \cdots \tag{1.69}$$

Lie proved that knowledge of all the generators of a group and the form their commutators allows one to construct the group, not just near $\hat{I}$, but over a finite part of the group manifold. We shall see an example of this in the next section.

[7] named for Marius Sophus Lie (1842-1899), the Norwegian mathematician who founded the subject of Lie groups and Lie algebras.

[8] named for their inventor Brook Taylor (1685-1731), the British mathematician who invented the calculus of finite differences, and proved his eponymous theorem (which Lagrange called "the main foundation of differential calculus"). Taylor also did work on mechanics.

Exercises:

1. Prove that unitary transformations leave the form of any commutation relations unchanged (invariant).

2. Prove that a unitary transformation of operators and states leaves all expectation values and scalar product between two states invariant.

3. Prove that the product of two unitary operators is unitary.

4. Using series prove that $\exp(\imath\hat{A})$ is a unitary operator if and only if $\hat{A}$ is Hermitian.

1.2.6 Translations

In classical mechanics the momentum of a system is the generator of an infinitesimal canonical transformation whose effect is to translate the system in configuration space. Here we work out the quantum version of this.

When we translate a point, $\boldsymbol{r} \to \boldsymbol{r} + \boldsymbol{\rho}$ where $\boldsymbol{\rho}$ is a constant vector. The collection of such translations is a group since $\boldsymbol{\rho}_1 + \boldsymbol{\rho}_2$ is also a translation, translations are associative, there is a zero translation (the group's identity), and every translation $\boldsymbol{\rho}$ has its inverse $-\boldsymbol{\rho}$. In addition translations commute ($\boldsymbol{\rho}_1 + \boldsymbol{\rho}_2 = \boldsymbol{\rho}_2 + \boldsymbol{\rho}_1$) which makes the group an Abelian group.[9] The group in question is called the *translation group*.

Passing to QT is reasonable to define the translated wave function ψ' by

$$\psi'(\boldsymbol{r}) = \psi(\boldsymbol{r} - \boldsymbol{\rho}). \tag{1.70}$$

The reason for the minus sign is that we take the value of ψ' from the value ψ had at the point which got translated to $\boldsymbol{r}$. Now take $\boldsymbol{\rho}$ in the x direction. The Taylor expansion,

$$\psi(x - \rho_x, y, z) = \psi(\boldsymbol{r}) - \rho\, \partial\psi/\partial x + \frac{1}{2}\rho^2\, \partial^2\psi/\partial x^2 - \cdots \tag{1.71}$$

[9] named for Niels Henrik Abel (1802-1829), a salient Norwegian mathematician, one of the originators of group theory. He applied this theory to prove that roots of polynomial equations of order higher than fourth cannot be solved for in terms of algebraic operations. He also did much work on elliptic functions.

can be formally summed (recall that one can define a function of an operator by its Taylor series) thus giving us

$$\psi'(\boldsymbol{r}) = e^{-\rho\,\partial/\partial x}\psi(\boldsymbol{r}). \tag{1.72}$$

Thus the translation in the x-direction by ρ_x is carried out by the operator

$$\hat{T}_{\rho_x} = e^{-\imath\rho_x\,\hat{p_x}/\hbar} \tag{1.73}$$

which is evidently a unitary operator because the operator $\hat{p}_x$ in the exponential is Hermitian (see Exercise 4 of Sec. 1.2.5). The collection of operators T_{ρ_x} form an Abelian unitary Lie group which is isomorphic to the *translation group* in one dimension (and is thus also referred to as the translation group).

When $\boldsymbol{\rho}$ has three nonvanishing components, we obviously have as translation operator

$$\hat{T}_{\boldsymbol{\rho}} = \hat{T}_{\rho_x}\,\hat{T}_{\rho_y}\,\hat{T}_{\rho_z} = e^{-\imath\boldsymbol{\rho}\cdot\hat{\boldsymbol{p}}/\hbar}, \tag{1.74}$$

the point being that exponentiation of a sum of commuting operators gives the product of the exponents of the operators, as happens for numbers. The group in question, a direct product of three one-dimensional translation groups, is isomorphic to the the translation group in 3 dimensions. It is obviously a 3-parameter unitary Abelian Lie group with three subgroups having like structure.

We now illustrate Lie's theorem that knowledge of the generators of a group and their commutators is sufficient to know the structure of the group well away from the identity. In the infinitesimal neighborhood of the identity, the translation operator can be written in terms of a triplet of generators $\hat{\boldsymbol{p}}$ as

$$\hat{T}_{\delta\boldsymbol{\rho}} = \hat{I} - \imath\,\delta\boldsymbol{\rho}\cdot\hat{\boldsymbol{p}}/\hbar\,. \tag{1.75}$$

This can be generalized to a collection of particles, with the total generator of rotation being the sum of momenta for the constituent particles, i.e., the total momentum.

To get a finite translation by $\boldsymbol{\rho} = N\delta\boldsymbol{\rho}$ with $N \gg 1$ we use the group property to write

$$\hat{T}_{\boldsymbol{\rho}} = (\hat{I} - \imath(\boldsymbol{\rho}/N)\cdot\hat{\boldsymbol{p}}/\hbar)^N \tag{1.76}$$

Comparing this with Euler's[10] result $\lim_{N\to\infty}(1 - s/N)^N = e^s$ we see that this $\hat{T}_{\boldsymbol{\rho}}$ takes the form (1.74). Thus in this case knowledge of the generators (which all commute) provides the structure of the group all over its manifold. This accords with Lie's theorem.

Exercises:

1. Prove that the $\hat{T}_{\boldsymbol{\rho}}$ form an Abelian group isomorphic to the translation group.

2. Prove directly that $\hat{T}_{\boldsymbol{\rho}}\,\hat{\boldsymbol{r}}\,\hat{T}^\dagger_{\boldsymbol{\rho}} = \hat{\boldsymbol{r}} - \boldsymbol{\rho}$.

3. Work out the operator for translations in momentum space?

1.2.7 Rotations

Consider a rotation by angle Ω around an axis in the direction of the unit vector $\boldsymbol{n}$. According to Euler's theorem in analytical mechanics, any rotation can be written this way. A vector $\boldsymbol{v}$ is transformed by said rotation into $R(\boldsymbol{\Omega})\boldsymbol{v}$, where $\boldsymbol{\Omega} \equiv \Omega\boldsymbol{n}$. What is the analog, $\hat{U}_{\boldsymbol{\Omega}}$, to the rotation of the operator $\hat{T}_{\boldsymbol{\rho}}$ for translation?

We can proceed by analogy with Exercise 2 of Sec. 1.2.6. We expect that

$$\hat{U}_{\boldsymbol{\Omega}}\,\hat{\boldsymbol{r}}\,\hat{U}^\dagger_{\boldsymbol{\Omega}} = R(-\boldsymbol{\Omega})\,\hat{\boldsymbol{r}}\,. \tag{1.77}$$

For classical $\boldsymbol{r}$ we know that for infinitesimal $\delta\boldsymbol{\Omega}$, $R(\boldsymbol{\delta\Omega})\,\boldsymbol{r} = \boldsymbol{r} + \delta\boldsymbol{\Omega}\times\boldsymbol{r}$. Thus we should have

$$\hat{U}_{\delta\boldsymbol{\Omega}}\,\hat{\boldsymbol{r}}\,\hat{U}^\dagger_{\delta\boldsymbol{\Omega}} = \hat{\boldsymbol{r}} - \delta\boldsymbol{\Omega}\times\hat{\boldsymbol{r}}\,. \tag{1.78}$$

Now in analogy with Eq. (1.75) we expand $\hat{U}_{\delta\boldsymbol{\Omega}}$ about the identity:

$$\hat{U}_{\delta\boldsymbol{\Omega}} = \hat{I} - \imath\,\delta\boldsymbol{\Omega}\cdot\hat{\boldsymbol{l}}/\hbar\,, \tag{1.79}$$

[10] derived by Leonhard Euler (1707-1783), greatest of Swiss mathematicians, and one of the founders of analytical mechanics and hydrodynamics.

where $\hat{\boldsymbol{l}}$ is the triplet of generators of rotation (required because there are 3 parameters in $\boldsymbol{\Omega}$). Substituting this equation into the preceding one gives

$$\imath[\delta\boldsymbol{\Omega}\cdot\hat{\boldsymbol{l}},\hat{\boldsymbol{r}}]/\hbar+\mathcal{O}(\delta\boldsymbol{\Omega}^2)=\delta\boldsymbol{\Omega}\times\hat{\boldsymbol{r}} \tag{1.80}$$

We only need to consider the above result to $\mathcal{O}(\delta\boldsymbol{\Omega})$. Thus if $\delta\boldsymbol{\Omega}$ is in the x direction, the Cartesian components[11] of the equation are

$$\imath[\hat{l}_x,\hat{x}]/\hbar=0;\qquad \imath[\hat{l}_x,\hat{y}]/\hbar=-\hat{z};\qquad \imath[\hat{l}_x,\hat{z}]/\hbar=\hat{y}. \tag{1.81}$$

By virtue of the fundamental commutation relations (1.52), the first of these tells us that $\hat{l}_x$ does not contain $\hat{p}_x$, the second that it contains the product $-\hat{p}_y\,\hat{z}$ and the last that it contains $\hat{p}_z\,\hat{y}$, the last two terms added together. Hence $\hat{l}_x=\hat{y}\,\hat{p}_z-\hat{z}\,\hat{p}_y+h(\hat{x},\hat{y},\hat{z})$, where h is some function.

Of course equations (1.77)-(1.78) have to be valid also with $\hat{\boldsymbol{p}}$ replacing $\hat{\boldsymbol{r}}$ (any vector operator is rotated according to the same rules as $\hat{\boldsymbol{r}}$). Repeating the above argument with $\hat{\boldsymbol{r}}\mapsto\hat{\boldsymbol{p}}$ gives us $\hat{l}_x=\hat{y}\,\hat{p}_z-\hat{z}\,\hat{p}_y+g(\hat{p}_x,\hat{p}_y,\hat{p}_z)$, where g is another function. Obviously both results can be correct only if $g=h=\text{const}$. Thus up to a constant, the generator of rotation around the x axis is the x component of angular momentum. The arbitrariness with which we assign the Cartesian coordinates means that the analogous results $\hat{l}_y=\hat{z}\,\hat{p}_x-\hat{x}\,\hat{p}_z+\text{const.}$ and $\hat{l}_z=\hat{x}\,\hat{p}_y-\hat{y}\,\hat{p}_x+\text{const.}$ (obtained by cyclic permutation) are equally valid. Thus up to a constant vector—call it $\boldsymbol{h}$—the generator $\hat{\boldsymbol{l}}$ here is identical to the orbital angular momentum $\hat{\boldsymbol{r}}\times\hat{\boldsymbol{p}}$.

The above is also true for a collection of particles, with the total generator of rotation being the sum of generators for the constituent particles. But if $\boldsymbol{h}\neq 0$ we get into trouble because each particle contributes $\boldsymbol{h}$ to the total generator. But what if we choose to combine two neighboring particles into one? Should we add $\boldsymbol{h}$ or $2\boldsymbol{h}$ to the generator? The arbitrariness suggests that $\boldsymbol{h}=0$. Another argument for this is that $\boldsymbol{h}$ is *not* a dynamical property of the system of particles (it is not built out of $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{p}}$), but an external vector. Such an external vector would imply a preferred direction in space, in contradiction to the fundamental assumption (in the absence of gravity)

[11] in honor of René Descartes (1596-1650), the French philosopher, mathematician and physicist who invented analytic geometry; his name was Latinized to *Cartesius*, hence the adjective Cartesian.

that space is isotropic. Thus whichever way we look at it, the generator of rotations for a system is its total orbital angular momentum observable.

When a particle has spin, the spin adds to $\hat{\boldsymbol{l}}$ to give the full angular momentum $\hat{\boldsymbol{j}}$; this last is the generator of joint rotations of $\hat{\boldsymbol{r}}, \hat{\boldsymbol{p}}$ and spin.

Exercises:

1. Derive angular momentum's commutation rule $\hat{\boldsymbol{l}} \times \hat{\boldsymbol{l}} = \imath\hbar\hat{\boldsymbol{l}}$ from the requirement that $\hat{U}_{\boldsymbol{\Omega}}$ rotates $\hat{\boldsymbol{l}}$ like any other vector operator.
2. Identify the generator of rotation as angular momentum by requiring that the rotated wave function $\hat{U}_{\boldsymbol{\Omega}}\,\psi(\boldsymbol{r})$ be related to $\psi(\boldsymbol{r})$ in analogy with Eqs. (1.70) and (1.72) for translations.
3. Starting from orbital angular momentum as generator, reconstruct the full $\hat{U}_{\boldsymbol{\Omega}}$ thus illustrating Lie's theorem anew.

1.2.8 Maximal set of mutually commuting observables

We have mentioned that it can happen that eigenstates of an observable are degenerate. One cannot thus distinguish them or label them by just the eigenvalues associated with them. But there usually are other observables whose eigenvalues help to remove the degeneracy. Now when two or more operators mutually commute, there are common eigentstates of all, so we can label states of the particle by such eigenvalues.

Consider a freely moving particle possessing spin. The observables that come up are $\hat{\boldsymbol{r}}, \hat{\boldsymbol{p}}$, orbital angular momentum $\hat{\boldsymbol{l}} = \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}}$, spin $\hat{\boldsymbol{s}} = \frac{1}{2}\hbar\boldsymbol{\sigma}$ and perhaps others. How many labels must the particle's state have in order to be singled out uniquely? We cannot use eigenvalues of all the observables mentioned because some, like $\hat{p}_x$ and $\hat{x}$, are not mutually compatible, that is, their operators do not commute. This has the effect that there is no state which is a mutual eigenstate, say, of $\hat{p}_x$ and $\hat{x}$. Under such circumstances there is always some *maximal set of mutually commuting observables* that can be used to label states. In the example above one could label a state as follows: $|\hat{\boldsymbol{p}}^2 = \boldsymbol{p}^2, \hat{p}_x = p_x, \hat{\boldsymbol{l}}^2 = 2\hbar^2, \hat{l}_x = -\hbar, \hat{\boldsymbol{s}}^2 = \frac{3}{4}\hbar^2, \hat{s}_x = +\frac{1}{2}\hbar\rangle$; there is no other state whose labels agree with these in every respect.

More generally speaking, if the maximal set of mutually commuting observables is $\hat{A}, \hat{B}, \hat{C}, \cdots$ with eigenvalues labeled by $\alpha, \beta, \gamma, \cdots$, respectively, a suitable decomposition of the identity for the system would be

$$\hat{I} = \sum_{\alpha,\beta,\gamma,\cdots} |\alpha, \beta, \gamma, \cdots\rangle\langle\alpha, \beta, \gamma, \cdots|. \tag{1.82}$$

where the sum is over all possible combinations of values $\{\alpha, \beta, \gamma, \cdots\}$.

1.3 Quantum dynamics

1.3.1 Schrödinger picture - the evolution operator

All that has been said concerned the states and operators of of systems at a given time. But how do these change in time? In investigating this question we assume that whereas states like $|\psi\rangle$ evolve, observables like $\hat{\boldsymbol{r}}, \hat{\boldsymbol{p}}$ and spin $\frac{1}{2}\hbar\boldsymbol{\sigma}$ do not. This viewpoint is called *Schrödinger picture*. Of course one can conceive other observables which are time varying, but from our viewpoint such time variation is externally induced.

So we write here $|\psi, t\rangle$. The first point is that the change of $|\psi, t_0\rangle$ at some initial time t_0 to $|\psi, t\rangle$ at some other time t must respect the superposition principle. Thus it must be a linear operation, carried out by a linear evolution operator $\hat{U}$, so we should write

$$|\psi, t\rangle = \hat{U}(t, t_0)|\psi, t_0\rangle. \tag{1.83}$$

Next we must require that the normalization of the initial state, be preserved in the course of time, since we agreed that normalization is connected with probability, and probability cannot be lost. Thus

$$\langle\psi, t|\psi, t\rangle = \langle\psi, t_0|\hat{U}(t, t_0)^\dagger\hat{U}(t, t, 0)|\psi, t_0\rangle = \langle\psi, t_0|\psi, t_0\rangle = 1 \tag{1.84}$$

Since the state in question is arbitrary, this result implies that

$$\hat{U}(t, t_0)^\dagger = \hat{U}(t, t_0)^{-1}, \tag{1.85}$$

that is, the evolution operator is unitary for any t and t_0.

Of course, if $\hat{U}(t,t_0)$ takes any state from t_0 to t_1, and $\hat{U}(t_2,t_1)$ does so from from t_1 to t_2 we must have

$$\hat{U}(t_2,t_1)\,\hat{U}(t_1,t_0)=\hat{U}(t_2,t_0) \tag{1.86}$$

so that we can compose evolutions. This composition law is evidently associative. Thus the collection of $\hat{U}(t,t')$ for all t and t' constitutes a group.

All this is general. To make progress we now specialize to a quantum system whose environment is stationary. In such situation changing the zero of time should make no difference, meaning that $\hat{U}(t+\xi,t_0+\xi)$ should be identical to $\hat{U}(t,t_0)$ for any real ξ. But this means that necessarily $U(t,t_0)=\hat{U}(t-t_0)$, namely, the evolution operator depends only on the time lapse. This together with Eq. (1.86) leaves no option but that $\hat{U}(t-t_0)$ depends *exponentially* on $t-t_0$. But according to Exercise 4 in Sec. 1.2.5, as a unitary operator $\hat{U}$ must be the exponential of $\imath$ times an Hermitian operator. Putting all this together we find that

$$\hat{U}(t-t_0)=e^{-\imath\hat{H}(t-t_0)/\hbar} \tag{1.87}$$

where we introduced $\hbar$ for convenience, and $\hat{H}$ is somes time independent Hermitian operator.

Consider now a particle or particles in a state with definite energy E. According to Bohr's rule[12] the wave function must have the time dependence $\exp(-\imath E/\hbar)$. Thus

$$|\psi,t\rangle_E=e^{-\imath\hat{H}(t-t_0)/\hbar}\,|\psi,t_0\rangle_E\sim\exp(-\imath E/\hbar). \tag{1.88}$$

It may be seen from this that the evidently generic state $|\psi,t_0\rangle_E$ must be an eigenstate of $\hat{H}$ with eigenvalue E. This singles out $\hat{H}$ as the energy observable, or *Hamiltonian*, to use the name of its cognate quantity in classical mechanics.

Drawing an analogy between the translation group and the group of quantum evolution we may say that the Hamiltonian is the generator of quantum evolution.

[12]introduced by Nobel laureate Niels Henrik David Bohr (1885-1962), the Danish Jewish theoretical physicist who is regarded as the most influential figure in the development of quantum mechanics. He also contributed importantly to nuclear physics.

1.3.2 The Schrödinger equation

Still considering closed systems only, let us differentiate the evolution equation as follows

$$\imath\hbar\frac{d}{dt}|\psi,t\rangle = \imath\hbar\frac{d}{dt}\left(e^{-\imath\hat{H}(t-t_0)/\hbar}\,|\psi,t_0\rangle\right) = \hat{H}e^{-\imath\hat{H}(t-t_0)/\hbar}\,|\psi,t_0\rangle = \hat{H}|\psi,t\rangle \tag{1.89}$$

(It is customary to use the notation d/dt rather than the perhaps more appropriate one $\partial/\partial t$). The resulting differential equation

$$\imath\hbar\frac{d}{dt}|\psi,t\rangle = \hat{H}|\psi,t\rangle \tag{1.90}$$

is called the Schrödinger equation.[13] With the initial value $|\psi,t=0\rangle = |\psi,t_0\rangle$ it yields as solution Eq. (1.83) with the choice (1.87). The Schrödinger equation is thus the quantum theoretic equation of motion for states.

To recover the Schrödinger wave equation from quantum mechanics, let us take the scalar product of Eq. (1.90) with $\langle\boldsymbol{r}|$ and insert the decomposition of the identity between $\hat{H}$ and $|\psi,t\rangle$:

$$\imath\hbar\frac{d}{dt}\psi(\boldsymbol{r},t) = \int\langle\boldsymbol{r}|\hat{H}|\boldsymbol{r}'\rangle\,\psi(\boldsymbol{r}',t)\,d^3r' \tag{1.91}$$

In classical mechanics a particle of mass m in a potential V has the Hamiltonian function $H = \boldsymbol{p}^2/2m + V(\boldsymbol{r})$. Hence we take $\hat{H} = \hat{\boldsymbol{p}}^2/2m + V(\hat{\boldsymbol{r}})$. Obviously $\langle\boldsymbol{r}|V(\hat{\boldsymbol{r}})|\boldsymbol{r}'\rangle = V(\boldsymbol{r})\delta(\boldsymbol{r}-\boldsymbol{r}')$. We recall the position representation form of momentum: $(\hbar/\imath)\boldsymbol{\nabla}$. Thus in notation where $\Delta \equiv \boldsymbol{\nabla}\cdot\boldsymbol{\nabla}$,

$$\langle\boldsymbol{r}|\hat{\boldsymbol{p}}^2|\boldsymbol{r}'\rangle = -\hbar^2\Delta\delta(\boldsymbol{r}-\boldsymbol{r}'). \tag{1.92}$$

Substituting all these results in (1.91) and doing an integration by parts of the $\hbar^2$ term (assuming that both ψ and $\boldsymbol{\nabla}\psi$ vanish asymptotically) gives the familiar form of the Schrödinger equation

$$\imath\hbar\frac{d}{dt}\psi(\boldsymbol{r},t) = -\frac{\hbar^2}{2m}\Delta\psi(\boldsymbol{r},t) + V(\boldsymbol{r})\psi(\boldsymbol{r},t). \tag{1.93}$$

[13] first obtained by Nobel laureate Erwin Rudolf Josef Alexander Schrödinger (1887-1961), Austrian theoretical physicist who also obtained the relativistic version (called Klein-Gordon equation today), discovered coherent states and the phenomenon of *Zitterbewegung* and pointed out that entanglement is one of the defining features of the quantum world. Schrödinger also contributed to the quantum field theory in a cosmological setting and to theoretical biology.

It is to be noted that this form was pretty much forced on us by very general arguments. The one restrictive assumption we made is that $\hat{H}$ is time independent. We shall assume—in harmony with all experimental evidence—that Eq. (1.90) is still valid when $\hat{H} = \hat{H}(t)$.

1.3.3 Heisenberg picture

The viewpoint adopted in the last two subsections is not really very intuitive from a classical perspective. In classical mechanics physical quantities like momentum and spin vary in time, but we usually speak of a fixed state of the system (specified by the initial values). This is just the opposite of the language adopted above. But Schrödinger picture is not the only possible viewpoint. We now describe *Heisenberg picture*, a viewpoint more analogous to classical mechanics.

For every state in $\mathcal{H}, |\psi, t\rangle$ let us define a parallel state, the *Heisenberg picture state*

$$|\psi\rangle_H = \hat{U}(t,0)^\dagger |\psi, t\rangle. \tag{1.94}$$

and for every operator $\hat{O}$ acting on $\mathcal{H}$ we define a corresponding operator, the *Heisenberg picture operator*

$$\hat{O}_H(t) = \hat{U}(t,0)^\dagger \hat{O}\, \hat{U}(t,0). \tag{1.95}$$

Because of Eqs. (1.83) and (1.85) it is clear that $|\psi\rangle_H = |\psi, 0\rangle$. In other words, the Heisenberg picture state of a system is fixed forever at the state in Schrödinger picture which held sway at the origin of time. It may also be seen from Eq. (1.95) that even when in Schrödinger picture an operator is fixed in time, its Heisenberg picture version will vary in time. This is just like in classical mechanics where physical quantities evolve in time (unless they are conserved).

Let us be more specific about the evolution of a Heisenberg picture operator, including the case when the Schrödinger picture operator is already time dependent. For brevity we shall write $\hat{U} = \hat{U}(t,0)$. If we differentiate Eq. (1.95) w.r.t. t we get

$$\imath\hbar \frac{d}{dt}\hat{O}_H = -\hat{H}\,\hat{U}^\dagger\,\hat{O}\,\hat{U} + U^\dagger\,\hat{O}\,\hat{U}\,\hat{H} + \imath\hbar\,\hat{U}^\dagger \frac{\partial \hat{O}}{\partial t}\,\hat{U} \tag{1.96}$$

or more compactly

$$\imath\hbar \frac{d}{dt}\hat{O}_H = [\hat{O}_H, \hat{H}] + \imath\hbar \left(\frac{\partial \hat{O}}{\partial t}\right)_H \tag{1.97}$$

(note that that $\hat{H}_H = \hat{H}$). This last is the *Heisenberg equation*, the equation of motion for Heisenberg picture. Its form agrees with what would be expected from Dirac's rule (see beginning of Sec. 1.2.3): it is the classical equation of motion in Poisson form with the Poisson bracket replaced by the corresponding commutator divided by $\imath\hbar$. Whenever the Schrödinger picture operator is time-independent, e.g. $\hat{\boldsymbol{r}}, \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}}$ etc., the evolution in Heisenberg picture is determined solely by the commutator. Thus any such operator which commutes with the Hamiltonian is a conserved quantity, just as in classical mechanics a quantity not explicitly time-dependent whose Poisson bracket with the Hamiltonian vanishes is conserved.

Since the passage from Schrödinger to Heisenberg picture is effected with a unitary operator, we see that the two pictures are related by a unitary time dependent transformation. It is important to distinguish between passage between two pictures and transformation between two different representations.

Let us now consider what happens to the spectrum of an operator $\hat{A}$ upon passage to Heisenberg picture. By premultiplying the eigenvalue equation

$$\hat{A}|a_i\rangle = a_i|a_i\rangle \tag{1.98}$$

by $\hat{U}^\dagger \equiv U(t,0)^\dagger$ we can obviously write it as

$$\hat{U}^\dagger\, \hat{A}\, \hat{U}\, \hat{U}^\dagger |a_i\rangle = a_i\, \hat{U}^\dagger\, |a_i\rangle, \tag{1.99}$$

or equivalently as

$$\hat{A}_H\, |a_i\rangle_H = a_i\, |a_i\rangle_H. \tag{1.100}$$

where $|a_i\rangle_H = \hat{U}^\dagger |a_i\rangle$ in harmony with definition (1.94). Thus the spectrum of $\hat{A}_H$ is exactly the same as that of $\hat{A}$. That is, the measured values of an observable are the same for both pictures. The eigenvectors of $\hat{A}_H$, however, are different from their Schrödinger picture analog, and will always be time dependent even when the later are not. As may be seen from Exercise 1 in this section, mean values and matrix elements of an operator, both of

which have observational consequences, are the same when calculated in the different pictures.

Another feature which does not change with the picture is the algebra of observables. According to Exercise 2 in this section the form of the commutator of two operators is the same in both pictures. The algebra of observables, the totality of commutators of the relevant observables, is thus invariant under the change of picture. This again shows that a change of picture leaves the physics unchanged since we know that the algebra defines a variety of measurable characteristics.

Exercises:

1. Prove that the mean value $\langle\phi|\hat{A}|\phi\rangle$ and the matrix element $\langle\phi|\hat{A}|\psi\rangle$ are identical when calculated in Schrödinger or Heisenberg picture.

2. Suppose $[\hat{A},\hat{B}]=\hat{C}$. Prove that $[\hat{A}_H,\hat{B}_H]=\hat{C}_H$.

3. The Schrödinger picture Hamiltonian of the isotropic harmonic oscillator is $\hat{H}=\frac{1}{2}\hat{\boldsymbol{p}}^2+\frac{1}{2}\omega^2\boldsymbol{r}^2$ where the units have been chosen appropriately and ω is a parameter. Integrate the Heisenberg equation for $\boldsymbol{r}$ in terms of $\boldsymbol{r}(0)$ and three phases (for the three coordinates).

1.3.4 Evolution with time independent Hamiltonian

We work in Schrödinger picture. Suppose the Hamiltonian $\hat{H}$ of a system is time independent (the system is not subject to external influence which varies in time). The evolution operator is then (1.87). Suppose we manage to determine the $\hat{H}$'s spectrum $\{E_1,E_2,\cdots\}$ as well as the corresponding eigenstates $\{|E_1\rangle,|E_2\rangle\cdots\}$. Then by the definition (1.19) we have

$$\hat{U}(t-t_0)=\sum_j e^{-\imath E_j(t-t_0)/\hbar}\,|E_j\rangle\langle E_j|, \tag{1.101}$$

where the sum must include every eigenstate, with the degenerate ones entering with like phase $\exp\big(-\imath E_j(t-t_0)\big)$. Now suppose the initial state is $|\psi, t_0\rangle$. We obtain $|\psi, t\rangle$ by operating on $|\psi, t_0\rangle$ with $\hat{U}(t-t_0)$. If we are interested in the wave function at time t we would form the matrix element

$$\psi(\boldsymbol{r}, t) = \langle \boldsymbol{r}| \sum_j e^{-\imath E_j(t-t_0)/\hbar}\, |E_j\rangle\langle E_j|\psi, t_0\rangle \tag{1.102}$$

We observe that the part of the initial state which is projected into $|E_j\rangle$ oscillates with frequency $E_j/\hbar$ just as required by the Bohr's rule.

Now suppose we insert the decomposition of the identity in the form (1.31) between $\langle E_j|$ and $|\psi, t_0\rangle$. We get (with $u_j(\boldsymbol{r}) \equiv \langle \boldsymbol{r}|E_j\rangle$ representing the eigen*function* of $\hat{H}$ with eigenvalue E_j)

$$\psi(\boldsymbol{r}, t) = \sum_j e^{-\imath E_j(t-t_0)/\hbar}\, \langle \boldsymbol{r}|E_j\rangle \int \langle E_j|\boldsymbol{r}'\rangle\, \psi(\boldsymbol{r}', t_0)\, d^3r' \tag{1.103}$$

$$= \sum_j \int u_j(\boldsymbol{r}')^*\, \psi(\boldsymbol{r}', t_0)\, d^3r' \cdot e^{-\imath E_j(t-t_0)/\hbar}\, u_j(\boldsymbol{r}) \tag{1.104}$$

which is a well known expression in quantum mechanics for the law of propagation of a wave function.

1.3.5 Time dependent Hamiltonian: subtleties

When the system is exposed to external time varying forces we cannot carry out the whole program outlined above. It is then simply *not* true that $U(t, t_0) = \hat{U}(t-t_0)$; therefore Eq. (1.87) fails us. As mentioned, one assumes that the differential Schrödinger Eq. (1.90) is still valid, albeit now with $\hat{H} = \hat{H}(t)$.

There is still an evolution operator; the arguments for unitarity and the composition law (1.86) still stand. Let us substitute Eq. (1.83) in (1.90). The arbitrariness of $|\psi, t_0\rangle$ means that

$$\imath\hbar \frac{d}{dt}\hat{U}(t, t_0) = \hat{H}(t)\, \hat{U}(t, t_0). \tag{1.105}$$

Thus $\hat{U}(t, t_0)$ for given t_0 also satisfies a Schrödinger equation. Evidently the initial value for this equation is $\hat{U}(t_0, t_0) = \hat{1}$.

Had we the solution of Eq. (1.105) on hand, we would know the evolution of any state by Eq. (1.83). But solving (1.105) is far from trivial. The naive solution

$$\hat{U}(t,t_0) = e^{-(\imath/\hbar)\int_{t_0}^{t}\hat{H}(t')dt'} \tag{1.106}$$

is actually wrong. When we differentiate it w.r.t. t, a factor $\hat{H}(t)$ comes down from the exponent. Shall we put it in front of the exponential or after it? When $\hat{H}$ was independent, the choice did not matter since $\hat{H}$ commutes with its exponential. So by putting the $\hat{H}$ in front of the exponential we got to satisfy Eq. (1.105). But with $\hat{H}(t)$, front and back are inequivalent because the integral involves $\hat{H}(t)$ at different times, and $\hat{H}(t)$s at two different times *do not necessarily commute*. We are unable to claim that the equation is satisfied regardless of ordering. We shall now study methods for correctly solving Eq. (1.105).

Exercises:

1. Relying on Eq. (1.105) show that if $\hat{U}(t_0,t_0)\,\hat{U}(t_0,t_0)^\dagger = \hat{I}$, then in the course of time $\hat{U}(t,t_0)\,\hat{U}(t,t_0)^\dagger = \hat{I}$ (unitarity of the evolution operator is preserved).

1.3.6 The sudden approximation

Perhaps the simplest type of time dependence of $\hat{H}$ is when the operator is constant in time save for a number of discontinuities. In the simplest case $\hat{H}_1(t)$ applies for $t<0$ and $\hat{H}_2(t)$ applies for $t>0$ with $\hat{H}_2(+\epsilon) \neq \hat{H}_1(-\epsilon)$ where $\epsilon>0$ is a tiny time which will be taken to zero in the end. Here $t_0<0$. If we integrate Eq. (1.105) over time from $t=-\epsilon$ to $t=\epsilon$ we find that

$$\hat{U}(+\epsilon,t_0) - \hat{U}(-\epsilon,t_0) = \mathcal{O}(\epsilon)\big[\hat{H}_2(+\epsilon) + \hat{H}_1(-\epsilon)\big]\,. \tag{1.107}$$

We conclude that $\hat{U}(t,t_0)$ goes through $t=0$ *continuously*. Before that time it is

$$\hat{U}_1(t,t_0) = \exp\big(-\imath\hat{H}_1\cdot(t-t_0)/\hbar\big) \tag{1.108}$$

while thereafter it is

$$\hat{U}_2(t,t_0) = \exp\big(-\imath\hat{H}_2\cdot t/\hbar\big)\,U_1(0,t_0)\,, \tag{1.109}$$

where we have employed the composition law Eq. (1.86). In the last equation we should refrain from writing the product as exponential of the sum of arguments of the two exponentials: since $\hat{H}_1$ and $\hat{H}_2$ may not commute, this rule for combining exponents does not work in the usual way.

According to Eq. (1.83) the state, and the wave function of the system also goes through $t = 0$ continuously. We calculate as $\hat{U}_1(t, t_0)|\psi, t_0\rangle$ for $t < 0$ and $\hat{U}_2(t, t_0)|\psi, t_0\rangle$ for $t > 0$.

Even when the Hamiltonian varies continuously in time except for a sudden jump, the above approximation may be employed. The evolution operators for before and after the jump are to be taken as $\hat{U}_1(t, t_0)$ and $\hat{U}_2(t, 0)\,\hat{U}_1(0, t_0)$, where the $\hat{U}_j(t, t')$ are computed by solving the evolution equation (1.105) with $\hat{H}_j(t)$ and suitable initial condition. The above procedure is Pauli's *sudden approximation*.

The following example illustrates the use of the sudden approximation taking into account certain realities.

Example: Atom flying in external field

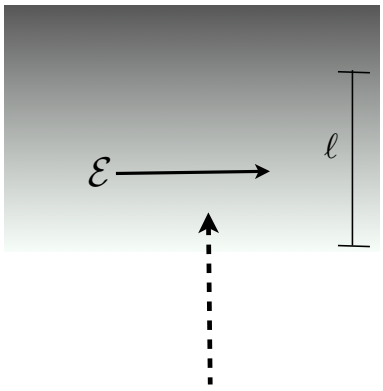

Figure 1.1: **The field $\mathcal{E}$ of fixed direction varies in strength, in accordance with the degree of graying shown, over a scale ℓ. The atom flies in the direction of the dashed arrow.**

Consider an hydrogen atom in the n-th Bohr state travelling at speed u that enters an external electric field $\mathcal{E}$ of fixed direction whose strength rises from zero to its full value over a distance ℓ, as illustrated in Fig. 1.1. We

know that the hydrogen's electron travels around the nucleus at a speed $\alpha c/n$ where $\alpha \approx 1/137$ is the fine structure constant. The n-th Bohr orbit has a radius $n^2 a_0$ with a_0 the Bohr radius. Thus the time-scale associated with the dynamics of that electron is of order $\alpha^{-1} n^3 a_0/c$. The time-scale for the change of the Hamiltonian (the part having to do with $\mathcal{E}$) is obviously ℓ/u. If $n^3 a_0 \gg \alpha \ell c/u$, the change in Hamiltonian can be regarded as instantaneous, and the sudden approximation applies. This will always be true for a sufficiently large n. For the atom initially in such a state we may apply the sudden approximation as follows.

The initial state at $t = t_0$ will be taken as $|E_n\rangle$, an eigenstate of the hydrogen hamiltonian $\hat{H}_1$ with eigenvalue E_n. This evolves as $\hat{U}_1(t, t_0)\,|E_n\rangle$ for $0 \geq t \geq t_0$. Thus at $t = 0$ the state is $e^{\imath E_n t_0/\hbar}|E_n\rangle$. The evolution just changed its phase. For $t > 0$ the state will evolve according to $\hat{U}_2(t, t_0)$, but by the sudden approximation, it will start from $e^{\imath E_n t_0/\hbar}|E_n\rangle$. We must expand this "initial state" in the basis of eigenstates $|\bar{E}_k, \mathcal{E}\rangle$ of the Hamiltonian $\hat{H}_2$ for hydrogen in the field $\mathcal{E}$. Using the decomposition of the identity according to these latter states we have

$$e^{\imath E_n t_0/\hbar}|E_n\rangle = e^{\imath E_n t_0/\hbar} \sum_k |\bar{E}_k, \mathcal{E}\rangle \,\langle \bar{E}_k, \mathcal{E}|E_n\rangle \,. \tag{1.110}$$

For $t > 0$ the evolution operator has the form $\hat{U}_2 = \exp(-\imath \hat{H}_2 t/\hbar)$ (for our purpose here the initial condition is $\hat{U}(0) = 0$). Thus the state for $t > 0$ is

$$e^{\imath E_n t_0/\hbar} \sum_k \, e^{-\imath \bar{E}_k t/\hbar} \langle \bar{E}_k, \mathcal{E}|E_n\rangle \, |\bar{E}_k, \mathcal{E}\rangle. \tag{1.111}$$

Thus, regardless of k, there is a finite probability, $|\langle \bar{E}_k, \mathcal{E}|E_n\rangle|^2$, for finding the atom in the state $|\bar{E}_k, \mathcal{E}\rangle$.

Exercises:

1. The Hamiltonian for a one-dimensional isotropic harmonic oscillator is $\hat{H} = \frac{1}{2}\hat{p}_x^2/m + \frac{1}{2}\omega^2 x^2$, where ω is the oscillator's frequency. At some moment ω doubles over a time span τ. What is the condition for applicability of the sudden approximation? If it is satisfied, what is the probability that the oscillator remains in its ground state (*persistence probability*)? The harmonic oscillator's ground state wave function is $\psi(x) = (m\omega/\pi\hbar)^{1/4} \exp(-m\omega x^2/2\hbar)$.

2. A tritium (H^3) atom's nucleus emits an electron at velocity v. The resulting nucleus is that of He^3. What is the condition on v so that one may use the sudden approximation to calculate probabilities of excitation of the various *electronic* levels of the once-ionized helium atom?

1.3.7 The adiabatic theorem

There is an important result applicable to a situation when the Hamiltonian changes very slowly in time; in mechanics a slow change of the Hamiltonian is called *adiabatic*.

In order to solve the Schrödinger equation (1.90) we first solve the eigenvalue problem for $\hat{H}(t)$ with t *regarded as a parameter*:

$$\hat{H}(t)|E_n, t\rangle = E_n(t)|E_n, t\rangle \tag{1.112}$$

The method works well only if there are no degeneracies; we assume this. An immediate consequence of this, and the Hermiticity of $\hat{H}(t)$ is that

$$\langle E_k|E_n\rangle = \delta_{nk}, \tag{1.113}$$

where here and henceforth we drop the argument t in each eigenket, and assume that the eigenstates $|E_n\rangle$ are properly normalized.

Now we make an *ansatz* or educated guess:

$$|\psi, t\rangle = \sum_n a_n(t)\, e^{-\imath \int^t E_n(t')\, dt'/\hbar}\, |E_n\rangle. \tag{1.114}$$

Substituting this in (1.90) and taking the scalar product with $\langle E_k|$ we have

$$\frac{da_k}{dt} = -\sum_n a_n(t) \langle E_k| \frac{\partial |E_n\rangle}{\partial t} e^{\imath \int^t \left(E_k(t') - E_n(t')\right) dt'/\hbar}. \tag{1.115}$$

To determine the unknown scalar product we differentiate Eq. (1.112) with respect to t, take the scalar product of the result with a $\langle E_k|$ with $k \neq n$, and use Eq. (1.113) and (1.112) :

$$\langle E_k|\frac{\partial|E_n\rangle}{\partial t} = \frac{\langle E_k|\frac{\partial\hat{H}}{\partial t}|E_n\rangle}{E_n - E_k}\,. \tag{1.116}$$

This makes most of the terms in Eq. (1.115) explicit; but what is $\langle E_k|\partial|E_k\rangle/\partial t$?

To find this last, we differentiate Eq. (1.113) with $n = k$:

$$\langle E_k|\frac{\partial|E_k\rangle}{\partial t} + \frac{\partial\langle E_k|}{\partial t}|E_k\rangle = 0. \tag{1.117}$$

By Eq. (1.4) the two terms here are complex conjugates of each other, and thus pure imaginary:

$$\langle E_k|\frac{\partial|E_k\rangle}{\partial t} = \imath\alpha_k(t) \tag{1.118}$$

where the α_k are real functions. We now reconsider the eigenvalue problem (1.112). Its solution does not fix the phase of $|E_k\rangle$; this is arbitrary and independent of the phase at other times (time at the level of this equation is a parameter, so we cannot speak of evolution of the phase). Thus we redefine our eigenkets as follows:

$$|E_k\rangle \to |E_k\rangle e^{\imath\beta_k(t)}. \tag{1.119}$$

This redefinition leads to a modification of Eq. (1.118):

$$\langle E_k|\frac{\partial|E_k\rangle}{\partial t} = \imath\alpha_k(t) \to \imath\big(\alpha_k(t) + \dot{\beta}_k(t)\big) \tag{1.120}$$

For every k we may now choose $\beta_k(t)$ in such a way that the r.h.s. of Eq. (1.120) vanishes. Thus there is no $n = k$ term in the sum in Eq. (1.115) which now takes the form

$$\frac{da_k}{dt} = \sum_{n\neq k} \frac{a_n}{\hbar\omega_{kn}(t)}\,\langle E_k|\frac{\partial\hat{H}}{\partial t}|E_n\rangle\, e^{\imath\int^t \omega_{kn}(t')\,dt'/\hbar}. \tag{1.121}$$

where $\omega_{kn}(t) \equiv \big(E_k(t) - E_n(t)\big)/\hbar$ is the Bohr transition frequency between states $|E_k\rangle$ and $|E_n\rangle$.

The above evolution equation is exact, and is equivalent to the Schrödinger equation. It may serve as a basis for time-dependent perturbation theory, but we shall not go into that here.

Suppose the system started at $t = 0$ in the state $|E_m\rangle$ which means $a_m(0) = 1$ while all other $a_n(0)$ vanish exactly. The assumed slow change of $\hat{H}(t)$ means that $\omega_{kn}(t)$ as well as as the matrix element in Eq. (1.121) can be taken, in first approximation, as constant. Thus for $k \neq m$ we have for a short time after $t = 0$

$$\frac{da_k}{dt} = \frac{1}{\hbar\omega_{km}} \langle E_k | \frac{\partial \hat{H}}{\partial t} | E_m \rangle \, e^{\imath \omega_{km} t} \tag{1.122}$$

which integrates to

$$a_k = -\frac{\imath}{\hbar\omega_{km}^2} \langle E_k | \frac{\partial \hat{H}}{\partial t} | E_m \rangle \, (e^{\imath \omega_{km} t} - 1) \tag{1.123}$$

It is obvious that none of the originally zero amplitudes grow systematically but rather they undergo sinusoidal oscillations. The typical amplitude of each such oscillation is equal to the ratio of the matrix element divided by $\hbar\omega_{km}^2$. This ratio can be roughly estimated as the change in $\hat{H}$ during the oscillation period $2\pi/\omega_{km}$ divided by the energy gap $|E_k - E_m|$. So for a sufficiently slowly varying Hamiltonian, all the a_k for $k \neq m$ will remain small even after $\hat{H}$ has changed a lot.

Substituting these expressions for the a_k into Eq. (1.121) with $k \to m$, we see that a_m changes very little and will remain near unity in magnitude. The conclusion is that, for *adiabatic change of the Hamiltonian* the system, if originally in an energy eigenstate, remains in it, even if the corresponding eigenvalue and position eigenfunction change significantly overall. This is sometimes called the *adiabatic theorem*.

Any time that we assume, on the basis of the above, that the state coincides with a particular energy eigenstate while the Hamiltonian changes slowly, we are using the *adiabatic approximation* due to Born[14] and Fock.[15] The adiabatic approximation is the opposite type of approximation to the sudden approximation.

[14]Max Born (1882-1970) was a German-British physicist of Jewish origin who contributed the probability interpretation of the wave function; a Nobel laureate, he mentored a large number of distinguished physicists, six of which won Nobel prizes

[15]Vladimir Aleksandrovich Fock (1898-1974) was a Russian theoretical physicist who contributed to early quantum mechanics and general relativity. The many particle Hilbert space in QT and quantum field theory is named after him.

Example: Born-Oppenheimer approximation

The Born-Oppenheimer[16] approximation, which clarified the quantum mechanics of molecules, is based on the adiabatic approximation. In a simple molecule we have two or more nuclei surrounded by a few electrons. Let the nuclear Hamiltonian be $\hat{H}_N(\hat{\boldsymbol{P}}^2, \hat{\boldsymbol{R}})$ with $\hat{\boldsymbol{P}}$ denoting collectively the momenta of the various nuclei, $\hat{\boldsymbol{R}}$, denoting the nuclear positions, and let the electronic Hamiltonian be $\hat{H}_e(\hat{\boldsymbol{p}}^2, \hat{\boldsymbol{r}})$ with $\hat{\boldsymbol{p}}$ the momenta of the various electrons and $\hat{\boldsymbol{r}}$ the electrons' positions. There is also a Coulomb interaction $\hat{V}(\hat{\boldsymbol{R}}, \hat{\boldsymbol{r}})$ *between nuclei and electrons.*

The nuclei being heavy move sluggishly. Therefore in $\hat{H}_e + \hat{V}$ we may regard $\hat{\boldsymbol{R}}$ as a slowly varying *parameter* and solve the restricted eigenvalue problem for the electrons

$$(\hat{H}_e + \hat{V})|E_k\rangle = E_k|E_k\rangle\,, \tag{1.124}$$

where both E_k and $|E_k\rangle$ will depend on $\hat{\boldsymbol{R}}$ (as well as on the electronic variables). The adiabatic theorem tells us that the electrons stay in the same state $|E_k\rangle$ regardless of the slow motion of the nuclei. Thus we may write the full state of the molecule as

$$|\psi\rangle = |\phi\rangle_N \otimes |E_k\rangle \tag{1.125}$$

where $|\phi\rangle_N$ is a nuclear state. Operating on $|\psi\rangle$ with $\hat{H}_N + \hat{H}_e + \hat{V}$ gives

$$\hat{H}_N|\phi\rangle_N \otimes |E_k\rangle + |\phi\rangle_N \otimes (\hat{H}_e + \hat{V})|E_k\rangle = (\hat{H}_N + E_k)|\phi\rangle_N \otimes |E_k\rangle \tag{1.126}$$

It is plain that to solve the nuclear eigenvalue problem, or to consider dynamical evolution of the nuclear state, we must use the effective Hamiltonian $\hat{H}_{\text{eff}} \equiv \hat{H}_N + E_k(\hat{\mathbf{R}})$, that is the electronic eigenvalue $E_k(\hat{\mathbf{R}})$ is like an extra potential between the nuclei.

Exercises:

1. An hydrogen atom is placed between the plates of a capacitor. A voltage pulse is applied to the last which causes the capacitor's electric

[16] Julius Robert Oppenheimer (1904-1967) was an American Jewish theoretical physicist who made contributions to the physics of molecules, quantum electrodynamics and the physics of black holes. He was the scientific director of the Manhattan project to produce the fission bomb, and later director of the Institute for Advanced Study in Princeton.

field to build up according to the law $\mathcal{E} = \mathcal{E}_0(1 - e^{-t/\tau})$ where $\mathcal{E}_0$ and τ are constants. What is the criterion on τ in order for the hydrogen atom *not* to become excited.

1.3.8 Berry's phase

Every quantum state can be assigned a phase arbitrarily, but this cannot always be done freely as time goes on. Suppose we start with the system in which the Hamiltonian depends on several parameters. Berry[17] showed that when the parameters are varied adiabatically in a closed cycle, the phase of the system's state does not necessarily return to its original value. This *Berry phase* is a good example of a topological phase in QT. Topological phases have assumed growing importance in QT and quantum field theory.

We write the Hamiltonian as $\hat{H}(\boldsymbol{R})$, where $\boldsymbol{R}$ is the collection of parameters; for simplicity we focus on the case of 3 parameters, and think of $\boldsymbol{R}(t)$ as a vector in the appropriate Euclidean space. Let the system start in eigenstate $|E_n, \boldsymbol{R}\rangle$ of the Hamiltonian (the relevant equation is (1.112)) to which we tack on a real phase $\gamma_n(0)$ at time $t = 0$. If $\boldsymbol{R}$ varies slowly we can use the adiabatic theorem to infer that at some later time the state is

$$|\psi, t\rangle = |E_n, \boldsymbol{R}\rangle e^{\imath \int_0^t E_n(\boldsymbol{R})/\hbar\, dt'} e^{\imath\gamma_n(t)} \tag{1.127}$$

where $\gamma_n(t)$ appears as a consequence of the introduction of $\gamma_n(0)$. To find the evolution of $\gamma_n(t)$ we just substitute this *ansatz* into the Schrödinger equation (1.90) and cancel out all common phases:

$$(E_n(\boldsymbol{R}) - \hbar\dot{\gamma}_n)|E_n, \boldsymbol{R}\rangle + \imath\hbar\dot{\boldsymbol{R}} \cdot \partial|E_n, \boldsymbol{R}\rangle/\partial\boldsymbol{R} = E_n(\boldsymbol{R})|E_n, \boldsymbol{R}\rangle \tag{1.128}$$

where $\dot{} \equiv \partial/\partial t$. Canceling $E_n(\boldsymbol{R})|E_n, \boldsymbol{R}\rangle$ and taking the scalar product with $\langle E_n, \boldsymbol{R}|$ we get

$$\dot{\gamma}_n = \imath\dot{\boldsymbol{R}} \cdot \langle E_n, \boldsymbol{R}|\partial|E_n, \boldsymbol{R}\rangle/\partial\boldsymbol{R} \tag{1.129}$$

By analogy with the conclusion drawn from Eq. (1.117) we see that $\dot{\gamma}_n(t)$ here is real. Hence $\gamma_n(t)$ itself is real.

[17] Sir Michael Victor Berry (1941-), a British Jewish mathematical physicist, has worked on the semiclassical approach to quantum theory and optics, and on quantum chaos.

Does $\gamma_n(t)$, the phase over and above the dynamical phase $\int_0^t E_n(\boldsymbol{R})/\hbar\, dt'$, return to its original value $\gamma_n(0)$ if we cause $\boldsymbol{R}$ to go through a closed path in *its* configuration space such that $\boldsymbol{R}(T) = \boldsymbol{R}(0)$? Why would an overall change $\Delta\gamma_n \equiv \gamma_n(T) - \gamma_n(0) \neq 0$ be interesting? Is it not true that the phase tacked on to a quantum state has no physical consequences? But consider a particular system which is put in a superposition of two states. Changes in the *difference* of phases or the appearance of a *relative phase* between them can be measured and shows up in the probabilties. A nonzero $\Delta\gamma_n$ is of the nature of a relative phase which could be measured and so have physical consequences.

Obviously

$$\Delta\gamma_n = \int_0^T \dot{\boldsymbol{R}} \cdot \imath \langle E_n, \boldsymbol{R}| \frac{\partial |E_n, \boldsymbol{R}\rangle}{\partial \boldsymbol{R}} dt' = \oint d\boldsymbol{R} \cdot \imath \langle E_n, \boldsymbol{R}| \frac{\partial |E_n, \boldsymbol{R}\rangle}{\partial \boldsymbol{R}}\,. \quad (1.130)$$

It is not clear whether the second *integrand* here, called the *Berry connection* $\boldsymbol{A}_B(\boldsymbol{R})$, is a gradient of a single-valued function ($\Delta\gamma_n = 0$) or not ($\Delta\gamma_n \neq 0$). To clarify this we use Stokes' theorem to rewrite $\Delta\gamma_n$ as follows:

$$\Delta\gamma_n = \imath \int d\boldsymbol{S} \cdot \frac{\partial \langle E_n, \boldsymbol{R}|}{\partial \boldsymbol{R}} \times \frac{\partial |E_n, \boldsymbol{R}\rangle}{\partial \boldsymbol{R}}\,. \quad (1.131)$$

One might wrongly think that the integrand here always vanishes, being a vector product of parallel "vectors". But this is not so. The gradient of $|E_n, \boldsymbol{R}\rangle$ is a complex object with vectorial properties which we might write as $\boldsymbol{a} + \imath\boldsymbol{b}$ with $\boldsymbol{a}$ and $\boldsymbol{b}$ distinct real "vector fields". Then the gradient of $\langle E_n, \boldsymbol{R}|$ must be $\boldsymbol{a} - \imath\boldsymbol{b}$ and the vector product would be

$$(\boldsymbol{a} + \imath\boldsymbol{b}) \times (\boldsymbol{a} - \imath\boldsymbol{b}) = \imath(\boldsymbol{b} \times \boldsymbol{a} - \boldsymbol{a} \times \boldsymbol{b}) = -2\imath\, \boldsymbol{a} \times \boldsymbol{b} \quad (1.132)$$

which has no reason to vanish automatically.

It follows that the Berry phase γ_n of a state might well change upon adiabatic transport of the corresponding system along a closed path in parameter space. One example where detailed calculation shows this refers to an electron's magnetic moment coupled to a uniform magnetic field $\boldsymbol{B}$. The relevant part of the Hamiltonian is $-g\hat{\boldsymbol{s}} \cdot \boldsymbol{B}$ with g the electron's gyromagnetic factor and $\hat{\boldsymbol{s}}$ the spin. If the magnetic field is rotated so that it ends up pointing oppositely, and then the rotation is continued so that it returns to its original

direction, the electron's spin state picks up a Berry phase factor $e^{\imath\pi} = -1$. This can be revealed by causing the electron to interfere with itself (in the manner of the two slit experiment) so that over one path it goes through the rotated magnetic field while over the other it feels a constant field.

Exercises:

1. Show that if the state $|E_n, \boldsymbol{R}\rangle$ is normalized to unity, the Berry connection is pure real.

2. Redefine the state by

$$|E_n, \boldsymbol{R}\rangle \mapsto |E_n, \boldsymbol{R}\rangle \, e^{\imath\lambda(\boldsymbol{R})} \tag{1.133}$$

   with λ an arbitrary real and single valued function. Show that the Berry connection changes according to the *gauge transformation*

$$\boldsymbol{A}_B(\boldsymbol{R}) \mapsto \boldsymbol{A}_B(\boldsymbol{R}) - \boldsymbol{\nabla}_{\boldsymbol{R}} \lambda(\boldsymbol{R}) \tag{1.134}$$

   while the Berry phase γ_n is left unchanged.

Chapter 2

Propagators and path integrals

2.1 The propagator

Let us take the scalar product of the evolution equation, Eq. (1.83), with a position eigenstate $\langle \boldsymbol{r}|$ and introduce the decomposition of the identity between $\hat{U}$ and $|\psi, t\rangle$:

$$\psi(\boldsymbol{r}, t) = \int K(\boldsymbol{r}, t; \boldsymbol{r}', t_0)\, \psi(\boldsymbol{r}', t_0)\; d^3r'; \tag{2.1}$$

$$K(\boldsymbol{r}, t; \boldsymbol{r}', t_0) \equiv \langle \boldsymbol{r}|\hat{U}(t, t_0)|\boldsymbol{r}'\rangle\,. \tag{2.2}$$

Evidently Eq. (2.1) is just the evolution equation in position representation. The matrix element of the evolution operator, $K(\boldsymbol{r}, t; \boldsymbol{r}', t_0)$, for given t and t_0 is the Feynman propagator.[1] Evidently the propagator must satisfy the identity

$$K(\boldsymbol{r}, t_0; \boldsymbol{r}', t_0) = \delta(\boldsymbol{r} - \boldsymbol{r}'), \tag{2.3}$$

that is the equal time propagator is a spatial delta function because in zero time nothing happens to the wave function.

[1] named for Richard Phillips Feynman (1918-1988), a Nobel Laureate Jewish American regarded widely as the greatest North American theoretical physicist of the 20th century. Apart from the notion of path integral he devised his eponymous diagrams for describing elementary processes, and generally developed quantum electrodynamics. He also contributed to the microscopic model of He^4 superfluidity, and to the theory of elementary particles (Feynman-Gellman V-A weak decay theory, parton concept).

Next we take the matrix element of Eq. (1.86) and again intercalate the decomposition of the identity between the $\hat{U}$'s:

$$K(\boldsymbol{r}, t_2; \boldsymbol{r}_0, t_0) = \int K(\boldsymbol{r}, t_2; \boldsymbol{r}', t_1)\, K(\boldsymbol{r}', t_1; \boldsymbol{r}_0, t_0)\, d^3\boldsymbol{r}' \,. \tag{2.4}$$

This is the composition law for the propagator; it is evidently consistent with Eq. (2.3). The time t_1 can be taken anywhere in (t_0, t_2). So far the propagator (2.2) is only defined for $t \geq t_0$.

What is the physical interpretation of $K(\boldsymbol{r}, t; \boldsymbol{r}', t_0)$?. Let us take the initial state as $|\psi, t_0\rangle = |\boldsymbol{r}_0\rangle$. Thus $\psi(\boldsymbol{r}, t_0) = \delta(\boldsymbol{r} - \boldsymbol{r}_0)$. According to Eq. (2.2), $\psi(\boldsymbol{r}, t) = K(\boldsymbol{r}, t; \boldsymbol{r}_0, t_0)$. Since $\psi(\boldsymbol{r}, t)$ is the amplitude to find the particle at $\boldsymbol{r}$ at time t, $K(\boldsymbol{r}, t; \boldsymbol{r}_0, t_0)$ is clearly the amplitude for a particle originating at $\boldsymbol{r}_0$ at time t_0 to end up at $\boldsymbol{r}$ at time t: the propagator is the probability amplitude of propagation of the particle between the first and second events it mentions.

2.1.1 Propagator for stationary system

For an immediate example of a propagator let us look at Eq. (1.104), the law of evolution of a wave function when the Hamiltonian is time-independent. From it we immediately indentify

$$K(\boldsymbol{r}, t; \boldsymbol{r}', t_0) = \sum_j e^{-\imath E_j (t - t_0)/\hbar}\, u_j(\boldsymbol{r})\, u_j(\boldsymbol{r}')^*, \tag{2.5}$$

where E_j and $u_j(\boldsymbol{r})$ are the eigenvalues and eigenfunctions of the relevant Hamiltonian. The reason why this propagator depends on t and t_0 only through their difference is the time-independence of the Hamiltonian which entails that it should be possible to shift the origin of time without any significant change.

Suppose we take the Fourier transform of $K(\boldsymbol{r}, \boldsymbol{r}', \tau)$, where we have changed the format slightly to underline that time appears only as $\tau = t - t_0$. Given that $\tau \geq 0$ we should write

$$\mathcal{F}_K(\omega) = \int_0^\infty K(\boldsymbol{r}, \boldsymbol{r}', \tau)\, e^{\imath\omega\tau}\, d\tau \,. \tag{2.6}$$

Substituting from Eq. (2.5) we get an integral which will convege so long as ω is complex with positive imaginary part:

$$\mathcal{F}_K(\omega) = \imath \sum_j \frac{u_j(\boldsymbol{r})\, u_j(\boldsymbol{r}')^*}{\omega - E_j/\hbar}\,. \tag{2.7}$$

Thus viewed as a function of the complex variable ω, the Fourier transform of the propagator is analytic in the upper complex plane, and has a pole at every energy eigenvalue, with residue $u_j(\boldsymbol{r})\, u_j(\boldsymbol{r}')^*$. The poles of the propagator signal the energy eigenvalues and the residues give the eigenfunctions. This is a very general feature in QT: the propagator knows everything about the spectrum of the Hamiltonian.

2.1.2 Propagator for a free particle

A free particle is one of the cases where the sum representing the propagator in Eq. (2.5) can be performed exactly. The free particle has $\hat{H} = \hat{\boldsymbol{p}}^2/2m$, and consequently the eigenvalues are $\boldsymbol{p}^2/2m$ for every vector $\boldsymbol{p}$. The corresponding eigenfunctions are given by Eq. (1.64) so that

$$K_{\mathrm{f}}(\boldsymbol{r}, t; \boldsymbol{r}', t_0) = \int \frac{d^3p}{(2\pi\hbar)^3}\; e^{\imath \boldsymbol{p}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)}\, e^{-\imath \frac{p^2(t-t_0)}{2m\hbar}}\,. \tag{2.8}$$

We have passed from a discrete sum over index j to an integral over $\boldsymbol{p}$ which is reasonable since momentum is a continuous variable. But how do we know that the measure of integration in momentum space is just d^3p? This last is clear from comparing the generic form of the decomposition of the identity Eq. (1.18) with Eq. (1.41) appropriate to momentum space.

To evaluate the integral we complete the square in the exponent, so that the whole exponent takes the form

$$-\imath \frac{(t-t_0)}{2m\hbar}\left[\boldsymbol{p} - \frac{m(\boldsymbol{r}-\boldsymbol{r}_0)}{t-t_0}\right]^2 + \imath \frac{m|\boldsymbol{r}-\boldsymbol{r}_0|^2}{2\hbar(t-t_0)} \tag{2.9}$$

Thus

$$K_{\mathrm{f}}(\boldsymbol{r}, t; \boldsymbol{r}', t_0) = e^{\imath \frac{m|\boldsymbol{r}-\boldsymbol{r}_0|^2}{2\hbar(t-t_0)}} \int \frac{d^3p}{(2\pi\hbar)^3}\, e^{-\imath \frac{(t-t_0)}{2m\hbar}\left[\boldsymbol{p} - \frac{m(\boldsymbol{r}-\boldsymbol{r}_0)}{t-t_0}\right]^2} \tag{2.10}$$

At this point we shift the origin of $\boldsymbol{p}$ so that the added term in the square in the exponential inside the integral disappears (the integration is over all $\boldsymbol{p}$ space so the shift does not change the integration domain). At this point we factor the exponential into p_x, p_y and p_z parts; the integration measure factors into $dp_x\, dp_y\, dp_z$. Thus

$$K_{\rm f}(\boldsymbol{r}, t; \boldsymbol{r}', t_0) = e^{\imath \frac{m|\boldsymbol{r}-\boldsymbol{r}_0|^2}{2\hbar(t-t_0)}} \left(\int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, e^{-\imath \frac{(t-t_0)}{2m\hbar} p^2} \right)^3 \tag{2.11}$$

The integral in question is a Gaussian[2] integral—named for its integrand being reminiscent of the famous probability distribution function. There are various ways of doing the integral. The example below illustrates the use of contour integration. Using its results we have, finally

$$K_{\rm f}(\boldsymbol{r}, t; \boldsymbol{r}', t_0) = \left(\frac{m}{2\pi\imath\hbar(t-t_0)} \right)^{3/2} \exp\left(\imath \frac{m|\boldsymbol{r}-\boldsymbol{r}_0|^2}{2\hbar(t-t_0)} \right). \tag{2.12}$$

This result is exact. It has the expected dependence on $t - t_0$ for a system with time independent Hamiltonian. Additionally, it depends, not separately on the points $\boldsymbol{r}$ and $\boldsymbol{r}_0$, but on the distance between them. Why? The particle is not subject to forces—the potential it feels is constant. It then follows from homogeneity of space that it should be possible to shift the origin without changes. This requires spatial dependence only on the vector $\boldsymbol{r} - \boldsymbol{r}_0$. In addition the isotropy of space allows a rotation without physical change. This means only the absolute magnitude of the vector may appear, namely $|\boldsymbol{r} - \boldsymbol{r}_0|$.

In terms of the physical interpretation of the propagator it is clear that the *probability amplitude* for the particle to go from $\boldsymbol{r}_0$ to $\boldsymbol{r}$ in a given time interval is sinusoidal in the square of the distance, but the probability itself is distance independent while inversely proportional to the cube of the time interval.

[2] Carl Friedrich Gauss (1777-1855), a German, was probably the greatest mathematician of the last two centuries. His interests ranged from number theory through non-Euclidean geometry and function theory to probability theory. He also contributed to the theory and experimental basis of electromagnetic theory and to the theory of measurement (least squares method).

Example: Contour evaluation of Gaussian integrals

The integral in question,

$$\int_{-\infty}^{\infty} e^{-\imath\alpha p^2}\, dp; \qquad \alpha > 0 \tag{2.13}$$

is over the real axis. Because of the oscillations of the imaginary exponent it is not even clear whether it converges (it does!). Let us employ Cauchy's theorem[3] that the closed contour integral of an *entire function* (analytic with no poles or cuts) vanishes. The function $e^{-\imath\alpha p^2}$ is entire. As the contour we start with the whole real axis, which we continue with an arc *at infinity* that sweeps down from the real point $+\infty$ to angle $\varphi = -\pi/4$ in the complex plane. The contour then proceeds as a straight line through the origin to the point at infinity at $\varphi = 3\pi/4$. From there the contour is an arc at infinity with φ growing to reach the real point $-\infty$, where the contour rejoins the real line.

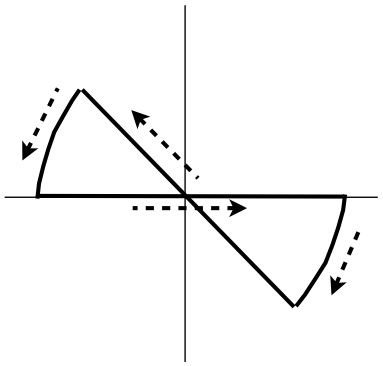

Figure 2.1: **The contour used in Cauchy's theorem to calculate the integral (2.13).**

At infinity we can write $p = Re^{\imath\varphi}$ with R positive and very large and $0 < \varphi \leq 2\pi$. Thus for the first arc $0 > 2\varphi \geq -\pi/2$ so that p^2 has there a negative imaginary part. Therefore the contribution of the arc to the integral vanishes, the integrand being $e^{-\alpha R^2|\sin 2\phi|}$. In like manner in the second arc

[3]named for the Baron Augustin-Louis Cauchy (1789-1857), a prolific French mathematician who contributed famously to complex function theory, but also to the theory of waves in elastic media. He was one of the first to introduce rigorous methods in mathematics.

$2\pi > 2\varphi \geq 3\pi/2$, so again p^2 has there a negative imaginary part and the contribution of that arc to the integral vanishes. By Cauchy's theorem the integral over the real line is equal to the integral along L, the infinite straight line from infinity in the second quadrant to the origin with $\varphi = 3\pi/4$, continuing straight to infinity in the fourth quadrant with $\varphi = -\pi/4$. On this line $p = ue^{-\imath\pi/4}$ with u real and ranging from $-\infty$ to ∞; $p^2 = -\imath u^2$. Therefore,

$$\int_L e^{-\imath\alpha p^2}\, dp = \int_{-\infty}^{\infty} e^{-\alpha u^2}\, e^{-\imath\pi/4}\, du = e^{-\imath\pi/4}\sqrt{\pi/\alpha} = \sqrt{\pi/\imath\alpha}. \tag{2.14}$$

Of course, once the integral is calculated for $\alpha > 0$, the result can be used for $\alpha < 0$ or even for complex α by virtue of analytic continuation.

Exercises:

1. Show that the composition of two free particle propagators with a common moment according to Eq. (2.4) produces the appropriate free particle propagator from $\boldsymbol{r}_0$ to $\boldsymbol{r}$ in time $t_2 - t_0$.
2. Show that the free particle propagator satisfies the identity (2.3).
3. A free particle has an initial Gaussian packet wave function, i.e. $\psi(\boldsymbol{r}, t_0) \propto e^{-\beta(\boldsymbol{r}-\boldsymbol{r}_0)^2}$ with $\beta > 0$. Show that the wave function continues to be Gaussian, but its width spreads, and find the law of spreading.
4. How would you tell if a given propagator describes a system with stationary Hamiltonian? And how would you check if the function $f(\boldsymbol{r}, t_0)$ is indeed the correct initial value for the wave function of an energy eigenstate?

2.1.3 The propagator as a path integral

Following an obscure remark by Dirac, Feynman hypothesized that quite in general the propagator of a system whose classical Lagrangian is $L(\dot{\boldsymbol{r}}, \boldsymbol{r}, t)$ can be written as

$$K(\boldsymbol{r}, t; \boldsymbol{r}', t_0) = \mathcal{N} \int_{\text{paths}} \mathcal{D}[\boldsymbol{r}(t)]\, \exp\left(\frac{\imath}{\hbar}\int_{t_0}^{t} L\left(\dot{\boldsymbol{r}}(t'), \boldsymbol{r}(t'), t'\right)\, dt'\right). \tag{2.15}$$

Here $\mathcal{N}$ is a normalization factor. The inner integral is taken for each continuous (but not necessarily smooth) path that goes from $\boldsymbol{r}(t)$ from $\boldsymbol{r}_0$ at t_0 to $\boldsymbol{r}$ at t; the outer integral is to be interpreted as a sum of the exponent over all possible paths with the $\mathcal{D}[\boldsymbol{r}(t)]$ denoting the measure over paths. We must use an integral with measure as the paths in question obviously make up a continuum.

Feynman's prescription looks so different from the definition of propagator as matrix element of $\hat{U}(t, t_0)$ that one needs some supporting evidence. One point is that the prescription is entirely consistent with the composition rule (2.4). This is seen as follows. When we multiply the two path integral expressions for the two propagators, we can move both exponents inside the double integral. The integral over $\boldsymbol{r}'$ taken at time t_1 from the composition rule converts the path integration to one over *all* paths from $\boldsymbol{r}_0$ at t_0 to $\boldsymbol{r}$ at t regardless of the intermediate point. In parallel the two exponents can be added to make the integral over the Lagrangian for a path from $\boldsymbol{r}_0$ at t_0 to $\boldsymbol{r}$ at t. Thus we obtain the Feynman recipe for the propagator from $\boldsymbol{r}_0$ at t_0 to $\boldsymbol{r}$ at t.

A second point concerns the classical limit of the path integral. The quantum of action $\hbar$ is very small. Any macroscopic system has an action $\int L dt$ very much larger than $\hbar$. Thus for a macroscopic system the exponent is a phase very large compared to 2π. As we add the contributions from many paths in Feynman's path integral, the fact that the phases vary wildly will cause most contributions to cancel one another. An exception is a path very close to the *classical trajectory* of the system (the one that satisfies Lagrange's equations) and goes from the initial to the final configuration. Of course, according to Hamilton's principle, such trajectory extremizes the classical action between initial and final configuration. This means that all nearby paths have essentially the same action. All these can contribute to the path integral without cancellation since phase varies little from path to path. Thus the path integral of a macroscopic system is dominated by almost classical paths. This agrees with the requirement that a macroscopic system should have classical dynamics.

What is the condition for a system to function classically. Let's go back to the case of a particle of mass m which moves over a distance L in time T. Obviously the kinetic energy is of order mL^2/T^2 and this is the full Lagrangian. So the classical action is of order mL^2/T. When this is large

compared to $\hbar$ the cancellation of phases will set in. A classical particle is one which satisfies

$$mL^2/T \gg \hbar. \tag{2.16}$$

One understands why it is usually the case that a very light particle does not behave classically. However, note that an electron flying a meter over a second is *quasiclassical*.

It is possible to derive the path integral prescription for the propagator (2.15) staring directly from the standard Eq. (2.2) and the Schrödinger equation (1.105). However this rather intricate derivation gives the Feynman prescription only for the case of a classical Hamiltonian corresponding to Lagrangian of the form

$$L = \frac{1}{2}m\big(\dot{\boldsymbol{r}} + a(\boldsymbol{r})\big)^2 - V(\boldsymbol{r}). \tag{2.17}$$

Nevertheless, when it comes to quantize dynamics in a completely new are of physics, it is customary to do this at first with Feynman's prescription, appropriately adapted, since it provides the clearest path for the transition from the classical physics.

To quell any doubts about the general validity of Feynman's path integral prescription, we provide the following derivation of Schrödinger's equation from the path integral for a simple Hamiltonian.

Exercises:

1. Show that another way to characterize the classical limit is to say that the particle's de Broglie wavelenth[4] is small compared to the dimension of the region in which it moves.

2. A solid disk has moment of inertia I about its axis of symmetry. Write the path integral for the propagator of the angular coordinate $\theta(t)$. Hint: This is not a trivial rewriting of Eq. (2.12) because θ is an angle.

3. An electron is emitted from a source at time t_0; in front of the source stands an opaque screen with two tiny holes at known positions. Write

[4]introduced by the French nobleman Louis Victor Pierre Raymond, 7th Duke de Broglie (1892-1987), one of the founders of quantum mechanics (wave aspect of matter) and a Nobel Laureate. De Broglie also proposed deterministic quantum theories.

the amplitude for arrival of the electron at a detector behind the screen at time t_1 in terms of the propagator $K_{\rm f}$.

4. Two particles with masses m_1 and m_2 interact through the potential $V(|\boldsymbol{r}_1 - \boldsymbol{r}_2|)$. Starting from the total Lagrangian separate the motion and write the propagator for the center-of-mass motion in closed form and the path integral for the relative motion.

5. A free particle starts from $\boldsymbol{r} = 0$ at $t = 0$ and ends at $\boldsymbol{r} = \boldsymbol{R}$ at $t = T$. Use the free propagator to express the mean value of its position at time $t = T/2$.

2.1.4 Schrödinger's equation from path integration

For simplicity we work in one dimension. The evolution equation (2.1) for a brief time $t - t_0 = \epsilon$ is

$$\psi(x, t_0 + \epsilon) = \int_{-\infty}^{\infty} K(x, t_0 + \epsilon; x', t_0)\, \psi(x', t_0)\, dx' \,. \tag{2.18}$$

In the one-dimensional version of Eq. (2.15) we shall take

$$L(\dot{x}, x, t) = \frac{1}{2} m \dot{x}^2 - V(x, t) \,. \tag{2.19}$$

We first look at the path that goes from (x', t_0) to $(x, t_0 + \epsilon)$ in a straight line with constant velocity—the uniform path. Its classical action $S[x, t; x', t_0]$ is

$$\int_{t_0}^{t_0+\epsilon} L\big(\dot{x}(t'), x(t'), t'\big) dt' = \frac{1}{2} m \frac{(x - x')^2}{\epsilon} - \int_{t_0}^{t_0+\epsilon} V\big(x(t'), t'\big)\, dt' \tag{2.20}$$

Obviously the kinetic term, that diverges as $\epsilon \to 0$, dominates over the potential term which vanishes in that limit. The same must be true for a non-uniform path since it must have an even bigger kinetic term (it gets from x' to x in the same time ϵ by a longer path). Thus the important factor in the short-time path integral is contributed by the kinetic energy.

Obviously the particle cannot go far in a short time ϵ so $\eta \equiv x - x'$ must be small also. Expanding by Taylor's theorem in the two variables

$$\psi(x, t_0 + \epsilon) = \psi(x, t_0) + \epsilon \frac{\partial \psi(x,t)}{\partial t}\Big|_{t=t_0} + \cdots , \tag{2.21}$$

$$\psi(x', t_0) = \psi(x, t_0) - \eta \frac{\partial \psi(x, t_0)}{\partial x} + \tfrac{1}{2}\eta^2 \frac{\partial^2 \psi(x, t_0)}{\partial x^2} + \cdots . \tag{2.22}$$

The reason for neglecting $\mathcal{O}(\epsilon^2)$ terms will be clear shortly.

Before substituting in Eq. (2.18) we shall write the short time path integral (2.15) with action (2.20) as

$$K(x, t_0 + \epsilon; x', t_0) = \mathcal{A} \exp\left(\frac{\imath m \eta^2}{2\hbar\epsilon}\right) \exp\left(-\frac{\imath\epsilon}{\hbar} V\left(x - \tfrac{1}{2}\eta, t_0 + \tfrac{1}{2}\epsilon\right)\right) . \tag{2.23}$$

The first exponent is the phase due to the uniform path. What is $\mathcal{A}$? Instead of integrating over paths, we have multiplied the exponent of the uniform path by a factor that "counts" the number of paths which are very like it. Paths which are very different contribute phases which vary rapidly; their exponents when summed over tend to cancel one another out. The product of $\mathcal{N}$ with thes count factor is $\mathcal{A}$; it will determined below. Next, we have approximated the time integral over V by ϵ times V taken in the middle of the uniform path in position and time. Because ϵ and η are small, this is a good approximation assuming that V is a continuous and smooth function of both its arguments.

And because ϵ and η are small we are allowed to Taylor expand the second exponent in Eq. (2.23), again to $\mathcal{O}(\epsilon)$ and $\mathcal{O}(\eta^2)$:

$$e^{-\frac{\imath\epsilon}{\hbar}V(x-\frac{1}{2}\eta, t_0+\frac{1}{2}\epsilon)} = 1 - \frac{\imath\epsilon}{\hbar}V(x, t_0) + \frac{\imath\epsilon\eta}{2\hbar}\frac{\partial V(x,t_0)}{\partial x} - \frac{\imath\epsilon\eta^2}{8\hbar}\frac{\partial^2 V(x,t_0)}{\partial x^2} . \tag{2.24}$$

We now substitute the last four equations into Eq. (2.18):

$$\psi + \epsilon\frac{\partial\psi}{\partial t_0} = \psi(1 - \frac{\imath\epsilon}{\hbar}V)\,\mathcal{A}\int_{-\infty}^{\infty} e^{\frac{\imath m\eta^2}{2\hbar\epsilon}}\, d\eta \tag{2.25}$$

$$+ \left[\frac{1}{2}(1 - \frac{\imath\epsilon}{\hbar}V)\frac{\partial^2\psi}{\partial x^2} - \frac{\imath\epsilon}{2\hbar}\frac{\partial V}{\partial x}\frac{\partial\psi}{\partial x} - \frac{\imath\epsilon}{8\hbar}\frac{\partial^2 V}{\partial x^2}\psi\right]\mathcal{A}\int_{-\infty}^{\infty}\eta^2 e^{\frac{\imath m\eta^2}{2\hbar\epsilon}}\, d\eta + \cdots \tag{2.26}$$

where the arguments of ψ and V are understood to be x and t_0, and we have passed from an integral over x to one over η.

It may seem strange that the integral extends to infinity given that we said that η is effectively small. But we can allow this because Eq. (2.23) shows that when η^2 grows beyond $\hbar\epsilon/m$, the consequent oscillations of the first exponential will erase contributions to the integral in Eq. (2.18). By the same token, we may regard the quantity η^2 to be of the same order of smallness as ϵ. This is the reason why we expanded to $\mathcal{O}(\epsilon)$ and $\mathcal{O}(\eta^2)$ but not to $\mathcal{O}(\epsilon^2)$. Likewise, we have not included terms multiplied by $\int_{-\infty}^{\infty} \eta \exp(\frac{\imath m\eta^2}{2\hbar\epsilon})\, d\eta$ because this integral vanishes.

We now appeal to the example of Sec. 2.1.2 to derive the result

$$\int_{-\infty}^{\infty} e^{\frac{\imath m\eta^2}{2\hbar\epsilon}}\, d\eta = \left(\frac{2\pi\imath\epsilon\hbar}{m}\right)^{1/2}, \tag{2.27}$$

while differentiation of both sides with respect to m gives

$$\int_{-\infty}^{\infty} \eta^2 e^{\frac{\imath m\eta^2}{2\hbar\epsilon}}\, d\eta = \frac{\imath\hbar\epsilon}{m}\left(\frac{2\pi\imath\epsilon\hbar}{m}\right)^{1/2}. \tag{2.28}$$

Let us substitute these in Eq. (2.26) and isolate the lowest order terms in ϵ. If we pretend that $\mathcal{A}$ is independent of ϵ, we cannot balance the $\mathcal{O}(\epsilon^0)$ terms consistently. But if we surmise that

$$\mathcal{A} = \left(\frac{m}{2\pi\imath\epsilon\hbar}\right)^{1/2} \tag{2.29}$$

then the $\mathcal{O}(\epsilon^0)$ terms cancel. The $\mathcal{O}(\epsilon)$ terms will cancel (we take the liberty to replace $t_0 \to t$) provided

$$\epsilon\frac{\partial\psi}{\partial t} = -\frac{\imath\epsilon}{\hbar}V(x,t)\psi + \frac{1}{2}\frac{\imath\hbar\epsilon}{m}\frac{\partial^2\psi}{\partial x^2}. \tag{2.30}$$

But this is evidently the Schrödinger equation for a particle of mass m in a potential $V(x,t)$. And should we proceed to calculate the $\mathcal{O}(\epsilon^2)$ terms we would just get the space derivative of the Schrödinger equation.

We have thus established that Feynman's ansatz (2.15) with the Lagrangian (2.19) is equivalent to standard quantum dynamics. It is not hard to see that the same is true in three dimensions, and for a system of several particles interacting via potential-derivable two-body forces. In effect, Fenman's prescription is equivalent to the Hamiltonian approach to quantum dynamics.

Another thing that we learned [see Eqs. (2.23) and (2.29)] is that for short times

$$K(x,t+\epsilon;x_0,t)=\left(\frac{m}{2\pi\imath\epsilon\hbar}\right)^{1/2}\exp\left(\frac{\imath m(x-x_0)^2}{2\hbar\epsilon}\right)\left(1+\mathcal{O}(\epsilon)\right), \tag{2.31}$$

which agrees in form with the exact free particle propagator (2.12) to lowest order in ϵ. Thus over short times the effect of an external force on a particle is not yet visible. Later we shall construct the corrections to this expression coming from the potential.

2.1.5 Propagator for the harmonic oscillator

Exercise 3 of Sec 1.3.3 gives the Hamiltonian of the 3-D harmonic oscillator. The corresponding Lagrangian (still with unit mass) in 1-D is

$$L=\tfrac{1}{2}\dot{x}^2-\tfrac{1}{2}\omega^2x^2\,. \tag{2.32}$$

The Lagrange equation

$$\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{x}}\right)=\frac{\partial L}{\partial x} \tag{2.33}$$

yields as equation of motion

$$\ddot{x}+\omega^2x=0, \tag{2.34}$$

whose general solution is

$$x(t')=X(t')\equiv A\sin\omega t'+B\cos\omega t' \tag{2.35}$$

with A and B real constants. Of course if we want the oscillator to start from x_0 at t_0 and end up at x at t we must set

$$x_0 = A\sin\omega t_0+B\cos\omega t_0\,, \tag{2.36}$$
$$x = A\sin\omega t+B\cos\omega t\,, \tag{2.37}$$

from which we solve

$$A=\frac{x_0\cos\omega t-x\cos\omega t}{\sin\omega(t-t_0)}\,, \tag{2.38}$$
$$B=\frac{x_0\sin\omega t-x\sin\omega t}{\sin\omega(t-t_0)}\,. \tag{2.39}$$

These define the classical motion of the oscillator.

To construct the path integral for the harmonic oscillator we have to consider all paths of the form

$$x(t') = X(t') + y(t'); \qquad y(t_0) = y(t) = 0 \tag{2.40}$$

with $y(t)$ continuous but otherwise arbitrary, one y for each distinct path. The Lagrangian (2.32) written with the path (2.40) takes the form

$$L = \tfrac{1}{2}\dot{X}^2 - \tfrac{1}{2}\omega^2 X^2 + \tfrac{1}{2}\dot{y}^2 - \tfrac{1}{2}\omega^2 y^2 + \dot{X}\dot{y} - \omega^2 Xy. \tag{2.41}$$

We note that

$$\dot{X}\dot{y} - \omega^2 Xy = \frac{d}{dt}(\dot{X}y) - y(\ddot{X} + \omega^2 X) = \frac{d}{dt}(\dot{X}y), \tag{2.42}$$

with the last result following from Eq. (2.34) or (2.35).

We now form the action,

$$\int_{t_0}^{t} L\,dt' = S[X] + S[y] + \dot{X}y\Big|_{t_0}^{t} \tag{2.43}$$

$$= \int_{t_0}^{t} \tfrac{1}{2}\left(\dot{X}^2 - \omega^2 X^2\right) dt' + \int_{t_0}^{t} \tfrac{1}{2}\left(\dot{y}^2 - \omega^2 y^2\right) dt' \tag{2.44}$$

where the contribution from $\dot{X}y\big|_{t_0}^{t}$ drops out by virtue of the boundary conditions in Eq. (2.40). The part $S[X]$ is the action of the classical oscillator path between x_0 at t_0 and x at t. The $S[y]$ is the contribution to the total oscillator action $\int L\,dt$ from the *deviations* of the possible paths from the classical path.

The $S[x]$ is calculated in Exercise 2. Thus, according to Eqs. (2.15) and (2.44),

$$K(x,t;x_0,t_0) = \mathcal{N}\exp\left(\frac{\imath}{\hbar}S[X]\right)\int \mathcal{D}[y(t')]\, e^{\frac{\imath}{\hbar}S[y]}. \tag{2.45}$$

The prefactor involving the classical action turns out to be ubiquitous in path integral theory. It is sometimes called the *semiclassical approximation* or *tree-level approximation* to the path integral.

How to evaluate $S[y]$? In view of the conditions in Eq. (2.40) it is appropriate to regard $y(t')$ as a periodic function with period $t - t_0$ which is, in

addition, odd ($y(t_0) = 0$). But in the theory of Fourier series[5] the representation of the generic odd periodic function with period $t - t_0$ is

$$y(t') = \sum_{n=1}^{\infty} a_n \, \sin\left(\frac{n\pi(t'-t_0)}{t-t_0}\right) . \tag{2.46}$$

Thus

$$\begin{aligned} \int_{t_0}^{t} y(t')^2 \, dt' &= \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} a_n a_m \int_{t_0}^{t} \sin\left(\frac{n\pi(t'-t_0)}{t-t_0}\right) \sin\left(\frac{m\pi(t'-t_0)}{t-t_0}\right) dt' \\ &= \frac{1}{2}(t-t_0)\sum_{n=1}^{\infty} {a_n}^2 . \end{aligned} \tag{2.47}$$

In like manner

$$\int_{t_0}^{t} \dot{y}(t')^2 \, dt' = \frac{1}{2}(t-t_0)\sum_{n=1}^{\infty} {a_n}^2 \frac{n^2\pi^2}{(t-t_0)^2} \tag{2.48}$$

so that

$$S[y] = \frac{1}{4}(t-t_0)\sum_{n=1}^{\infty} {a_n}^2 \left[\frac{n^2\pi^2}{(t-t_0)^2} - \omega^2\right] . \tag{2.49}$$

The Fourier coefficients a_n are normally a fixed set depending on the function being represented. But here we want to sum over all continuous functions $y(t')$; thus each a_n will be allowed to take all real values. Therefore we envision the replacement

$$\int \mathcal{D}[y(t')] \Longrightarrow \lim_{N\to\infty} \prod_{n=1}^{N} \int_{-\infty}^{\infty} da_n \, . \tag{2.50}$$

But something is missing! When in integrating one changes from one set $\{x_1, x_2, \cdots\}$ of variables to another, $\{y_1, y_2, \cdots\}$, one includes as a factor the Jacobian determinant $J \equiv |\partial y_i/\partial x_j|$. Here the suitable Jacobian is

[5] Jean Baptiste Joseph Fourier (1768-1830) was the French mathematician and physicist who invented the eponymous series and transform and used them to give the first quantitative theory of heat conduction. He is thought to have invented dimensional analysis and to have proposed the greenhouse effect. He accompanied Napoleon to Egypt and was governor of Lower Egypt until the French withdrawal.

$|\partial y(t')/\partial a_n|$; we shall denote it by J_N because at first it refers to a finite set of N coefficients a_n. From Eq. (2.46) it is clear that J_N depends only on $t-t_0$ and not on $\hbar$. In practice there is no need to compute the J_N explicitly.

We are thus faced with the multiple integral

$$\tilde{I} \equiv \lim_{N\to\infty} J_N \prod_{n=1}^{N} \int_{-\infty}^{\infty} da_n \exp\left(\frac{\imath}{4\hbar}(t-t_0)\sum_{n=1}^{\infty} {a_n}^2 \left[\frac{n^2\pi^2}{(t-t_0)^2} - \omega^2\right]\right). \tag{2.51}$$

According to the result Eq. (2.14) each Gaussian integral here equals

$$\left(\frac{\imath\, 4\pi\hbar}{t-t_0}\right)^{1/2} \left[\frac{n^2\pi^2}{(t-t_0)^2} - \omega^2\right]^{-\frac{1}{2}}. \tag{2.52}$$

Thus

$$\tilde{I} = \lim_{N\to\infty} J_N \left(\frac{\imath\, 4\pi\hbar}{t-t_0}\right)^{N/2} \prod_{n=1}^{N} \left(\frac{t-t_0}{n\pi}\right) \prod_{n=1}^{N} \left[1 - \frac{\omega^2(t-t_0)^2}{n^2\pi^2}\right]^{-\frac{1}{2}}. \tag{2.53}$$

At this point we recall Euler's identity,

$$\prod_{n=1}^{N} \left(1 - \frac{x^2}{n^2\pi^2}\right) = \frac{\sin x}{x} \tag{2.54}$$

which means that

$$\tilde{I} = F(t-t_0,\hbar) \left(\frac{\omega(t-t_0)}{\sin\omega(t-t_0)}\right)^{1/2} \tag{2.55}$$

for some function F (which may not converge). Combining this with the result of Exercise 2 in Eq. (2.45) we get

$$K(x,t;x_0,t_0) = \mathcal{N}F\cdot \left(\frac{\omega(t-t_0)}{\sin\omega(t-t_0)}\right)^{1/2} \exp\left[\frac{\imath m\omega}{2\hbar}\,\frac{(x^2+x_0^2)\cos\omega(t-t_0) - 2xx_0}{\sin\omega(t-t_0)}\right], \tag{2.56}$$

where we have restored the mass m by dimensional considerations.

To determine $\mathcal{N}F$ we now compare this expression in the limit $\omega \to 0$ with the free particle propagator [Eq. (2.12) in 1-D] which should emerge in

this limit. This will be true only if

$$\mathcal{N}F(t-t_0,\hbar)=\left[\frac{m}{2\pi\imath\hbar(t-t_0)}\right]^{1/2}. \tag{2.57}$$

By accepting this consistency argument we sidestep the problems of determining the normalization factor $\mathcal{N}$ as well as the J_N. The final result is

$$K(x,t;x_0,t_0)=\left(\frac{m\omega}{2\pi\imath\hbar\sin\omega(t-t_0)}\right)^{1/2}\exp\left[\frac{\imath m\omega}{2\hbar}\,\frac{(x^2+x_0^2)\cos\omega(t-t_0)-2xx_0}{\sin\omega(t-t_0)}\right]. \tag{2.58}$$

Through the complex form of Eq. (2.58) one observes two things. First, the propagator is fully periodic in time with frequency ω just as is the motion of the classical oscillator. Second, if we let $t-t_0$ become infinitesimal, this propagator reduces to the free particle propagator (2.12). This is another example of the rule [see Eq. (2.31)] that interactions are not felt over a short time.

As Exercise 3 shows, the work we have done in computing the path integral over $y(t')$ (the quantum factor in Eq. (2.45)) can be used *unchanged* for obtaining propagators for the whole class of Lagrangians quadratic in x and $\dot{x}$. All these lead to the same Gaussian integrals, and the difference between one case and another is restricted to the semiclassical part.

Exercises

1. Prove that for every Lagrangian quadratic in x and $\dot{x}$ (even with time varying coefficients) we obtain a split like in Eqs. (2.43)- (2.44).

2. By use of trigonometric identities prove that the classical action (the first term on the r.h.s. of Eq. (2.44)) is given by

$$S[X]=\omega\frac{(x^2+x_0^2)\cos\omega(t-t_0)-2x\,x_0}{2\sin\omega(t-t_)}. \tag{2.59}$$

3. A particle's Lagrangian is

$$L=\tfrac{1}{2}(m\dot{x}^2-\omega^2x^2)+\alpha(t)x+\beta(t)\dot{x}. \tag{2.60}$$

Explain why this describes a forced harmonic oscillator. Prove that in calculating the propagator for this oscillator, all we need to recalculate is the classical action $S[X]$; the integral in Eq. (2.45) is the same as for $\alpha = \beta = 0$.

4. A particle with mass m and charge e moves in one dimension in a uniform electric field of strength $\mathcal{E}$ pointed in the $-z$ direction. Show that the *probability* of transition from x_0 at t_0 to x at t does *not* depend on x or x_0. What is its dependence on t and t_0?

2.1.6 Spectrum and eigenfunctions

In a case like ours for which the Hamiltonian is time-independent the propagator can be expanded in terms of the former's eigenvalues and eigenfunctions according to Eq. (2.5). This allows to infer eigenvalues and eigenfunctions of the harmonic oscillator's Hamiltonian directly from Eq. (2.58). To start we rewrite

$$\sin\omega(t-t_0) = \frac{e^{\imath\,\omega(t-t_0)}}{2\imath}\left[1-e^{-2\imath\,\omega(t-t_0)}\right], \tag{2.61}$$

$$\frac{\cos\omega(t-t_0)}{\sin\omega(t-t_0)} = \imath\frac{1+e^{-2\imath\,\omega(t-t_0)}}{1-e^{-2\imath\,\omega(t-t_0)}}. \tag{2.62}$$

In terms of this we get

$$K(x,t;x_0,t_0) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\frac{1}{2}\imath\,\omega(t-t_0)}\; W(e^{-\imath\,\omega(t-t_0)}) \tag{2.63}$$

where

$$W(\xi) \equiv \frac{1}{\sqrt{1-\xi^2}}\exp\left\{-\frac{m\omega}{2\hbar}\left[(x^2+x_0^2)\left(\frac{1+\xi^2}{1-\xi^2}\right)-\frac{4x\,x_0\,\xi}{1-\xi^2}\right]\right\}. \tag{2.64}$$

At this point we expand $W(\xi)$ in a series in ξ. Because $\xi = e^{-\imath\,\omega(t-t_0)}$ it is obvious that the propagator is a series of whole powers of $e^{-\imath\,\omega(t-t_0)}$ multiplied by the factor $e^{-\frac{1}{2}\imath\,\omega(t-t_0)}$ with $(t-t_0)$ appearing nowhere else. Comparing with Eq. (2.5) we see that the spectrum of the harmonic oscillator is

$$E = (n+\tfrac{1}{2})\,\hbar\omega; \qquad n = 0,1,2,\cdots \tag{2.65}$$

which, of course, is the correct result. In addition, by comparing the $\mathcal{O}(\xi^0)$ term of the series for $K(x,t;x_0,t_0)$ with Eq. (2.5), we identify the first eigenfunction,

$$u_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left[-\frac{m\omega}{2\hbar}x^2\right] \tag{2.66}$$

which is indeed the ground state of the harmonic oscillator.

Exercise

1. Use a computer algebra program to verify that expanding $W(\xi)$ to higher orders will give the correct eigenfunctions for energies $\frac{3}{2}\hbar\omega$ and $\frac{5}{2}\hbar\omega$

2.1.7 Perturbation theory for the propagator

Thus far we use the propagator only for $t \geq t_0$; we shall insist on this by imagining that it is to carry an overall factor $\Theta(t-t_0)$ where $\Theta(x)$ is the Heaviside or step function,[6] $\Theta(x) = 1$ for $x \geq 0$ and $\Theta(x) = 0$ otherwise. In particular, we write instead of $K_{\rm f}(\boldsymbol{r},t;\boldsymbol{r}',t_0)$ from Eq. (2.12) the form

$$G_{\rm f}^{(+)}(\boldsymbol{r},t;\boldsymbol{r}',t_0) = -\imath\Theta(t-t_0)\left(\frac{m}{2\pi\imath\hbar(t-t_0)}\right)^{3/2}\exp\left(\imath\frac{m|\boldsymbol{r}-\boldsymbol{r}_0|^2}{2\hbar(t-t_0)}\right), \tag{2.67}$$

with the plus sign referring to the property of propagation into the *future*.

Next we operate on $G_{\rm f}^{(+)}$ with

$$\hat{D}_0 \equiv \imath\,\hbar\,\partial/\partial t - \hat{\boldsymbol{p}}^2/2m\,. \tag{2.68}$$

[6] named after Oliver Heaviside (1850-1925), a non-mainstream British electrical engineer, mathematician and physicist. He introduced both complex numbers and vectors to electromagnetism, deviced the theory of transmission lines ("telegrapher's equation") and invented the coaxial cable.

This is done is steps. First we note that

$$(\imath\,\hbar\,\partial/\partial t - \hat{p}_x{}^2/2m)\left\{\left(\frac{m}{2\pi\imath\hbar(t-t_0)}\right)^{1/2}\exp\left(\imath\frac{m(x-x_0)^2}{2\hbar(t-t_0)}\right)\right\} = 0\,. \quad (2.69)$$

It is then immediate that

$$\hat{D}_0\left\{\left(\frac{m}{2\pi\imath\hbar(t-t_0)}\right)^{3/2}\exp\left(\imath\frac{m|\boldsymbol{r}-\boldsymbol{r}_0|^2}{2\hbar(t-t_0)}\right)\right\} = 0\,. \quad (2.70)$$

So if we apply $\hat{D}_0$ to $G_{\rm f}^{(+)}(\boldsymbol{r},t;\boldsymbol{r}',t_0)$, the $\imath\,\hbar\,\partial/\partial t$ acting on $-\imath\Theta(t-t_0)$ produces a term which is $\hbar\,\delta(t-t_0)$ multiplied by $K_{\rm f}(\boldsymbol{r},t;\boldsymbol{r}',t_0)$ of Eq. (2.12). But we know this last reduces to $\delta(\boldsymbol{r}-\boldsymbol{r}_0)$ when the $\delta(t-t_0)$ forces $t=t_0$. In summary

$$\hat{D}_0\; G_{\rm f}^{(+)}(\boldsymbol{r},t;\boldsymbol{r}',t_0) = \hbar\,\delta(t-t_0)\delta(\boldsymbol{r}-\boldsymbol{r}_0)\,. \quad (2.71)$$

This shows that the free propagator as newly defined in Eq. (2.67) is a Green function[7] for the free Schrödinger equation $\hat{D}_0\psi = 0$ (generically a Green function obeys the original *linear* differential equation supplemented by a point "source" on the r.h.s.).

If we now define $\hat{D} \equiv \hat{D}_0 - V$ with the potential energy $V(\boldsymbol{r},t)$ appropriate to the problem of a particle moving in an external force, we can demand that the Green function for that problem, now denoted $G^{(+)}(\boldsymbol{r},t;\boldsymbol{r}',t_0)$, satisfy

$$\hat{D}\,G^{(+)}(\boldsymbol{r},t;\boldsymbol{r}',t_0) = \hbar\,\delta(t-t_0)\delta(\boldsymbol{r}-\boldsymbol{r}_0)\,. \quad (2.72)$$

We now guess that $G^{(+)}(\boldsymbol{r},t;\boldsymbol{r}',t_0)$ satisfies the following Fredholm type 1 integral equation:[8]

$$G^{(+)}(\boldsymbol{r},t;\boldsymbol{r}_0,t_0) = G_{\rm f}^{(+)}(\boldsymbol{r},t;\boldsymbol{r}_0,t_0)$$
$$+\frac{1}{\hbar}\int G_{\rm f}^{(+)}(\boldsymbol{r},t;\boldsymbol{r}',t')\,V(\boldsymbol{r}',t')\,G^{(+)}(\boldsymbol{r}',t';\boldsymbol{r}_0,t_0)\,d^3r'dt'\,. \quad (2.73)$$

[7] invented by George Green (1793-1841), a British miller's son, during his mathematics studies in Cambridge where he also proved his eponymous theorem. The wide usefulness of Green functions was first pointed out by William Thomson (Lord Kelvin).

[8] Erik Ivar Fredholm (1866-1927), a Swedish mathematician, was the founder of the theory of integral equations and helped to found operator theory.

To show this let us operate on this last with $\hat{D}_0$ and employ Eq. (2.71):

$$\begin{aligned}\hat{D}_0\, G^{(+)}(\boldsymbol{r},t;\boldsymbol{r}_0,t_0) &= \hbar\,\delta(t-t_0)\delta(\boldsymbol{r}-\boldsymbol{r}_0)\\ +\quad &\int \delta(t-t')\delta(\boldsymbol{r}-\boldsymbol{r}')\,V(\boldsymbol{r}',t')\,G^{(+)}(\boldsymbol{r}',t';\boldsymbol{r}_0,t_0)\,d^3r'dt' \qquad (2.74)\\ &= \hbar\,\delta(t-t_0)\delta(\boldsymbol{r}-\boldsymbol{r}_0) + V(\boldsymbol{r},t)\,G^{(+)}(\boldsymbol{r},t;\boldsymbol{r}_0,t_0). \qquad (2.75)\end{aligned}$$

This demonstrates that the integral equation is equivalent to Eq. (2.72).

We introduce abbreviated notation for Eq. (2.73):

$$G^{(+)} = G_{\rm f}^{(+)} + \frac{1}{\hbar}\overbrace{G_{\rm f}^{(+)}VG^{(+)}}\,. \qquad (2.76)$$

If we iterate this equation by repeatedly substituting its l.h.s. at the right of the preceding equation we get

$$\begin{aligned}G^{(+)} = G_{\rm f}^{(+)} + \frac{1}{\hbar}\overbrace{G_{\rm f}^{(+)}VG_{\rm f}^{(+)}} + \frac{1}{\hbar^2}\overbrace{G_{\rm f}^{(+)}VG_{\rm f}^{(+)}VG_{\rm f}^{(+)}}\\ + \frac{1}{\hbar^3}\overbrace{G_{\rm f}^{(+)}VG_{\rm f}^{(+)}VG_{\rm f}^{(+)}VG_{\rm f}^{(+)}} + \cdots \qquad (2.77)\end{aligned}$$

where every internal *pair* of arguments $\boldsymbol{r},t$ are integrated over their full ranges. We observe from this last that since $G_{\rm f}^{(+)}(\boldsymbol{r},t;\boldsymbol{r}_0,t_0)$ carries a factor $\Theta(t-t_0)$, the $G^{(+)}(\boldsymbol{r},t;\boldsymbol{r}_0,t_0)$ carries one too. We may thus infer that $G^{(+)}(\boldsymbol{r},t;\boldsymbol{r}_0,t_0)$ is of the form $-\imath\Theta(t-t_0)\,K(\boldsymbol{r},t;\boldsymbol{r}_0,t_0)$.

Eq. (2.77) is the *perturbation series* for the full Green function (the one describing the effects of forces on the particle). The series involves integrals over known functions. If it is carried out up to the term with n-th power of $\hbar^{-1}$, one is said to work with n-th order perturbation theory. One can conceive of the series as one in powers of the presumed small potential energy. What is the physical interpretation of the series?

One can break the propagator for a particle in a potential V into a sum of terms. The first corresponds to free propagation. The second to free propagation followed by interaction with V at a generic point and time which is then followed by free propagation. The first integral in Eq. (2.77) takes care to sum up the contributions for this single interaction at all points in space and at all times in $[t_0,t]$. The third term in Eq. (2.77) involves

free propagation punctuated just twice by interaction with V at two generic points and times; there is also integration over these, but the temporal order among them is respected. The idea is repeated to all orders. Perturbation to $\mathcal{O}(n)$ means that the particle interacts briefly and locally with the potential just n times and moves freely otherwise.

It is possible to derive the perturbation series directly from the path integral (2.15) using the 3-D form of Lagrangian (2.19), expanding the exponential in a Taylor series in V, and simplifying the various terms. The procedure is more complicated than the one used here.

Exercises

1. A particle moves in a uniform electric field $\mathcal{E}$ pointed in the $-z$ direction. To first order in perturbation write down the wave function that develops from $\psi_0(\boldsymbol{r}, t_0)$ in the course of time. Perform the integrals as far as possible.

2. Derive Eq. (2.76) directly from the path integral. Understand the precise form of the $\mathcal{O}(\hbar^{-2})$ term in Eq. (2.77) by consulting Feynman and Hibbs' book.

2.1.8 Operator derivation of the perturbation series

We can think of Eq. (2.72) as the matrix element with respect to $|\boldsymbol{r}'\rangle$ and $\langle \boldsymbol{r}|$ of the operator equation [with $\hat{H}_0 = \hat{\boldsymbol{p}}^2/(2m)$]

$$\left(\imath\frac{\partial}{\partial t} - \frac{1}{\hbar}\hat{H}_0 - \frac{1}{\hbar}\hat{V}\right)\hat{G}(t,t') = \hat{I}. \tag{2.78}$$

We may *formally* solve this last by

$$\hat{G} = \left(\imath\frac{\partial}{\partial t} - \frac{1}{\hbar}\hat{H}_0 - \frac{1}{\hbar}\hat{V}\right)^{-1}. \tag{2.79}$$

Now when $\hat{V} = 0$ we may write

$$\hat{G}_{\rm f} = \left(\imath \frac{\partial}{\partial t} - \frac{1}{\hbar} \hat{H}_0 \right)^{-1} , \tag{2.80}$$

so that Eq. (2.79) can be written as

$$\hat{G} = \left(\hat{G}_{\rm f}^{-1} - \frac{1}{\hbar} \hat{V} \right)^{-1} = \left(\left(\hat{I} - \frac{1}{\hbar} \hat{V}\, \hat{G}_{\rm f} \right) \hat{G}_{\rm f}^{-1} \right)^{-1} = \hat{G}_{\rm f} \left(\hat{I} - \frac{1}{\hbar} \hat{V}\, \hat{G}_{\rm f} \right)^{-1} . \tag{2.81}$$

Now we may formally expand the last factor assuming $\hat{V}$ is in some sense small:

$$\hat{G} = \hat{G}_{\rm f} + \frac{1}{\hbar} \hat{G}_{\rm f} \hat{V} \hat{G}_{\rm f} + \frac{1}{\hbar^2} \hat{G}_{\rm f} \hat{V} \hat{G}_{\rm f} \hat{V} \hat{G}_{\rm f} + \cdots \tag{2.82}$$

This is analogous to Eq. (2.77): it is the operator version of the equation obtained by iterating Eq. (2.73). In addition, we may factor the series (2.82) in the form

$$\hat{G} = \hat{G}_{\rm f} + \frac{1}{\hbar} \hat{G}_{\rm f} \hat{V} \left(\hat{G}_{\rm f} + \frac{1}{\hbar} \hat{G}_{\rm f} \hat{V} \hat{G}_{\rm f} + \cdots \right) , \tag{2.83}$$

and by looking at Eq. (2.82) recognize the brackets as $\hat{G}$, so that we have recovered the operator version of the integral equation (2.73). We see that it is possible to obtain correct results about Green function by cautious manipulations of operator equations. However, we now have to confront the fact that there are at least two different Green functions, both represented by series of the form of (2.82).

2.1.9 Retarded and advanced Green functions

It is useful to write the propagation equation (2.1) as

$$\Theta(t - t_0)\, \psi(\boldsymbol{r}, t) = \imath \int G^{(+)}(\boldsymbol{r}, t; \boldsymbol{r}', t_0)\, \psi(\boldsymbol{r}', t_0)\; d^3 r' \,; \tag{2.84}$$

this reduces to Eq. (2.1) for $t > t_0$, while for $t < t_0$ both sides of it obviously vanish. We thus call $G^{(+)}(\boldsymbol{r}, t; \boldsymbol{r}', t_0)$ the *retarded Green function* of Schrödinger's equation (retarded because it determines the wave function at times *after* that of the initial wave function). Of course $G_{\rm f}^{(+)}(\boldsymbol{r}, t; \boldsymbol{r}', t_0)$ is the retarded Green function of the free (without potential) Schrödinger equation.

It is easy to see that if $\psi(\boldsymbol{r},t)$ solves the Schrödinger equation with a *real* Hamiltonian, e.g. $\hat{H}=\hat{\boldsymbol{p}}^2/2m+V(\boldsymbol{r},t)$ with $V^*=V$, then $\psi(\boldsymbol{r},-t)^*$, the conjugated wave function with the progress of time reversed, is also a solution of the same equation. The conjugation is critical because of the factor $\imath$ in the Schrödinger equation. In summary, the *time reversed wave function* $\psi(\boldsymbol{r},-t)^*$ is also a solution of the Schrödinger equation.

For the task of evolving the time reversed wave function (propagating back in time) we invent a new Green function, $G^{(-)}(\boldsymbol{r},t;\boldsymbol{r}',t_0)$, for which

$$\Theta(t_0-t)\,\psi(\boldsymbol{r},t)=-\imath\int G^{(-)}(\boldsymbol{r},t;\boldsymbol{r}',t_0)\,\psi(\boldsymbol{r}',t_0)\;d^3r'\,. \tag{2.85}$$

The l.h.s. vanishes for $t>t_0$ so we infer that $G^{(-)}(\boldsymbol{r},t;\boldsymbol{r}',t_0)$ carries a factor $\imath\Theta(t_0-t)$ [just the reverse from $G^{(+)}(\boldsymbol{r},t;\boldsymbol{r}',t_0)$] in front of $K(\boldsymbol{r},t;\boldsymbol{r}',t_0)$. $G^{(-)}(\boldsymbol{r},t;\boldsymbol{r}',t_0)$ is called the *advanced Green function* of the full Schrödinger's equation (it determines the wave function at times prior to that of the final wave function). There is a corresponding advanced free Green function $G_{\rm f}^{(-)}(\boldsymbol{r},t;\boldsymbol{r}',t_0)$.

Eq. (2.85) carries an overall minus sign for the following reason. If we operate with $\hat{D}$ on both sides of it we get a $-\imath\hbar\delta(t_0-t)\,\psi(\boldsymbol{r},t)$ on the l.h.s. (since $\hat{D}\,\psi(\boldsymbol{r},t)=0$) and

$$-\,\imath\int\hat{D}\,G^{(-)}(\boldsymbol{r},t;\boldsymbol{r}',t_0)\,\psi(\boldsymbol{r}',t_0)\;d^3r' \tag{2.86}$$

on the r.h.s. The two sides agree provided $G^{(-)}(\boldsymbol{r},t;\boldsymbol{r}',t_0)$ obeys Eq. (2.72) just as does $G^{(+)}(\boldsymbol{r},t;\boldsymbol{r}',t_0)$. So with the choice of sign in Eq. (2.85) both Green functions obey one equation but, of course, satisfy different boundary conditions. Multiplicity of Green functions is common for partial differential equations of the hyperbolic type, of which wave equations are an example.

We observe from Eq. (2.12) that

$$K_{\rm f}(\boldsymbol{r}',t_0;\boldsymbol{r},t)^*=K_{\rm f}(\boldsymbol{r},t;\boldsymbol{r}',t_0) \tag{2.87}$$

Therefore,

$$G_{\rm f}^{(+)}(\boldsymbol{r}',t_0;\boldsymbol{r},t)^*=G_{\rm f}^{(-)}(\boldsymbol{r},t;\boldsymbol{r}',t_0) \tag{2.88}$$

where, as usual, the $G_{\rm f}^{(\pm)}$ are free Green functions (for the equation $\hat{D}_0\,\psi=0$). We now show that an analogous relation applies for $G^{(\pm)}(\boldsymbol{r},t;\boldsymbol{r}',t_0)$.

First since both Green function obey the same differential equations, they must both be subject to the integral equation (2.76) and to the series (2.77). In the proof below it is essential that $V(\boldsymbol{r},t)$ is real. Let us take the complex conjugate of Eq. (2.77), as applied to $G^{(+)}$, and interchange $\boldsymbol{r},t$ with $\boldsymbol{r}_0,t_0$. On the l.h.s. we now have $G^{(+)}(\boldsymbol{r}_0,t_0;\boldsymbol{r},t)^*$. On the r.h.s. the first term is $G_{\rm f}^{(+)}(\boldsymbol{r}_0,t_0;\boldsymbol{r},t)^*$. The next term will be

$$\frac{1}{\hbar}\int\int_t^{t_0} G_{\rm f}^{(+)}(\boldsymbol{r}_0,t_0;\boldsymbol{r}',t')^*\,V(\boldsymbol{r}',t')\,G_{\rm f}^{(+)}(\boldsymbol{r}',t';\boldsymbol{r},t)^*\,d^3r'dt'\,. \tag{2.89}$$

Because there are dummy arguments, the outcome in this last is as if we had interchanged the pairs of arguments in both $G_f^{(+)}$'s under the integral. It is easy to check that this pattern continues to be true for higher orders. Then by virtue of Eq. (2.88) the r.h.s. of our equation becomes a series of the form (2.77) but in $G_{\rm f}^{(-)}(\boldsymbol{r},t;\boldsymbol{r}_0,t_0)$. We know that such a series defines a Green function of Eq. (2.72), and since that the new Green's function carries a factor $\Theta(t_0-t)$ in every term of the series, it must be $G^{(-)}(\boldsymbol{r},t;\boldsymbol{r}_0,t_0)$. Hence

$$G^{(+)}(\boldsymbol{r}',t_0;\boldsymbol{r},t)^* = G^{(-)}(\boldsymbol{r},t;\boldsymbol{r}',t_0). \tag{2.90}$$

Exercises

Prove the following identities:

1. $\int G^{(+)}(\boldsymbol{r},t;\boldsymbol{r}',t')\,G^{(+)}(\boldsymbol{r}',t';\boldsymbol{r}_0,t_0)\,d^3r' = -\imath G^{(+)}(\boldsymbol{r},t;\boldsymbol{r}_0,t_0).$
2. $\int G^{(-)}(\boldsymbol{r},t;\boldsymbol{r}',t')\,G^{(-)}(\boldsymbol{r}',t';\boldsymbol{r}_0,t_0)\,d^3r' = \imath G^{(-)}(\boldsymbol{r},t;\boldsymbol{r}_0,t_0).$
3. $\int G^{(-)}(\boldsymbol{r},t;\boldsymbol{r}',t')\,G^{(+)}(\boldsymbol{r}',t';\boldsymbol{r}_0,t)\,d^3r' = \delta(\boldsymbol{r}-\boldsymbol{r}_)).$

Chapter 3

Collision theory

Much of what we know about molecules, atoms, nuclei, nucleons and elementary particles was learned by scattering projectiles off these objects, or bombarding other objects with them. The theory dealing with scattering is known as scattering or collision theory.

3.1 The Scattering matrix (S-matrix)

There are a variety of equivalent ways of developing the theory; we shall start with use of the S-matrix because of its ubiquitous presence in theoretical physics, as well as other areas, e.g. electrical engineering.

3.1.1 Definition and interpretation

The S-matrix for a system contains, in principle, all the information about the system implicit in its Hamiltonian. It can, however, be used even when the Hamiltonian is not fully known. This accounts for the popularity enjoyed by the S-matrix in various branches of physics. The S-matrix was invented by Wheeler[1] for use in nuclear physics and was introduced later into elementary

[1]John Archibald Wheeler (1911-2008) was an American physicist who contributed importantly to quantum electrodynamics (lifetime of positronium), nuclear physics (existence

particle theory by Heisenberg.

To define the S-matrix we need a *complete set* of mutual eigenstates $|\phi_k\rangle$ of a commuting set of observables, not all of which need commute with the Hamiltonian. An often-found example uses the eigenvectors of momentum in a system with a potential. We consider all the states $|\phi_k^{(+)}, t\rangle$, where the state $|\phi_j^{(+)}, t\rangle$ evolves from a particular $|\phi_j\rangle$ at $t = -\infty$. Thus in terms of the evolution operator of Sec. 1.3.1

$$|\phi_j^{(+)}, t\rangle = \hat{U}(t, -\infty)|\phi_j\rangle, \tag{3.1}$$

or

$$\phi_j^{(+)}(\boldsymbol{r}, t) = \imath \int G^{(+)}(\boldsymbol{r}, t; \boldsymbol{r}', -\infty)\, \phi_j(\boldsymbol{r}')\, d^3r' \,, \tag{3.2}$$

where for finite t the Θ function in $G^{(+)}$ is surely unity.

The S-matrix is the matrix whose elements are defined by

$$S_{ij} \equiv \lim_{t\to\infty} \langle \phi_i | \phi_j^{(+)}, t\rangle. \tag{3.3}$$

Using the two previous equations we have

$$S_{ij} = \langle \phi_i | \hat{U}(\infty, -\infty) | \phi_j \rangle \tag{3.4}$$

$$= \lim_{\substack{t\to\infty \\ t_0\to-\infty}} \imath \int \phi_i(\boldsymbol{r})^*\, G^{(+)}(\boldsymbol{r}, t; \boldsymbol{r}', t_0)\, \phi_j(\boldsymbol{r}')\, d^3r\, d^3r' \,. \tag{3.5}$$

Thus in one interpretation the S-matrix is the matrix representation of the evolution operator over an infinite time interval. Alternatively, we can say that the S-matrix is the array of probability amplitudes for the transitions during an infinite time interval between any pair of states $|\phi_j\rangle$ and $|\phi_i\rangle$. Another interpretation follows from choosing the position basis: $|\phi_j\rangle = |\boldsymbol{r}_j\rangle$ or $\phi_j(\boldsymbol{r}) = \delta(\boldsymbol{r} - \boldsymbol{r}_j)$. Then

$$S_{ij} = \imath\, G^{(+)}(\boldsymbol{r}_i, \infty; \boldsymbol{r}_j, -\infty) \,, \tag{3.6}$$

so that the S-matrix in position representation is essentially the retarded Green function with its two events separated by infinite time.

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of μ-mesic atoms, the theory of nuclear fission with N. Bohr), gravitation theory (nature of gravitational collapse, black holes), astrophysics (spinning neutron star a must for Crab Nebula) and the foundations of quantum theory (concept of the Delayed Choice experiment). Feynman was one of his earlier students.

3.1.2 Unitarity of the S-matrix

A very important fact in QT (as well as a quantum field theory) is that the S matrix is a unitary matrix. When in these subjects one says "unitarity" without specifying unitarity of what, one invariably means unitarity of the S-matrix. This unitarity applies whether the two indices of the matrix are of the same kind, or whether one is discrete and one continuous.

Our demonstration of the unitarity property assumes that both indices are discrete, but it can be easily adapted to the other cases. We start with Eq. (3.4). Use of Eq. (1.7) gives

$$S^\dagger_{ki} = \langle\phi_i|\hat{U}(\infty,-\infty)|\phi_k\rangle^* = \langle\phi_k|\hat{U}(\infty,-\infty)^\dagger|\phi_i\rangle. \tag{3.7}$$

Therefore, on account of the completeness of the states $|\phi_i\rangle$,

$$\sum_i S^\dagger_{ki}\, S_{ij} = \sum_i \langle\phi_k|\hat{U}(\infty,-\infty)^\dagger|\phi_i\rangle\, \langle\phi_i|\hat{U}(\infty,-\infty)|\phi_j\rangle \tag{3.8}$$

$$= \langle\phi_k|\hat{U}(\infty,-\infty)^\dagger\hat{U}(\infty,-\infty)|\phi_j\rangle = \langle\phi_k|\phi_j\rangle = \delta_{kj}\,. \tag{3.9}$$

In a similar manner one can show (see Exercises) that

$$\sum_i S_{ki}\, S^\dagger_{ij} = \delta_{kj}. \tag{3.10}$$

We have shown that S_{ij} is a unitary matrix.

The significance of S-matrix unitarity is complicated; right now we can clarify just a couple of points. First we set $j = k$ in Eq. (3.9) to get

$$\sum_i S^*_{ik}\, S_{ik} = \sum_i |S_{ik}|^2 = 1. \tag{3.11}$$

Given that S_{ik} is the probability amplitude that the particle (or system) passes from $|\phi_k\rangle$ to $|\phi_i\rangle$ in infinite time, we see that this result tells us that the probability that it passed from $|\phi_k\rangle$ to *any* state is unity. This is just conservation of probability, a feature which has to be included since the dynamics of the theory can be described by Schrödinger's equation.

Now suppose we take in Eq. (3.10) $k \neq j$. Then we get

$$\sum_i S_{ki}\, S^*_{ji} = 0. \tag{3.12}$$

This says that the two amplitudes for transition *from a common state to two different states* are subject to a specific constraint. We can complement this result with the other relation that comes out of Eq. (3.9) when $k \neq j$:

$$\sum_i S_{ik}^* S_{ij} = 0. \tag{3.13}$$

This says that the two amplitudes to pass *from two different states to a common state* are constrained in a particular way. Another way of stating the last two equations is that unitarity demands certain *correlations* between distinct transition amplitudes. There is more to unitarity than conservation of probability.

Exercises

1. Prove Eq. (3.10)

2. Prove that the determinant of S-matrix has modulus unity.

3. Prove that if the S-matrix if fully diagonal, its elements are just phases.

3.1.3 Symmetries and the S-matrix

A lot of free information can be obtained about the structure of the S-matrix (consequently about the systematics of scattering) from consideration of the symmetries of the Hamiltonian, even when full form of this last is unknown.

Let us recall the subject of translations from Sec. 1.2.6. Translations are implemented by the unitary operators $\hat{T}_{\boldsymbol{\rho}} = e^{-\imath \boldsymbol{\rho} \cdot \hat{\mathbf{p}}/\hbar}$ for all real vectors $\boldsymbol{\rho}$. The totality of the $\hat{T}_{\boldsymbol{\rho}}$ forms a continuous unitary group.

It is a similar story for all symmetries. According to a famous theorem of

Wigner[2] in order for the norms of states (probabilities) and the magnitude of scalar products between states (transition probability amplitudes) to be unchanged by a symmetry operation, it is necessary that the operations be carried out by either a unitary or an antiunitary operator. As mentioned in Sec. 1.2.5 for general unitary transformations, under a symmetry operation whose operator $\hat{U}$ is unitary, the states change according to $|\psi\rangle \to \hat{U}\,|\psi\rangle$ while operators (including observables) change according to $\hat{O} \to \hat{U}\,\hat{O}\,\hat{U}^\dagger$. These two rules are observed by translations [see Sec. 1.2.6, Eqs. (1.72), (1.73) and Exercise 2].

How do we characterize a symmetry operation from the viewpoint of QT? After a symmetry operation the system should look the same as before. But this does not mean the system's state $|\psi\rangle$ is invariant under a symmetry operation. However, the symmetry should act on the system in the same way today as yesterday. What this means is that if at time t_0 we perform the symmetry operation with the particular unitary operator $\hat{U}_\xi$ and then let the system evolve to time t, we should get the same system that would appear if we first let it evolve from t_0 to t and then apply $\hat{U}_\xi$. We, of course, assume all along that $\hat{U}_\xi$ is time-independent. Thus $\hat{U}_\xi$ represents a symmetry of the system whose evolution operator is $\hat{U}(t,t_0)$ if

$$\hat{U}_\xi\,\hat{U}(t,t_0) = \hat{U}(t,t_0)\,\hat{U}_\xi \quad \text{or} \quad [\hat{U}_\xi, \hat{U}(t,t_0)] = 0\,. \tag{3.14}$$

The time derivative of Eq. (3.14) gives

$$\hat{U}_\xi\,\frac{d\hat{U}(t,t_0)}{dt} = \frac{d\hat{U}(t,t_0)}{dt}\,\hat{U}_\xi\,, \tag{3.15}$$

which in view of the equation of motion of $\hat{U}(t,t_0)$, Eq. (1.105), becomes

$$\hat{U}_\xi\,\hat{H}\,\hat{U}(t,t_0) = \hat{H}\,\hat{U}(t,t_0)\,\hat{U}_\xi\,. \tag{3.16}$$

If we multiply from the right both sides of this by $\hat{U}(t,t_0)^\dagger$ and recall Eq. (3.14) we get

$$\hat{U}_\xi\,\hat{H} = \hat{H}\,\hat{U}_\xi \quad \text{or} \quad [\hat{U}_\xi, \hat{H}] = 0. \tag{3.17}$$

[2]Nobel laureate Eugene Paul Wigner (1902-1995) was an Hungarian-American theoretical physicist of Jewish origin. He did much to exploit the use of groups in quantum theory (Wigner-Eckart theorem), and made important contributions to atomic, nuclear and particle physics and solid state theory.

Thus every symmetry operator must commute with the Hamiltonian. According to Sec. 1.3.3 this means that $\hat{U}_\xi$ must be conserved. Note that all this is true regardless of whether the Hamiltonian depends on time or not.

Let us ask what is the S-matrix element between initial state $|\phi_{i'}\rangle \equiv \hat{U}_\xi|\phi_i\rangle$ and final state $|\phi_{j'}\rangle \equiv \hat{U}_\xi|\phi_j\rangle$. Obviously

$$S_{j'i'} = \langle\phi_j|\hat{U}_\xi^\dagger\, U(\infty,-\infty)\,\hat{U}_\xi|\phi_i\rangle = \langle\phi_j|\hat{U}_\xi^\dagger\,\hat{U}_\xi\, U(\infty,-\infty)\,|\phi_i\rangle = S_{ji} \quad (3.18)$$

where in the second step we have used Eq. (3.14). This is a general result: symmetry operations leave the S-matrix invariant For example, if i denotes the momentum $\boldsymbol{p}_i$ etc. then the amplitude for the particle to be scattered from the momentum $\boldsymbol{p}_i$ that has been rotated in a particular way to the momentum $\boldsymbol{p}_j$, equally rotated in angle and direction, that amplitude is the same as the amplitude between the original $\boldsymbol{p}_i$ and $\boldsymbol{p}_j$. This is true provided the rotation is a symmetry of the system, for example a rotation around the symmetry axis of a potential with azimuthal symmetry.

If the potential is spherically symmetric we can further conclude that all scatterings by the same angle have the same S-matrix element (and the same probability). This formalizes our intuitive guess.

Let us look at one more example of a continuous symmetry. Consider a system with time-independent Hamiltonian. This means the system is the same today and tomorrow; it is invariant under *time translation*. By analogy with $\hat{T}_{\boldsymbol{\rho}}$ for spatial translate, we guess that the corresponding class of unitary operators here is $\hat{U}_{\Delta t} = \exp(\imath\hat{H}\Delta t/\hbar)$. The reason for invoking the Hamiltonian is that we know that when $\hat{H}$ does not vary with time, $\exp(-\imath\hat{H}\Delta t/\hbar)$ serves to evolve the state $|\psi,t\rangle$ to $|\psi,t+\Delta t\rangle$. Hence $\hat{U}_{\Delta t}|\psi,t\rangle = |\psi,t-\Delta t\rangle$. This result is entirely analogous to the relation $\hat{T}_{\boldsymbol{\rho}}\,\psi(\boldsymbol{r}) = \psi(\boldsymbol{r}-\boldsymbol{\rho})$ [see Eqs. (1.70) and (1.72)]. Hence our $\hat{U}_{\Delta t}$ is indeed the operator of time translation by Δt, and is a member of a unitary group (see Exercises). The group's generator is $-\hat{H}$.

Spherically symmetric potentials automatically permit the extra symmetry of *space inversion*: the Hamiltonian is left unchanged by the joint replacements $\boldsymbol{r}\to-\boldsymbol{r}$ and $\boldsymbol{p}\to-\boldsymbol{p}$. More general potentials may also display this symmetry. Let us call the unitary operator that does this $\hat{U}_P$; we mean that $\hat{U}_P\,\boldsymbol{r}\,\hat{U}_P^\dagger = -\hat{\boldsymbol{r}}$, etc. This $\hat{U}_P$ is obviously its own inverse. We make no attempt to actually construct it; it is not as easy as it is for the opera-

tors associated with continuous transformations. As mentioned in Sec. 1.2.5, the collection $\{\hat{U}_P, \hat{I}\}$ constitutes a finite group, the *space inversion* group. Mathematicians call it Z_2.

If the potential has inversion symmetry, then by Eq. (3.17) $\hat{U}_P$ commutes with the Hamiltonian. Thus if $|E\rangle$ is any eigenstate of the Hamiltonian, $\hat{U}_P|E\rangle$ is also one, and has the same eigenvalue E. Then $|E\rangle + \hat{U}_P\,|E\rangle$ is also an eigenstate of $\hat{H}$ (not yet normalized) with E as eigenvalue, and is simultaneously an eigenstate of $\hat{U}_P$ with eigenvalue $+1$. It is called a state of *even parity*. $|E\rangle - \hat{U}_P\,|E\rangle$ is very much like it, except the eigenvalue of the inversion is -1. This is called a state of *odd parity*. The argument shows that in the presence of spatial inversion symmetry, the Hamiltonian always has eigenstates of *definite parity*.

If the energy spectrum is nondegenerate, e.g., the 1-D harmonic oscillator, then there are only definite parity eigenstates. For suppose the above mentioned $|E\rangle$ had no definite parity. Then, as we saw, $\hat{U}_P\,|E\rangle$ must have the same E, yet there are no two states with the same eigenvalue E. Thus nondegeneracy forbids eigenstates of $\hat{H}$ lacking definite parity. In our example all states of the harmonic oscillator are either of even or odd parity (their by wave functions are either even or odd functions). However, when there is degeneracy there can exist states with definite energy and states with *indefinite parity*.

In the case of space inversion we learn from Eq. (3.18) that the S-matrix element from $\hat{U}_P\,|\phi_i\rangle$ to $\hat{U}_P\,|\phi_j\rangle$ equals that from to $|\phi_i\rangle$ to $|\phi_j\rangle$. We shall see a consequence of this in Sec. 3.2.7.

Symmetry under time reversal comes under the rubric of antiunitary transformations. Eq. (3.18) is not correct for it as it stands. The next section develops the necessary formalism to treat time reversal.

Exercises:

1. Prove that any generator of the Lie group involved in a symmetry is a conserved quantity.
2. Prove that the $\hat{U}_{\Delta t}$ for all (real) Δt constitute a unitary group.
3. We define the electric dipole operator of an atom as $\hat{d} = e\sum_j \hat{\boldsymbol{r}}_j$ where

e is the electron charge and $\hat{\boldsymbol{r}}_j$ is the position of the j-th electron. Prove that the mean value of $\hat{d}$ always vanishes in a state of definite parity.

4. Suppose $\hat{H}$'s spectrum is degenerate, but $\hat{H}, \hat{U}_P$ and some other observable $\hat{O}$ are a maximal set of mutually commuting observables. If eigenstates degenerate in energy can be distinguished by their $\hat{O}$ eigenvalues, does the theorem in Exercise 3 apply to all joint $\hat{H}$ and $\hat{O}$ eigenstates?

3.1.4 Time reversal invariance

We mentioned in Sec. 2.1.9 that if $\psi(\boldsymbol{r}, t)$ solves the Schrödinger equation with a real potential, then $\psi(\boldsymbol{r}, -t)^*$ is also a solution, called the time-reversed wave function. We say that the Schrödinger equation has *time-reversal invariance* or *time-reversal symmetry*. According to Wigner, in QT every symmetry operation is to be performed by a unitary or antiunitary operator. Which do we have here? What does the time-reversal operater $\hat{\tau}$ look like?

Consider the evolution

$$|\psi, t\rangle = e^{-\imath \hat{H} t/\hbar} |\psi, 0\rangle \tag{3.19}$$

Let's say that at time t_1 we time-reverse the system so that the state becomes

$$\hat{\tau} e^{-\imath \hat{H} t_1/\hbar} |\psi, 0\rangle \tag{3.20}$$

If the system is time-reversal symmetric we should get the same thing by time-reversing at $t = 0$ and the propagating the system backwards in time for an interval t_1. Thus we must get

$$\hat{\tau} e^{-\imath \hat{H} t_1/\hbar} |\psi, 0\rangle = e^{\imath \hat{H} t_1/\hbar} \hat{\tau} |\psi, 0\rangle. \tag{3.21}$$

Since $|\psi, 0\rangle$ is arbitrary we must here have equality of the operator products on the l.h.s. and r.h.s., certainly to $\mathcal{O}(t_1)$:

$$-\hat{\tau}\, \imath\, \hat{H} = \imath\, \hat{\tau}\, \hat{H}. \tag{3.22}$$

We have two choices now. One is to assume that $\hat{\tau}$ is unitary (that is linear) so that $\hat{\tau}\, \imath = \imath\, \hat{\tau}$. We then conclude from the above equation that

$\hat{H}$ anticommutes with $\hat{\tau}$. But this leads to a paradox. Suppose $\hat{H}$ has an eigenstate $|E\rangle$ with energy E. Then by the above $\hat{\tau}|E\rangle$ is an eigenstate of $\hat{H}$ with energy $-E$. This is contrary to many examples, e.g. the harmonic oscillator has only positive energy eigenvalues. Thus our choice has led to an impasse. We must instead assume that $\hat{\tau}$ is antilinear, and thus antiunitary:

$$\hat{\tau}\,\imath = -\imath\,\hat{\tau}. \tag{3.23}$$

Then Eq. (3.22) tells us that

$$\hat{\tau}\,\hat{H} = \hat{H}\,\hat{\tau}, \tag{3.24}$$

i.e., $\hat{\tau}$ commutes with the Hamiltonian just as in the other symmetries we have considered earlier.

We see from Eq. (3.23) that $\hat{\tau}$ conjugates both numbers and functions: regarding its action on states, $\hat{\tau}$ can be regarded as identical to the conjugating operator which we call $\hat{K}$. But what about operators? First if we work in the position representation, $\hat{\boldsymbol{r}}$ can be regarded a real vector and so we have

$$\hat{\tau}\,\hat{\boldsymbol{r}} = \hat{\boldsymbol{r}}\,\hat{\tau} \tag{3.25}$$

which agrees with the intuition that time-reversal does not move a particle. We say that $\hat{\boldsymbol{r}}$ is *time-reversal invariant* or *time-reversal even*. Now we look at momentum: $\hat{\boldsymbol{p}} = (\hbar/\imath)\boldsymbol{\nabla}$ so that

$$\hat{\tau}\,\hat{\boldsymbol{p}} = -\hat{\boldsymbol{p}}\,\hat{\tau} \tag{3.26}$$

which again agrees with the intuition that time-reversal reverses the direction of all momenta. We say that $\hat{\boldsymbol{p}}$ is *time-reversal odd*. From all this it follows that for orbital angular momentum

$$\hat{\tau}\,\hat{\boldsymbol{l}} = -\hat{\boldsymbol{l}}\,\hat{\tau} \tag{3.27}$$

which again agrees with the expectation that time reversal inverts the direction of rotation and of the angular momentum vector. Orbital angular momentum is time-reversal odd.

However, if we go over to the momentum representation, $\hat{\boldsymbol{p}}$ is just a real vector and *commutes* with $\hat{K}$ so that the definition $\hat{\tau} = \hat{K}$ is inappropriate. The same is obvious from $\hat{\boldsymbol{r}} = \imath\hbar\boldsymbol{\nabla}_{\boldsymbol{p}}$. We conclude that the precise form of

$\hat{\tau}$ depends on the representation (making time reversal unique among transformation operators of interest). An appropriate choice for the momentum representation is

$$\hat{\tau} = \hat{U}_\tau \, \hat{K} \tag{3.28}$$

where $\hat{U}_\tau$ is a unitary operator which *commutes* with $\hat{K}$ but *anticommutes* with $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{p}}$. Then Eqs. (3.25)-(3.27) are satisfied.

As an application we show that eigenfunctions belonging to nondegenerate eigenvalues of an observable $\hat{\mathcal{O}}$ which is time-reversal even can be chosen to be real functions.

We work in position representation. The assumption above means that

$$\hat{K} \, \hat{\mathcal{O}} = \hat{\mathcal{O}} \, \hat{K}. \tag{3.29}$$

We now consider an eigenfunction $u_n(\boldsymbol{x})$ such that $\hat{\mathcal{O}} \, u_n(\boldsymbol{x}) = \lambda_n u_n(\boldsymbol{x})$ (λ_n is, of course, real). It is obvious that $\hat{K} \, u_n(\boldsymbol{x})$ is also an eigenfunction of $\hat{\mathcal{O}}$ with the same eigenvalue λ_n. However, $\hat{K} \, u_n(\boldsymbol{x}) = u_n(\boldsymbol{x})^*$. Since the particular eigenvalue is assumed nondegenerate, we must have $u_n(\boldsymbol{x})^* = c \, u_n(\boldsymbol{x})$ where c is a complex constant. For if this were not true there would be two distinct eigenfunctions with eigenvalue λ_n. Writing out the real and imaginary parts of this last equation we get

$$\mathcal{R}u_n(\boldsymbol{x}) = \mathcal{R}c \; \mathcal{R}u_n(\boldsymbol{x}) - \mathcal{I}c \; \mathcal{I}u_n(\boldsymbol{x}) \tag{3.30}$$

$$-\mathcal{I}u_n(\boldsymbol{x}) = \mathcal{R}c \; \mathcal{I}u_n(\boldsymbol{x}) + \mathcal{I}c \; \mathcal{R}u_n(\boldsymbol{x}) \tag{3.31}$$

These equations show that $\mathcal{I}u_n(\boldsymbol{x}) \propto \mathcal{R}u_n(\boldsymbol{x})$ so that $u_n(\boldsymbol{x})$ can be written as a real function times a *constant phase* $e^{i\gamma}$. However, a constant phase can always be discarded. Hence it is possible to write $u_n(\boldsymbol{x})$ as a real function.

One example is provided by the harmonic oscillator; its Hamiltonian has a fully nondegenerate spectrum. Indeed, all eigenfunctions of the harmonic oscillator are commonly written as purely real. A second example is provided by the hydrogen atom. All common eigenfunctions of $\hat{H}$ and $\hat{l}^2$ (both time-reversal even operators) with vanishing azimuthal quantum number μ are each specified by a unique pair of Bohr's quantum numbers n and l. There is no degeneracy here, and indeed these eigenfunctions are just real radial functions.

When the system has spin, its time reversal properties require special handling. Of course we must demand that

$$\hat{\tau}\,\hat{\boldsymbol{s}} = -\hat{\boldsymbol{s}}\,\hat{\tau} \tag{3.32}$$

in order that the total angular momentum $\hat{\boldsymbol{j}} = \hat{\boldsymbol{l}} + \hat{\boldsymbol{s}}$ shall be time-sreversal odd just as $\hat{\boldsymbol{l}}$.

We shall work in the position representation. First, suppose there is only one spin-$\frac{1}{2}$ particle. We recall that $\hat{\boldsymbol{s}} = \frac{1}{2}\hbar\boldsymbol{\sigma}$ in terms of the Pauli matrices (1.12) which may be seen to satisfy the algebra

$$\sigma_i^2 = \mathcal{I}; \qquad \sigma_i\sigma_j = \imath\sum_{k=1}^{3}\varepsilon_{ijk}\,\sigma_k \quad \text{for } i \neq j\,, \tag{3.33}$$

where ε_{ijk} is the totally antisymmetric symbol with $\epsilon_{123} = 1$. It is obvious that the Pauli matrices are mutually anticommuting. We now define

$$\hat{\tau} = \hat{U}_\tau\,\hat{K} = -\imath\sigma_2\hat{K} \tag{3.34}$$

where it is easily seen that

$$-\imath\sigma_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{3.35}$$

is indeed unitary. It is now obvious that $\hat{\tau}$ fits the commutation relations (3.25) and (3.26) since σ_2 operates in an Hilbert space different from that in which $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{p}}$ operate, and so commutes with them. Obviously

$$\hat{\tau}\sigma_1 = -\sigma_1\hat{\tau} \quad \text{and} \quad \hat{\tau}\sigma_3 = -\sigma_3\hat{\tau} \tag{3.36}$$

since σ_1 and σ_3 are real and Eq. (3.33) holds while

$$\hat{\tau}\sigma_2 = -\sigma_2\hat{\tau} \tag{3.37}$$

because σ_2 is pure imaginary. Thus is Eq. (3.32) implemented.

When there are N spin-$\frac{1}{2}$ particles we must write

$$\hat{\boldsymbol{s}} = \tfrac{1}{2}\hbar\Big(\underbrace{\sigma^{(1)} \oplus \sigma^{(2)} \oplus \sigma^{(3)} \oplus \cdots}_{N \text{ terms}}\Big)\,, \tag{3.38}$$

$$\hat{\tau} = (-\imath)^N\,\underbrace{\sigma_2^{(1)} \otimes \sigma_2^{(2)} \otimes \sigma_2^{(3)} \otimes \cdots}_{N \text{ factors}}\hat{K}\,, \tag{3.39}$$

where the exterior sum and product are taken because each spin-$\frac{1}{2}$ has its own Hilbert space (we assume $\hat{K}$ conjugates in all such spaces simultaneously). Now Eqs. (3.36) and (3.37) apply separately for each $\sigma^{(j)}$ and Eq. (3.32) is obeyed.

Example: Kramers' theorem

A curious consequence of time reversal invariance of the Hamiltonian in systems with an odd number of spin-$\frac{1}{2}$ particles is the necessary existence of energy degeneracy. This is called Kramers' degeneracy.[3]

We consider a situation where the Hamiltonian is time-reversal even, i.e.,

$$\hat{\tau}\hat{H} = \hat{H}\hat{\tau}. \tag{3.40}$$

This holds if the Hamiltonian is purely real, e.g., $\hat{H} = \hat{\boldsymbol{p}}^2/2m + V(\hat{\boldsymbol{r}})$. It is not however, a law of nature, and presence of magnetic fields will make it void. Now consider a eigenstate $|E\rangle$ of $\hat{H}$ of energy E. What is $\hat{\tau}|E\rangle$? Obviously by the last equation

$$\hat{H}\hat{\tau}|E\rangle = \hat{\tau}\hat{H}|E\rangle = \hat{\tau}E|E\rangle = E\,\hat{\tau}|E\rangle \tag{3.41}$$

so that $\hat{\tau}|E\rangle$ is also an eigenstate of $\hat{H}$ with energy E.

Now *assume* that the eigenvalue E is nondegenerate. Then $\hat{\tau}|E\rangle$ must be $C|E\rangle$ ($\hat{\tau}$ is antiunitary) and $|C|^2 = 1$ since time reversal cannot change the norm of a state. Thus

$$\hat{\tau}^2|E\rangle = \hat{\tau}\,C|E\rangle = C^*\hat{\tau}|E\rangle = |C|^2\,|E\rangle = |E\rangle. \tag{3.42}$$

We now calculate $\hat{\tau}^2$ directly sfrom Eq. (3.39). We know that $\sigma_2^{(i)}$ commutes with itself, $\hat{K}^2 = \hat{I}$, $\hat{K}\imath\sigma_2^{(i)} = \sigma_2^{(i)}\imath\hat{K}$, and ${\sigma_k}^2 = \hat{\mathcal{I}}$. Thus

$$\hat{\tau}^2 = (-1)^N\hat{I}\,. \tag{3.43}$$

[3]Hendrik Anthony Kramers (1894-1952) was a Dutch theoretical physicist known for the Kramers-Kronig dispersion relations, the Wentzel-Kramers-Brillouin (WKB) approximation, the Kramers-Heisenberg formula for scattering of photons by atomic electrons, the Kramers opacity law in astrophysics and important contributions to solid state theory.

We see that when N is odd, $\hat{\tau}^2 = -\hat{I}$ and Eq. (3.42) is self-contradictory. Thus the assumption that the eigenvalue E is nondegenerate was wrong. This means that the spectrum of a real $\hat{H}$ must be at least doubly degenerate throughout. This is Kramers' theorem.

Our conclusion that a time-reversal odd operator like $\hat{\boldsymbol{p}}$, $\hat{\boldsymbol{l}}$ or $\hat{\boldsymbol{s}}$ anticommutes with $\hat{\tau}$ has an important consequence. In an eigenstate of any such operators, say $|\phi_j\rangle$ (perhaps a joint eigenstate of other operators), the eigenvalue j pertaining to the odd operator flips its sign under time reversal:

$$\hat{\tau}|\phi_i\rangle = |\phi_{-i}\rangle\,. \tag{3.44}$$

We shall use this notation even if the index i also represents eigenvalues of time-reversal even operators which, of course, do not flip sign. If the state being time reversed depends on time, the conjugation inherent in $\hat{\tau}$ will enforce the flip $t \to -t$ as well. As an example, in position representation, we mention the eigenstate of momentum and energy

$$\phi_{\boldsymbol{p}}(\boldsymbol{r}, t) = (2\pi\hbar)^{-3/2}\, e^{\imath(\boldsymbol{p}\cdot\boldsymbol{r} - \imath\varepsilon_{\boldsymbol{k}}t)/\hbar}\,. \tag{3.45}$$

Applying $\hat{\tau} = \hat{K}$ to it yields the state $\phi_{-\boldsymbol{p}}(\boldsymbol{r}, -t)$ with the same energy as the original state because $\hat{H}$ is a time-reversal even operator, so $\varepsilon_{\boldsymbol{p}}$ does not change upon time reversal.

Exercises

1. If $|\chi\rangle \equiv \hat{\tau}|\psi\rangle$ and $|\nu\rangle \equiv \hat{\tau}|\phi\rangle$ show that $\langle\nu|\chi\rangle = \langle\psi|\phi\rangle$.
2. Show that if $\mathcal{O}$ is a time-reversal odd operator, $\langle\nu|\mathcal{O}|\chi\rangle = -\langle\psi|\mathcal{O}|\phi\rangle$. What is the analog for a time-reversal even operator?
3. Show that when N is odd, $\hat{\tau}|E\rangle$ is in fact orthogonal to $|E\rangle$.
4. Identify the Kramers degeneracy in the spectrum of Li: which states are necessarily degenerate?
5. Hydrogen atoms are trapped at interstitial sites in a crystal of NaCl. The electric field of the sodium and chlorine ions perturb the hydrogen spectrum. Discuss the degeneracies of the perturbed H spectrum.

3.2 Formal scattering theory

We shall only deal here with the scattering of one particle on a second one. We know from classical mechanics that if the two-body interaction is described by a potential of the form $V(\boldsymbol{r}_2 - \boldsymbol{r}_1, t)$, then we can replace the problem of motion of the two particles with masses m_1 and m_2 by that of the motion of an effective particle of mass m with $m^{-1} \equiv m_1^{-1} + m_2^{-2}$ which moves in the potential $V(\boldsymbol{r}, t)$ where $\boldsymbol{r} \equiv \boldsymbol{r}_2 - \boldsymbol{r}_1$. The same transformation is true in non-relativistic QT. Hence we need deal only with scattering of one particle from a potential.

3.2.1 The scattering scenario

The discussion of the S-matrix in Sec. 3.1.1 prompts us to identify the eigenvectors $|\phi_i\rangle$. We would like these to be momentum eigenvectors of Sec. 1.2.2 whose space representation is Eq. (1.64). However these functions are spread all over space; they certainly overlap the center of the potential, and so in no sense can they be the states $|\phi_i\rangle$ which, to make things simple, have to be states of a noninteracting particle. There are two ways of removing this impediment to the use of the S-matrix formalism. One is to use wave-packets with a range of momenta as the $|\phi_i\rangle$. Of course this complicates matters because such wave-packets do not have sharply defined momentum or energy. We cannot speak of scattering from this to that momentum at this energy. The second way is to use momentum eigenstates for the $|\phi_i\rangle$ but to regard the potential as turning on and slowly reaching its "static" form $V(\boldsymbol{r})$, maintaining it for a while, and then slowly turning off. In this manner the momentum states are exact states of the system before the potential and after the potential, and one can speak of a transition from one momentum to another. We shall go by the second way.

We thus use the Hamiltonian

$$\hat{H} = \hat{\boldsymbol{p}}^2/2m + V(\boldsymbol{r})\, g(t) \tag{3.46}$$

where the function $g(t)$, pictured in Fig. 3.1, turns on in a gradual (adiabatic) way, reaches a long flat plateau where $g = 1$, and then turns off in an adiabatic way.

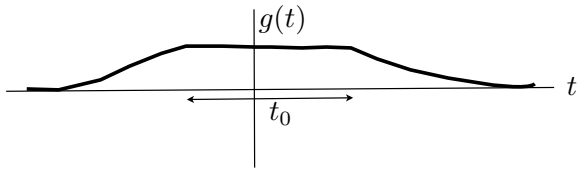

Figure 3.1: **The shape of the function $g(t)$ used in Eq. (3.46)**

We shall now write the function corresponding to $|\phi_i\rangle$ in a time dependent format:

$$\phi_{\boldsymbol{k}}(\boldsymbol{r},t) = \frac{1}{(2\pi)^{3/2}}\, e^{\imath \boldsymbol{k}\cdot\boldsymbol{r} - \imath\varepsilon_{\boldsymbol{k}} t/\hbar}, \tag{3.47}$$

that is, compared with Eq. (1.64) we use wave-vector rather than momentum $\hbar\boldsymbol{k}$ to label the eigenfunctions. The $\phi_{\boldsymbol{k}}$ are normalized according to

$$\int \phi_{\boldsymbol{k}'}(\boldsymbol{r},t)^*\, \phi_{\boldsymbol{k}}(\boldsymbol{r},t)\, d^3\boldsymbol{r} = \delta(\boldsymbol{k}-\boldsymbol{k}')\,. \tag{3.48}$$

The function $\phi_{\boldsymbol{k}}$ satisfies the free Schrödinger equation, but not the full Schrödinger equation; thus as time goes on it evolves into a superposition of $\phi_{\boldsymbol{k}}$ with a variety of $\boldsymbol{k}$ (because the set of $\phi_{\boldsymbol{k}}$ is complete). In terms of the full Green function this can be written

$$\phi^{(+)}_{\boldsymbol{k}}(\boldsymbol{r},t) = \imath \int G^{(+)}(\boldsymbol{r},t;\boldsymbol{r}',t_0)\, \phi_{\boldsymbol{k}}(\boldsymbol{r}',t_0)\, d^3r'\,, \tag{3.49}$$

where $\phi^{(+)}_{\boldsymbol{k}}$ denotes the true solution of Schrödinger's equation which grows out from $\phi_{\boldsymbol{k}}$.

3.2.2 The T-matrix

We now rewrite the expression (3.5) for the S-matrix as

$$S_{\boldsymbol{k}'\boldsymbol{k}} = \lim_{\substack{t\to\infty \\ t_0\to-\infty}} \imath \int \phi_{\boldsymbol{k}'}(\boldsymbol{r},t)^*\, G^{(+)}(\boldsymbol{r},t;\boldsymbol{r}',t_0)\, \phi_{\boldsymbol{k}}(\boldsymbol{r}',t_0)\, d^3r\, d^3r'\,. \tag{3.50}$$

Now we replace the $G^{(+)}$ here by Eq. (2.73) to get (time limits being understood)

$$S_{\boldsymbol{k}'\boldsymbol{k}} = \imath \int \phi_{\boldsymbol{k}'}(\boldsymbol{r},t)^*\, G_{\rm f}^{(+)}(\boldsymbol{r},t;\boldsymbol{r}',t_0)\, \phi_{\boldsymbol{k}}(\boldsymbol{r}',t_0)\, d^3r\, d^3r' \tag{3.51}$$
$$+\frac{\imath}{\hbar}\int \phi_{\boldsymbol{k}'}(\boldsymbol{r},t)^* G_{\rm f}^{(+)}(\boldsymbol{r},t;\boldsymbol{r}',t')\, V(\boldsymbol{r}',t')\, G^{(+)}(\boldsymbol{r}',t';\boldsymbol{r}_0,t_0)\, \phi_{\boldsymbol{k}}(\boldsymbol{r}_0,t_0)\, d^3r\, d^3r'\, d^3r_0\, dt'$$

Because the retarded free Green function appears in the first term, the integral over $\boldsymbol{r}'$ there gives $\phi_{\boldsymbol{k}}(\boldsymbol{r},t)$ and thus in view of Eq. (3.48) the first term is $\delta(\boldsymbol{k}-\boldsymbol{k}')$.

In regard to the second term, let us first look at the integral over $\boldsymbol{r}$ by itself:

$$\imath \int \phi_{\boldsymbol{k}'}(\boldsymbol{r},t)^* G_{\rm f}^{(+)}(\boldsymbol{r},t;\boldsymbol{r}',t')\, d^3r = \imath \left[\int \phi_{\boldsymbol{k}'}(\boldsymbol{r},t)\, G_{\rm f}^{(+)}(\boldsymbol{r},t;\boldsymbol{r}',t')^*\, d^3r\right]^* \tag{3.52}$$

But in view of Eqs. (2.88) and (2.85) we can write this as

$$\left[-\imath \int G_{\rm f}^{(-)}(\boldsymbol{r}',t';\boldsymbol{r},t)\, \phi_{\boldsymbol{k}'}(\boldsymbol{r},t)\, d^3r\right]^* = \phi_{\boldsymbol{k}'}(\boldsymbol{r}',t')^* \tag{3.53}$$

Note that the Green function $G_{\rm f}^{(-)}$ carries the free function $\phi_{\boldsymbol{k}'}$ from t (a late time) back to t' (an early time) where it is still a free function.Thus we have

$$S_{\boldsymbol{k}'\boldsymbol{k}} = \delta(\boldsymbol{k}-\boldsymbol{k}')+\frac{1}{\hbar}\int \phi_{\boldsymbol{k}'}(\boldsymbol{r}',t')^*\, V(\boldsymbol{r}',t')\, G^{(+)}(\boldsymbol{r}',t';\boldsymbol{r}_0,t_0)\, \phi_{\boldsymbol{k}}(\boldsymbol{r}_0,t_0)\, d^3r\, d^3r_0\, dt'\,. \tag{3.54}$$

Now making use of Eq. (3.49) this can be put more compactly:

$$S_{\boldsymbol{k}'\boldsymbol{k}} = \delta(\boldsymbol{k}-\boldsymbol{k}') - \frac{\imath}{\hbar}\int \phi_{\boldsymbol{k}'}(\boldsymbol{r}',t')^*\, V(\boldsymbol{r}',t')\, \phi_{\boldsymbol{k}}^{(+)}(\boldsymbol{r}',t')\, d^3r'\; dt'\,. \tag{3.55}$$

It is important that in this exact equation the two kinds of $\phi_{\boldsymbol{k}}$ function appear.

One thing that this last result says is that in scattering there is always some *forward scattering* since $S_{\boldsymbol{k}'\boldsymbol{k}}$ *does not* vanish for $\boldsymbol{k} = \boldsymbol{k}'$. This is

analogous to the light that appears at the center of the shadow cast by a sphere illuminated from one side.[4]

Let us write the full solution $\phi_{\boldsymbol{k}}^{(+)}$ in the form (c.f. Eq. (3.47))

$$\phi_{\boldsymbol{k}}^{(+)}(\boldsymbol{r},t) = u_{\boldsymbol{k}}^{(+)}(\boldsymbol{r})\, e^{-\imath\varepsilon_{\boldsymbol{k}}t/\hbar}\,. \tag{3.56}$$

We are allowed to assume an harmonic time dependence only because by assumption the potential $V(\boldsymbol{r})\, g(t)$ varies very slowly, on some long timescale T. To be precise, if ε_0 is the smallest energy (in absolute value) we are interested in, then we must require that $\varepsilon_0 T \gg \hbar$. This permits the harmonic factor in Eq. (3.56) to oscillate significantly while the potential hardly changes. Substituting from Eq. (3.56) into Eq. (3.55) we have

$$S_{\boldsymbol{k}'\boldsymbol{k}} = \delta(\boldsymbol{k}-\boldsymbol{k}') - \frac{\imath}{\hbar}\, T_{\boldsymbol{k}'\boldsymbol{k}} \int_{-\infty}^{\infty} g(t)\, e^{\imath(\varepsilon_{\boldsymbol{k}'}-\varepsilon_{\boldsymbol{k}})t/\hbar}\, dt \tag{3.57}$$

where

$$T_{\boldsymbol{k}'\boldsymbol{k}} \equiv \int \frac{e^{-\imath\boldsymbol{k}'\cdot\boldsymbol{r}'}}{(2\pi)^{3/2}}\, V(\boldsymbol{r}')\, u_{\boldsymbol{k}}^{(+)}(\boldsymbol{r}')\, d^3r' \tag{3.58}$$

is called the *transition matrix* or T-matrix. This matrix is obviously the nontrivial part of the S-matrix.

At this point we assume that $t_0 \to \infty$ without the ramps in Fig. 3.1 changing much. Then it is obvious that the integral in Eq. (3.57) produces a Dirac delta function. In detail

$$S_{\boldsymbol{k}'\boldsymbol{k}} = \delta(\boldsymbol{k}-\boldsymbol{k}') - 2\pi\imath\, T_{\boldsymbol{k}'\boldsymbol{k}}\, \delta(\varepsilon_{\boldsymbol{k}'}-\varepsilon_{\boldsymbol{k}})\,. \tag{3.59}$$

This is an often seen expression, and it is easy to generalize to relativistic scattering theory. We observe that the S-matrix is diagonal in energy. For if $\varepsilon_{\boldsymbol{k}'} \neq \varepsilon_{\boldsymbol{k}}$, then obviously $\boldsymbol{k} \neq \boldsymbol{k}'$ so $S_{\boldsymbol{k}'\boldsymbol{k}}$ vanishes. Scattering in an essentially stationary potential conserves energy.

[4] In 1818 the notable French mathematician and physicist Simeon Denis Poisson ridiculed young Augustine Fresnel's wave theory of diffraction because it would have predicted an illuminated spot in the shadow of the sphere; in fact this had already been observed a century earlier by Joseph-Nicolas Delisle. It is variously called Delisle's spot or Arago's spot (Francoise Arago defended Fresnel's claim and proved it by experiment).

3.2.3 Scattering cross section

Experimentalists know how to measure the *differential cross section* for a scattering process as a function of scattering angle and incident momentum. Let us see how this quantity is related to the T-matrix.

First let us now relate the T-matrix to the probability of scattering from $\phi_{\boldsymbol{k}}$ to $\phi_{\boldsymbol{k}'}$ with $\boldsymbol{k}' \neq \boldsymbol{k}$. Were we to calculate $|S_{\boldsymbol{k}'\boldsymbol{k}}|^2$ directly from Eq. (3.59) we would meet the square of $\delta(\varepsilon_{\boldsymbol{k}'} - \varepsilon_{\boldsymbol{k}})$ which is ill defined. Instead we return to the form (3.57) and taking care to write each integral over its own time variable we end up with

$$|S_{\boldsymbol{k}'\boldsymbol{k}}|^2 = \frac{1}{\hbar^2} |T_{\boldsymbol{k}'\boldsymbol{k}}|^2 \int_{-\infty}^{\infty} e^{-\imath(\varepsilon_{\boldsymbol{k}'} - \varepsilon_{\boldsymbol{k}})\tau/\hbar}\, d\tau \int_{-\infty}^{\infty} g(t)\, g(t+\tau)\, dt\,. \tag{3.60}$$

With the form $g(t)$ in Fig. 3.1 we see that the inner integral is approximately $(t_0 - \tau)\,\Theta(t_0 - \tau)$. When t_0 becomes large, the Heaviside function is unity for all τ, we may approximate $t_0 - \tau \approx t_0$, and thus since the outer integral gives a Dirac delta function,

$$|S_{\boldsymbol{k}'\boldsymbol{k}}|^2 = \frac{1}{\hbar^2} |T_{\boldsymbol{k}'\boldsymbol{k}}|^2\, 2\pi\hbar\, t_0\, \delta(\varepsilon_{\boldsymbol{k}'} - \varepsilon_{\boldsymbol{k}})\,. \tag{3.61}$$

The fact that the probability comes out proportional to the time t_0 during which the potential is "on" allows us to compute the scattering *rate* of probability:

$$W_{\boldsymbol{k}\to\boldsymbol{k}'} = \frac{1}{t_0} |S_{\boldsymbol{k}'\boldsymbol{k}}|^2 = \frac{2\pi}{\hbar}\, |T_{\boldsymbol{k}'\boldsymbol{k}}|^2\, \delta(\varepsilon_{\boldsymbol{k}'} - \varepsilon_{\boldsymbol{k}})\,. \tag{3.62}$$

This expression resembles Fermi's[5] *golden rule* from time-dependent perturbation theory, although the last is a first order result while Eq. (3.62) is exact. To overcome its essentially singular form, we ask, what is the probability rate at which the particle with initial momentum $\boldsymbol{k}$ gets scattered by the potential into a small solid angle $\Delta\Omega_{\boldsymbol{k}'}$. Recall now that the number of

[5]Italian Nobel laureate Enrico Fermi (1901-1954) emigrated to the United States under the pressure of fascism. He is known for many theoretical and experimental achievements: Fermi-Dirac statistics, the harmonic oscillator method for quantization of the electromagnetic field, the (old) theory of weak decay, the theory of acceleration of cosmic rays, etc. He also carried out the first artificial nuclear chain reaction.

quantum states which a particle found in a volume $\mathcal{V}$ and possessing wave-vector in an interval d^3k' about $\boldsymbol{k}'$ can be in is given by Weyl's[6] expression $\mathcal{V}d^3k'/(2\pi)^3$. To answer our question we just multiply $W_{\boldsymbol{k}\to\boldsymbol{k}'}$ by this last expression and integrate over the angle $\Delta\Omega_{\boldsymbol{k}'}$:

$$\sum_{\boldsymbol{k}'\in\Delta\Omega_{\boldsymbol{k}'}} W_{\boldsymbol{k}\to\boldsymbol{k}'} = \frac{2\pi}{\hbar}\int_{\boldsymbol{k}'\in\Delta\Omega_{\boldsymbol{k}'}} |T_{\boldsymbol{k}'\boldsymbol{k}}|^2\,\delta(\varepsilon_{\boldsymbol{k}'}-\varepsilon_{\boldsymbol{k}})\frac{\mathcal{V}\,d^3k'}{(2\pi)^3}\,. \tag{3.63}$$

But, of course, since

$$\varepsilon_{\boldsymbol{k}} = \hbar^2\,k^2/(2m) \tag{3.64}$$

as well as $\varepsilon_{\boldsymbol{k}'} = \hbar^2\,k'^2/(2m)$, we can rewrite

$$\begin{aligned}\sum_{\boldsymbol{k}'\in\Delta\Omega_{\boldsymbol{k}'}} W_{\boldsymbol{k}\to\boldsymbol{k}'} &= \frac{m\mathcal{V}}{4\pi^2\hbar^3}\int_{\boldsymbol{k}'\in\Delta\Omega_{\boldsymbol{k}'}} k'\,|T_{\boldsymbol{k}'\boldsymbol{k}}|^2\,\delta(\varepsilon_{\boldsymbol{k}'}-\varepsilon_{\boldsymbol{k}})\,d\varepsilon_{\boldsymbol{k}'}\,d\Omega_{\boldsymbol{k}'}\\ &= \frac{m\mathcal{V}k}{4\pi^2\hbar^3}\,|T_{\boldsymbol{k}'\boldsymbol{k}}|^2\,\Delta\Omega_{\boldsymbol{k}'}\end{aligned} \tag{3.65}$$

where it is assumed that $|T_{\boldsymbol{k}'\boldsymbol{k}}|^2$ varies little over the angle $\Delta\Omega_{\boldsymbol{k}'}$. The scattering rate of probability is also the rate of particle scattering.

The cross section corresponding to the solid angle $\Delta\Omega_{\boldsymbol{k}'}$, denoted $\Delta\sigma(\boldsymbol{k}')$, is the area of the incident beam that must be blocked to intercept just the rate of particles scattering into $\Delta\Omega_{\boldsymbol{k}'}$. Thus if $\mathcal{J}$ is the flux of particles hitting the target, all with wave vector $\boldsymbol{k}$, then $\mathcal{J}\,\Delta\sigma(\boldsymbol{k}') = \sum_{\boldsymbol{k}'\in\Delta\Omega_{\boldsymbol{k}'}} W_{\boldsymbol{k}\to\boldsymbol{k}'}$. In light of Eq. (3.47), the density of incident particles is $(2\pi)^{-3}$ and their speed is $\hbar\,k/m$. The product of these two factors is $\mathcal{J}$ [see Eq. (3.84)]. We also infer that the effective volume per particle is $\mathcal{V} = (2\pi)^3$. Thus from Eq. (3.65) we see that

$$\frac{\Delta\sigma(\boldsymbol{k}')}{\Delta\Omega_{\boldsymbol{k}'}} = \left(\frac{4\pi^2 m}{\hbar^2}\right)^2 |T_{\boldsymbol{k}'\boldsymbol{k}}|^2\,. \tag{3.66}$$

The limit of this ratio as $\Delta\Omega_{\boldsymbol{k}'}\to 0$ is called the *differential scattering cross section*, and written

$$\frac{d\sigma}{d\Omega} = \left(\frac{4\pi^2 m}{\hbar^2}\right)^2 |T_{\boldsymbol{k}'\boldsymbol{k}}|^2\,, \tag{3.67}$$

[6]The German Hermann Klaus Hugo Weyl (1885-1955), a student of Hilbert, was one of the great mathematicians of the 20th century. He also contributed to theoretical physics applying group theory to quantum mechanics and contributing to general relativity. He originated the notions of gauge symmetry and gauge field, and the theory of the two component neutrino.

with the directions of $\boldsymbol{k}$ and $\boldsymbol{k}'$ understood in the l.h.s. The $d\sigma/d\Omega$ is measurable by comparing the rate of particles scattered into a particular direction per unit solid angle with the incident flux. We have shown that knowing the T-matrix allows to make a prediction for the differential cross sections. However, we still have to calculate $u^{(+)}_{\boldsymbol{k}}(\boldsymbol{r})$.

3.2.4 The Lippmann-Schwinger equation

To do that we abandon temporarily the scenario of Sec. 3.2.1 and regard the potential as fully static. It is clear that the function $u^{(+)}_{\boldsymbol{k}}(\boldsymbol{r})$ of Eq. (3.56) satisfies the full time-independent Schrödinger equation. Using the definition (3.64) we can write this last as

$$(\Delta + k^2)\, u^{(+)}_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{2m}{\hbar^2}\, V(\boldsymbol{r})\, u^{(+)}_{\boldsymbol{k}}(\boldsymbol{r})\,. \tag{3.68}$$

The equation here is Helmholtz's equation[7] with a source term on the right. We may solve it by the method of Green functions. A Green function of the Helmholtz equation, $g(\boldsymbol{r}, \boldsymbol{r}')$, satisfies

$$(\Delta + k^2)\, g_k(\boldsymbol{r}, \boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}') \tag{3.69}$$

together with the requirement that $\lim_{r\to\infty} g_k(\boldsymbol{r}, \boldsymbol{r}') = 0$. The obvious "solution" of Eq. (3.68) is

$$u^{(+)}_{\boldsymbol{k}}(\boldsymbol{r}) = C\, e^{\imath \boldsymbol{k}\cdot\boldsymbol{r}} + \frac{2m}{\hbar^2} \int g_k(\boldsymbol{r}, \boldsymbol{r}')\, V(\boldsymbol{r}')\, u^{(+)}_{\boldsymbol{k}}(\boldsymbol{r}')\, d^3r', \tag{3.70}$$

where the first term solves the homogeneous Helmholtz equation. In principle C can be arbitrary, but since we expect $u^{(+)}_{\boldsymbol{k}}(\boldsymbol{r})$ in the region of large $\boldsymbol{r}$ preceding the potential to correspond to the wave (3.47), we set $C = (2\pi)^{-3/2}$ and take $\boldsymbol{k}$ to be the wave vector of the incident particle. Eq. (3.70) is

[7] Hermann Ludwig Ferdinand von Helmholtz (1821-1894) was the greatest German physicist of the 19th century. He is remembered for his work in thermodynamics (law of conservation of energy, Helmholtz free energy), hydrodynamics (the laws of vortices), electrodynamics (electric resonance, von Helmholtz's coil). He also did work in physiology (the speed of impulses in the nerves, mathematical theory of vision and color perception, and theory of hearing) being a physician as well.

an integral equation of Fredholm type 1 called the Lippman[8]-Schwinger[9] equation.

Example: Calculating a Green function of Helmholtz's equation

We now have to find $g_k(\boldsymbol{r}, \boldsymbol{r}')$. Since Eq. (3.69) does not contain a position dependent potential, we can write $g_k(\boldsymbol{r} - \boldsymbol{r}')$ instead of $g_k(\boldsymbol{r}, \boldsymbol{r}')$ [see the argument following Eq. (2.12)]. We may simplify the problem by representing the Green function by a Fourier integral:

$$g_k(\boldsymbol{r} - \boldsymbol{r}') = \int \mathcal{G}_k(\boldsymbol{k}')\, e^{\imath \boldsymbol{k}' \cdot (\boldsymbol{r} - \boldsymbol{r}')}\, d^3k' \,. \tag{3.71}$$

We substitute this in Eq. (3.69) and write $\delta(\boldsymbol{r} - \boldsymbol{r}')$ as an integral by means of Eq. (3.48) getting

$$\int \mathcal{G}_k(\boldsymbol{k}')\, (\Delta + k^2)\, e^{\imath \boldsymbol{k}' \cdot (\boldsymbol{r} - \boldsymbol{r}')}\, d^3k' = \frac{1}{(2\pi)^3} \int e^{\imath \boldsymbol{k}' \cdot (\boldsymbol{r} - \boldsymbol{r}')}\, d^3k' \,. \tag{3.72}$$

But of course $\Delta\, e^{\imath \boldsymbol{k}' \cdot (\boldsymbol{r} - \boldsymbol{r}')} = -k'^2\, e^{\imath \boldsymbol{k}' \cdot (\boldsymbol{r} - \boldsymbol{r}')}$. Therefore

$$\int \left[\mathcal{G}_k(\boldsymbol{k}')\, (-k'^2 + k^2) - \frac{1}{(2\pi)^3} \right] e^{\imath \boldsymbol{k}' \cdot (\boldsymbol{r} - \boldsymbol{r}')}\, d^3k' = 0 \,. \tag{3.73}$$

However, the Fourier transform of 0 is 0. Thus

$$\mathcal{G}_k(\boldsymbol{k}') = \frac{1}{(2\pi)^3} \frac{1}{k^2 - k'^2} \,. \tag{3.74}$$

Accordingly

$$g_k(\boldsymbol{r} - \boldsymbol{r}') = \frac{1}{(2\pi)^3} \int \frac{e^{\imath \boldsymbol{k}' \cdot (\boldsymbol{r} - \boldsymbol{r}')}}{k^2 - k'^2}\, d^3k' \,. \tag{3.75}$$

[8] named for Bernard A. Lippmann (1915-1988), an American Jewish physicist who developed the said equation in his thesis as a Ph. D. student of Schwinger.

[9] Julian Seymour Schwinger (1918-1994) was a prominent American Jewish theoretical physicist and Nobel Laureate. We owe to him much of quantum field theory including its variational formulation, the first calculation of the anomalous magnetic moment of the electron, the Schwinger model of confinement, the theory of fields with spin 3/2 (with W. Rarita) and the first suggestion that neutrinos come in several speciess. Four of his students received the Nobel prize.

Orient now the coordinates with the z axis along $\boldsymbol{r}-\boldsymbol{r}'$, write $\boldsymbol{r}-\boldsymbol{r}'=\boldsymbol{z}$, and perform the angular part of the last integral (using $d^3k'=k'^2\,dk'\,d\Omega_{\boldsymbol{k}'}$):

$$\int_0^{2\pi}\int_{-1}^{1} e^{\imath k'\,|\boldsymbol{z}|\cos\theta}\,d\cos\theta\,d\varphi=\frac{2\pi}{\imath\,k'\,|\boldsymbol{z}|}\left(e^{\imath k'|\boldsymbol{z}|}-e^{-\imath k'|\boldsymbol{z}|}\right). \tag{3.76}$$

In performing the k' integral, the second term here can be used to convert that integral into one from $-\infty$ to ∞. We thus get

$$g_k(\boldsymbol{z})=\frac{1}{4\pi^2\imath|\boldsymbol{z}|}\int_{-\infty}^{\infty}\frac{e^{\imath k'|\boldsymbol{z}|}\,k'\,dk'}{k^2-k'^2}\,. \tag{3.77}$$

The integrand here has two singularities, at $k'=\pm k$. Either one causes the corresponding integral to diverge. This does not mean we cannot obtain the Green function this way. It is possible to deform the contour of integration, now running exactly along the k' axis, to deviate from it into the complex k' plane to sidestep the singularities. When this is done a finite result is obtained. Different $g_k(\boldsymbol{z})$ can be obtained, depending on how the contour bypasses the singularities.

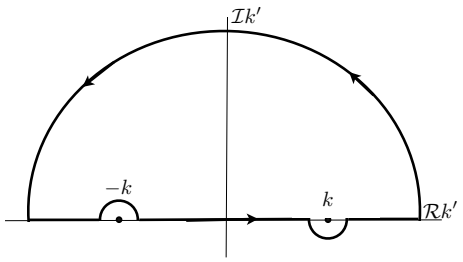

Figure 3.2: **The contour employed to calculate integral (3.77)**

Consider the way illustrated in Fig. 3.2; the contour has been extended from the real $\pm\infty$ where it used to end into the far upper k' plane and closed there. The piece of contour where k' has an imaginary part that tends to $+\infty$ does not contribute because the exponential $e^{\imath k'|\boldsymbol{z}|}$ vanishes provided $|\boldsymbol{z}|\neq 0$. Thus the closed contour integral is equivalent to the integral taken along the real k' axis but bypassing the singularities.

According to Cauchy's theorem the integral (3.77) is equal to $2\pi\imath$ times the *residue* of the integral at $k'=k$ (this being the location of the only pole

of the integrand within the contour). This residue is $-\frac{1}{2}e^{\imath k|\boldsymbol{z}|}$. Putting all these parts together we get, in the original variable,

$$g_k^{(+)}(\boldsymbol{r}-\boldsymbol{r}') = -\frac{e^{\imath k\,|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\,. \tag{3.78}$$

We have decorated the symbol for the Green function with a (+) because when this Green function is used in Eq. (3.70), it causes the second term of the wave function to behave, for large r, like $e^{+\imath kr}/r$ (outward propagating spherical waves) which corresponds to the physical expectation that the plane wave $e^{\imath \boldsymbol{k}\cdot\boldsymbol{r}}$, upon hitting the potential, will scatter *outward* in all directions (see Fig. 3.3) To see this explicitly we must look at the asymptotic limit of the Lippmann-Schwinger equation.

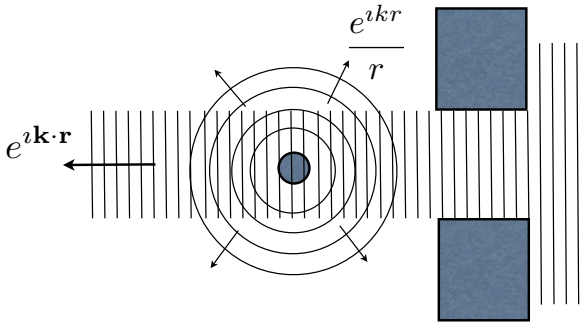

Figure 3.3: **Illustrating the breakup of the incident wave into a forward plane wave and a spherical outgoing wave as in Eq. (3.80).**

Consider the series expansion of $|\boldsymbol{r}-\boldsymbol{r}'|$ for large $\boldsymbol{r}$:

$$|\boldsymbol{r}-\boldsymbol{r}'| = (r^2 + r'^2 - 2\boldsymbol{r}\cdot\boldsymbol{r}')^{1/2} = r - \boldsymbol{r}\cdot\boldsymbol{r}'/r + \cdots \tag{3.79}$$

We substitute this full expression in the exponent of Eq. (3.78), but only r for its denominator, thus obtaining

$$u_{\boldsymbol{k}}^{(+)}(\boldsymbol{r}) \approx \frac{1}{(2\pi)^{3/2}}\left[e^{\imath \boldsymbol{k}\cdot\boldsymbol{r}} - \frac{(2\pi)^{1/2}m}{\hbar^2}\,\frac{e^{\imath kr}}{r}\int e^{-\imath \boldsymbol{k}'\cdot\boldsymbol{r}'}\,V(\boldsymbol{r}')\,u_{\boldsymbol{k}}^{(+)}(\boldsymbol{r}')\,d^3r'\right], \tag{3.80}$$

where $\boldsymbol{k}'$ has magnitude k and the radial direction $\boldsymbol{r}/r$, i.e., $\boldsymbol{k}'$ is the wavevector after scattering (assuming the center of the potential is at $\boldsymbol{r}=0$).

We see that for large r ($r \gg$ the range of the potential and so large compared to the r' contributing significantly to the integral) and relative to $\exp(\imath \boldsymbol{k}\cdot\boldsymbol{r})$, the scattered part of the wave has the form $e^{\imath kr}/r$ multiplied by a function of $\boldsymbol{k}$ and $\boldsymbol{k}'$, popularly known as the *scattering amplitude*:

$$f(\boldsymbol{k}\to\boldsymbol{k}') \equiv -\frac{4\pi^2 m}{\hbar^2}\int \frac{e^{-\imath \boldsymbol{k}'\cdot\boldsymbol{r}'}}{(2\pi)^{3/2}}\, V(\boldsymbol{r}')\, u_{\boldsymbol{k}}^{(+)}(\boldsymbol{r}')\, d^3r' \,. \tag{3.81}$$

Comparing with Eq. (3.58) we see that $f(\boldsymbol{k}\to\boldsymbol{k}')$ and $T_{\boldsymbol{k}'\boldsymbol{k}}$ differ only by a constant factor. This gives us another interpretation for an element of the T-matrix: it is the amplitude of the spherical outgoing wave with the mentioned $\boldsymbol{k}'$ when a plane wave of wavevector $\boldsymbol{k}$ is incident on the potential.

Exercises:

1. Reproduce the result given in the text for the residue of the integrand in Eq. (3.77).

2. Deform the contour in Fig. 3.2 in a different way in order to obtain the Green function
$$g_k^{(-)}(\boldsymbol{r}-\boldsymbol{r}') = -\frac{e^{-\imath k\,|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|} \,. \tag{3.82}$$

3. Discuss the relation between $g_k^{(+)}(\boldsymbol{r}-\boldsymbol{r}')$ and $g_k^{(-)}(\boldsymbol{r}-\boldsymbol{r}')$ as compared to that between $G^{(-)}(\boldsymbol{r},t;\boldsymbol{r}',t')$ and $G^{(+)}(\boldsymbol{r},t;\boldsymbol{r}',t')$ in Sec. 2.1.9.

3.2.5 Alternative way to the scattering cross section

We return to the Lippman-Schwinger equation (3.80) describing implicitly the scattering wave function $u_{\boldsymbol{k}}^{(+)}$. The first term of $u_{\boldsymbol{k}}^{(+)}$ represents the particle with momentum $\hbar\boldsymbol{k}$ incident from afar onto the potential whose center we take to be at the origin. Recall that in quantum mechanics the flux of probability is given by

$$\boldsymbol{j} = \frac{\hbar}{2m\imath}(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*) \,. \tag{3.83}$$

From Eq. (3.83) we see that the incident flux of probability is

$$\boldsymbol{j}_0 = (2\pi)^{-3}\,\hbar\boldsymbol{k}/m\,. \tag{3.84}$$

What is the flux of probability of the scattered particle into a solid angle $\Delta\Omega_{\boldsymbol{k}'}$? If we substitute the full expression on the r.h.s. of Eq. (3.80) in Eq. (3.83) we shall get interference terms which confuse the issue. So suppose the incident particle has to go through a collimator which allows only the part of the wave function within some radius R off the axis of $\boldsymbol{k}$ to continue to the target (see Fig. 3.3). We take $R \gg 1/k$ (to minimize diffraction of the wave) and $R \gg b$, the range of the potential, so that its effects are fully taken into account. Then if we look for the scattered flux at distances large compared to R, only the second term in $u^{(+)}_{\boldsymbol{k}}$ need to be substituted in Eq. (3.83).

The scattered flux is

$$\boldsymbol{j}_{\rm sc} = (2\pi)^{-3}\,\frac{\hbar k}{mr^2}|f(\boldsymbol{k}\to\boldsymbol{k}')|^2\,\boldsymbol{r}/r\,. \tag{3.85}$$

The rate of probability of the scattered particle into a solid angle $\Delta\Omega_{\boldsymbol{k}'}$ at distance r from the origin is $|\boldsymbol{j}_{\rm sc}|r^2\,\Delta\Omega_{\boldsymbol{k}'}$. The cross section $\Delta\sigma(\boldsymbol{k}')$ is this rate divided by the magnitude of the incident flux, Eq. (3.84), and so the differential cross section is

$$\frac{d\sigma}{d\Omega} = |f(\boldsymbol{k}\to\boldsymbol{k}')|^2\ . \tag{3.86}$$

Of course this result coincides with Eq. (3.67), though the new derivation is entirely different in concept.

3.2.6 The optical theorem

Bohr, Peierls[10] and Placzek[11] derived a very useful theorem connecting the scattering amplitude for forward scattering to the *total scattering cross section*. The theorem relies only on unitarity of the S-matrix.

[10]Rudolf Ernst Peierls (1907-1995), a German-British theoretical physicist of Jewish origin who made great contributions to solid state physics and to nuclear theory. He was also deeply involved on the British side in the nuclear bomb project during World War II.

[11]Georg Placzek (1905-1955) was a Czech Jewish theoretical physicist who made important contributions to optics, quantum mechanics and nuclear physics. He participated in the Manhattan project.

Our starting point is the unitarity condition, Eq. (3.9), in the form

$$\int d^3k''\, S_{\boldsymbol{k}\boldsymbol{k}''}{}^{\dagger}\, S_{\boldsymbol{k}''\boldsymbol{k}'} = \int d^3k''\, S_{\boldsymbol{k}''\boldsymbol{k}}{}^{*}\, S_{\boldsymbol{k}''\boldsymbol{k}'} = \delta(\boldsymbol{k}-\boldsymbol{k}') \tag{3.87}$$

where $\hbar\boldsymbol{k}$ is the momentum of the incident particle and $\hbar\boldsymbol{k}'$ that of the scattered one. We substitute for $S_{\boldsymbol{k}\boldsymbol{k}'}$ the definition (3.59) of the T-matrix to get

$$\begin{aligned} & 2\pi\imath \int d^3k''\, \delta(\boldsymbol{k}'-\boldsymbol{k}'')\, T_{\boldsymbol{k}''\boldsymbol{k}}{}^{*}\, \delta(\varepsilon_{\boldsymbol{k}''}-\varepsilon_{\boldsymbol{k}}) - 2\pi\imath \int d^3k''\, \delta(\boldsymbol{k}-\boldsymbol{k}'')\, T_{\boldsymbol{k}''\boldsymbol{k}'}\, \delta(\varepsilon_{\boldsymbol{k}''}-\varepsilon_{\boldsymbol{k}'}) \\ + \;& 4\pi^2 \int d^3k''\, T_{\boldsymbol{k}''\boldsymbol{k}'}\, T_{\boldsymbol{k}''\boldsymbol{k}}{}^{*}\, \delta(\varepsilon_{\boldsymbol{k}''}-\varepsilon_{\boldsymbol{k}})\, \delta(\varepsilon_{\boldsymbol{k}''}-\varepsilon_{\boldsymbol{k}'}) \\ + \;& \int d^3k''\, \delta(\boldsymbol{k}''-\boldsymbol{k}')\, \delta(\boldsymbol{k}-\boldsymbol{k}'') = \delta(\boldsymbol{k}-\boldsymbol{k}')\,. \end{aligned} \tag{3.88}$$

It is plain that the terms with only delta functions cancel out.

In the second line of Eq. (3.88)

$$\delta(\varepsilon_{\boldsymbol{k}''}-\varepsilon_{\boldsymbol{k}})\, \delta(\varepsilon_{\boldsymbol{k}''}-\varepsilon_{\boldsymbol{k}'}) = \delta(\varepsilon_{\boldsymbol{k}'}-\varepsilon_{\boldsymbol{k}})\, \delta(\varepsilon_{\boldsymbol{k}''}-\varepsilon_{\boldsymbol{k}})\,. \tag{3.89}$$

Now in the first integral the $\delta(\boldsymbol{k}'-\boldsymbol{k}'')$ can be used to replace $\delta(\varepsilon_{\boldsymbol{k}''}-\varepsilon_{\boldsymbol{k}}) \mapsto \delta(\varepsilon_{\boldsymbol{k}'}-\varepsilon_{\boldsymbol{k}})$ under the integral, while the $\delta(\boldsymbol{k}-\boldsymbol{k}'')$ in the second integral permits the replacement $\delta(\varepsilon_{\boldsymbol{k}''}-\varepsilon_{\boldsymbol{k}}) \mapsto \delta(\varepsilon_{\boldsymbol{k}}-\varepsilon_{\boldsymbol{k}'})$. Thus every integrand in Eq. (3.88) has a factor $\delta(\varepsilon_{\boldsymbol{k}}-\varepsilon_{\boldsymbol{k}'})$, and all these can be taken out of the integrals. They say that the equation we are about to obtain is nullified unless $\varepsilon_{\boldsymbol{k}} = \varepsilon_{\boldsymbol{k}'}$, i.e. there must be conservation of energy. That clear we factor out all the $\delta(\varepsilon_{\boldsymbol{k}}-\varepsilon_{\boldsymbol{k}'})$ and are left with

$$\imath(T_{\boldsymbol{k}\boldsymbol{k}'} - T_{\boldsymbol{k}'\boldsymbol{k}}{}^{*}) = 2\pi \int d^3k''\, T_{\boldsymbol{k}''\boldsymbol{k}'}\, T_{\boldsymbol{k}''\boldsymbol{k}}{}^{*}\, \delta(\varepsilon_{\boldsymbol{k}''}-\varepsilon_{\boldsymbol{k}})\,. \tag{3.90}$$

We now replace all T-matrix elements by their equivalent scattering amplitude f based on the comparison of Eq. (3.58) and formula (3.81):

$$\imath\,[f(\boldsymbol{k}\to\boldsymbol{k}')^{*} - f(\boldsymbol{k}'\to\boldsymbol{k})] = \frac{\hbar^2}{2\pi m} \int d^3k'' f(\boldsymbol{k}'\to\boldsymbol{k}'')\, f(\boldsymbol{k}\to\boldsymbol{k}'')^{*} \delta(\varepsilon_{\boldsymbol{k}''}-\varepsilon_{\boldsymbol{k}}) \tag{3.91}$$

But in view of Eq. (3.64), $d^3k'' = k''^2\, dk''\, d\Omega'' = (m/\hbar^2)k''d\Omega''d\varepsilon_{\boldsymbol{k}''}$. Carrying out the k'' integral we get

$$\int d\Omega'' f(\boldsymbol{k}' \to \boldsymbol{k}'')\, f(\boldsymbol{k} \to \boldsymbol{k}'')^* = \frac{4\pi}{k} \frac{f(\boldsymbol{k}' \to \boldsymbol{k}) - f(\boldsymbol{k} \to \boldsymbol{k}')^*}{2i}\,. \tag{3.92}$$

This is sometimes called the *generalized optical theorem*.

As an application of it consider a rather weak potential. In view of Eq. (3.81) f can be regarded as small? Now f has units of length, so small can mean small compared to $1/k$ or compared to the range of the potential b. In Eq. (3.92) we can then neglect the l.h.s. if f is small compared to $1/k$ and conclude that for sufficiently weak potential we have the *approximate* symmetry property

$$f(\boldsymbol{k}' \to \boldsymbol{k})^* \approx f(\boldsymbol{k} \to \boldsymbol{k}')\,. \tag{3.93}$$

Let us now consider the special case of Eq. (3.92) with $\boldsymbol{k}' = \boldsymbol{k}$. Of course $f(\boldsymbol{k} \to \boldsymbol{k})$ means the forward scattering cross section, and we see its imaginary part appearing in the r.h.s. In the l.h.s. and under the integral we have $|f(\boldsymbol{k} \to \boldsymbol{k}'')|^2$ which by Eq. (3.86) is the differential scattering cross section; its integral over solid angle is the total cross section σ. Hence

$$\sigma = \int \frac{d\sigma}{d\Omega}\, d\Omega = \frac{4\pi}{k} \mathcal{I} f(\boldsymbol{k} \to \boldsymbol{k}) \tag{3.94}$$

which is known widely as the *optical theorem*.

One consequence of the optical theorem is that if there is any scattering at all ($\sigma \neq 0$), there must be forward scattering (again Delisle's spot—see footnote in Sec. 3.2.2), because at least the imaginary part of the forward amplitude does not vanish. This reminds us that the qualifier "optical" applied to our theorem here arises because an analogue of it exists in optics, and in fact in any theory of waves.

3.2.7 Consequences of symmetries for the scattering amplitude

Here we discuss symmetries in scattering in the language of $f(\boldsymbol{k} \to \boldsymbol{k}')$. We learned in Sec. 3.1.3 that the S-matrix element from $\hat{U}_\xi\,|\phi_i\rangle$ to $\hat{U}_\xi\,|\phi_j\rangle$ is

the same as for the scattering $|\phi_i\rangle$ to $|\phi_j\rangle$. When we discuss scattering of momentum states this symmetry of $S_{\boldsymbol{k}'\boldsymbol{k}}$ is passed on to $f(\boldsymbol{k} \to \boldsymbol{k}')$ by virtue of Eqs. (3.59), (3.58) and formula (3.81). Examples follow.

Assume the potential has spatial inversion symmetry. Then

$$f(-\boldsymbol{k} \to -\boldsymbol{k}') = f(\boldsymbol{k} \to \boldsymbol{k}')\,. \tag{3.95}$$

Why is this true? Because aside from a factor $\hbar$, $\boldsymbol{k}$ is an eigenvalue of $\hat{\boldsymbol{p}}$ and we know that spatial inversion changes the sign of $\hat{\boldsymbol{p}}$, hence of its eigenvalues. By the theorem in Sec. 3.1.3, the spatial inversion does not change the elements of the S-matrix, so Eq. (3.95) follows.

Let us now consider spherical symmetry of the potential. In that case an arbitrary rotation by angle Ω around an axis $\boldsymbol{n}$, denoted in Sec. 1.2.7 as $R(\boldsymbol{\Omega})\boldsymbol{v}$, is a symmetry of the Hamiltonian. Then it is clear from the general theorem of Sec. 3.1.3 that

$$f\big(R(\boldsymbol{\Omega})\boldsymbol{k} \mapsto R(\boldsymbol{\Omega})\boldsymbol{k}'\big) = f(\boldsymbol{k} \to \boldsymbol{k}'). \tag{3.96}$$

Now when two vectors $\boldsymbol{k}$ and $\boldsymbol{k}'$ are rotated together, the angle ϑ between them is unchanged. Since scattering on a static potential conserves the energy, we must have $|\boldsymbol{k}| = |\boldsymbol{k}'| = k$. Hence we can write the scattering amplitude for a spherically symmetric potential as a function of just two variables:

$$f(\boldsymbol{k} \to \boldsymbol{k}') = \tilde{f}(k, \vartheta). \tag{3.97}$$

We shall henceforth drop the tilde over f.

According to Eq. (3.17) every symmetry operator commutes with the Hamiltonian, and is thus a conserved quantity provided it has no explicit time dependence. If we write the rotation operator for infinitesimal rotation angle as in Eq. (1.79), it is clear that $\hat{\boldsymbol{l}}$ itself commutes with the Hamiltonian and is thus conserved. One knows that $\hat{\boldsymbol{l}}^2$ and $\hat{l}_z$ commute. hence the set $\{\hat{H}, \hat{\boldsymbol{l}}^2, \hat{l}_z\}$ is a maximally commuting set of observables. (If there were spin, we could add $\hat{\boldsymbol{s}}^2$ and $\hat{s}_z$.) One can thus contemplate initial and final scattering states which, instead of the form $|\boldsymbol{k}\rangle$, are of the type $|kl\mu\rangle$ where l and μ are the angular momentum eigenvalues (more precisely the eigenvalues of $\hat{\boldsymbol{l}}^2$ are $l(l+1)\hbar^2$; $l = 0, 1, 2, \cdots$ and those of $\hat{l}_z$ are $\mu\hbar$; $\mu = -l, -l+1, \cdots -1, 0, 1, \cdots l$). The k plays the role of energy eigenvalue

since $\varepsilon = \hbar^2 k^2/2m$. There is a unitary transformation which transforms from the basis of $|\boldsymbol{k}\rangle$ to that of $|kl\mu\rangle$.

What is special about the basis of $|kl\mu\rangle$ is that all its eigenvalues are conserved during scattering. This means that in this representation the S-matrix is completely diagonal:

$$S_{k'l'\mu';kl\mu} = \tilde{S}_{kl\mu}\,\delta(k'-k)\,\delta_{l'l}\,\delta_{\mu'\mu} \tag{3.98}$$

The delta function for k is a Dirac one because k is a continuous variable.

We now further show that $\tilde{S}_{kl\mu}$ does not depend on μ. The *raising and lowering operators* $\hat{l}_+ \equiv \hat{l}_x + \imath\,\hat{l}_y$ and $\hat{l}_- \equiv \hat{l}_x - \imath\,\hat{l}_y$ are each other's Hermitian conjugates. It is known from the theory of angular momentum that

$$\hat{l}_\pm\,|kl\mu\rangle = \sqrt{l(l+1)-\mu(\mu\pm1)}\,\hbar\,|kl,\mu\pm1\rangle\,. \tag{3.99}$$

Since both $\hat{l}_+$ and $\hat{l}_-$ are built from the generator of rotations, they must, according to Eqs. (1.79) and (3.17), commute with the evolution operator. Thus by Eq. (3.99)

$$\begin{aligned}&\langle kl\mu'|\,[\hat{l}_+,\hat{U}(t,t_0)]\,|kl\mu\rangle = \\ &\sqrt{l(l+1)-\mu'(\mu'-1)}\langle kl,\mu'-1|\hat{U}(t,t_0)|kl\mu\rangle \\ -\quad &\sqrt{l(l+1)-\mu(\mu+1)}\langle kl\mu'|\hat{U}(t,t_0)|kl,\mu+1\rangle = 0\,.\end{aligned} \tag{3.100}$$

Of course because of the conservation of angular momentum the first matrix element on the r.h.s. survives only if $\mu'-1=\mu$ while the second does so only if $\mu'=\mu+1$; namely, in both cases we need $\mu'=\mu+1$ to get a nonzero result. Putting $\mu'=\mu+1$ everywhere we obtain

$$\langle kl,\mu+1|\,\hat{U}(t,t_0)\,|kl,\mu+1\rangle = \langle kl\mu|\,\hat{U}(t,t_0)\,|kl\mu\rangle\,. \tag{3.101}$$

This says that the S-matrix element between states of type $|kl\mu\rangle$ cannot depend on μ. Thus Eq. (3.98) becomes

$$S_{k'l'\mu';kl\mu} = \tilde{S}_{kl}\,\delta(k'-k)\,\delta_{l'l}\,\delta_{\mu'\mu} \tag{3.102}$$

There is one further thing we can say. Because the S-matrix is diagonal in the klm basis and has a factor equivalent to the unit matrix $\mathcal{I}$, the unitarity condition $S\,S^\dagger = \mathcal{I}$ can be written

$$\tilde{S}_{kl}\,\tilde{S}^*_{kl} = 1 \tag{3.103}$$

which means each S_{kl} is just a phase. Thus we can write

$$S_{k'l'\mu';kl\mu} = e^{2\imath\delta_l(k)}\,\delta(k'-k)\,\delta_{l'l}\,\delta_{\mu'\mu} \tag{3.104}$$

where the $\delta_l(k)$ are real and receive the name *phase-shifts*. These contain all the information about spherically symmetric scattering.

We now return to time reversal invariance; it obtains when the Hamiltonian is time independent and real. Free plane waves like that in Eq. (3.47) will undergo time-reversal according to the rule (3.44) with j meaning $\boldsymbol{k}$. By analogy the scattering wave (3.49) or (3.56) will transform under time-reversal as

$$\hat{\tau}\phi^{(+)}_{\boldsymbol{k}}(\boldsymbol{r},t) = \phi^{(-)}_{-\boldsymbol{k}}(\boldsymbol{r},-t) \tag{3.105}$$

where $\phi^{(-)}_{-\boldsymbol{k}}(\boldsymbol{r},t)$ is obtained from $\phi_{-\boldsymbol{k}}(\boldsymbol{r},t)$ by the action of the advanced Green function $G^{(-)}(\boldsymbol{r},t;\boldsymbol{r}',t')$. Physically $\phi^{(-)}_{-\boldsymbol{k}}(\boldsymbol{r},t)$ develops in the far future into $\phi_{-\boldsymbol{k}}(\boldsymbol{r},t)$, or what amounts to the same thing, $\phi_{-\boldsymbol{k}}(\boldsymbol{r},t)$ develops into $\phi^{(-)}_{-\boldsymbol{k}}(\boldsymbol{r},t)$ as we go back into the far past. The time independent part of $\phi^{(-)}_{-\boldsymbol{k}}(\boldsymbol{r},t)$, namely $u^{(-)}_{-\boldsymbol{k}}(\boldsymbol{r})$, comprises a scattered part that behaves as $e^{-\imath kr}/r$ rather than as $e^{\imath kr}/r$, i.e. $u^{(-)}_{-\boldsymbol{k}}(\boldsymbol{r})$ is obtained from the Lippmann-Schwinger equation (3.70) by use of the Green function $g^{(-)}_{\boldsymbol{k}}$ of Eq. (3.82).

In giving the proof of the modification of Eq. (3.18) applicable for time reversal symmetry we shall consider $\hat{\tau}$ to include the unitary operator $\hat{U}_\tau$ introduced in Sec. 3.1.4. We shall also use the notation $\langle\hat{O}\psi_j|$ to denote the bra state corresponding to the wave function $\hat{O}\psi_j(\boldsymbol{r})$. The j is here a generic time-reversal odd eigenvalue, of which $\boldsymbol{k}$ is just one example.

In Eq. (3.3) we defined the element of S-matrix as

$$S_{ji} = \lim_{t\to\infty}\langle\phi_j,t|\phi^{(+)}_i,t\rangle \tag{3.106}$$

We now use Eq. (1.4) to get

$$\langle\phi_j,t|\phi^{(+)}_i,t\rangle = \langle\hat{K}\phi^{(+)}_i,t|\hat{K}\phi_j,t\rangle\,. \tag{3.107}$$

Now we introduce a unity factor $\hat{U}^\dagger_\tau\hat{U}_\tau$ between ket and bra to get

$$\langle\hat{K}\phi^{(+)}_i,t|\hat{K}\phi_j,t\rangle = \langle\hat{K}\phi^{(+)}_i,t|\hat{U}^\dagger_\tau\hat{U}_\tau|\hat{K}\phi_j,t\rangle = \langle\hat{U}_\tau\hat{K}\phi^{(+)}_i,t|\hat{U}_\tau\hat{K}\phi_j,t\rangle \tag{3.108}$$

(use of unitarity of $\hat{U}_\tau$). In view of Eq. (3.28) we have

$$\langle \hat{U}_\tau \hat{K} \phi_i^{(+)}, t | \hat{U}_\tau \hat{K} \phi_j, t \rangle = \langle \hat{\tau} \phi_i^{(+)}, t | \hat{\tau} \phi_j, t \rangle = \langle \phi_{-i}^{(-)}, -t | \phi_{-j}, -t \rangle \tag{3.109}$$

where we have used Eq. (3.105). The chaining of the last four equations gives

$$S_{ji} = \lim_{t \to -\infty} \langle \phi_{-i}^{(-)}, t | \phi_{-j}, t \rangle \tag{3.110}$$

But we said that $\phi_{-\boldsymbol{k}}(\boldsymbol{r}, t)$ develops into $\phi_{-\boldsymbol{k}}^{(-)}(\boldsymbol{r}, t)$ as we go back into the far past. For a generic eigenvalue this means $|\phi_{-j}, t\rangle$ develops in the far past into $|\phi_{-j}^{(-)}, t\rangle$. Hence the last scalar product is to be interpreted as $S_{-i,-j}$ (the evolution backwards in time is the reason why the order of free and full states is reversed).

We have obtained the *principle of microscopic reversibility* or *principle of reciprocity*,

$$S_{ji} = S_{-i,-j}\,; \tag{3.111}$$

this replaces Eq. (3.18) which applies only to unitary operator symmetries. Of course the *probabilities* of direct and inverse processes with opposite sign for the time-reversal odd eigenvalues will be the same. This is called the *principle of detailed balance*.

The result (3.111) means that when the Hamiltonian is time-reversal invariant, the amplitude of a process equals the amplitude of the inverse process but with all eigenvalues of the time-reversal odd observables entering with opposite sign. To give an example, in scattering of a spin-$\frac{1}{2}$ particle with definite momentum $\hbar\boldsymbol{k}$ and z-projection of spin μ_s by a static real potential (which makes the Hamiltonian time-reversal even), we would have

$$S_{\boldsymbol{k}',\mu_s';\boldsymbol{k},\mu_s} = S_{-\boldsymbol{k},-\mu_s;-\boldsymbol{k}',-\mu_s'}\,. \tag{3.112}$$

In terms of the scattering amplitude we would write microscopic reversibility as

$$f(\boldsymbol{k}, \mu_s \to \boldsymbol{k}', \mu_s') = f(-\boldsymbol{k}', -\mu_s' \to -\boldsymbol{k}, -\mu_s)\,. \tag{3.113}$$

Exercises:

1. Suppose a spin-$\frac{1}{2}$ particle with definite $\boldsymbol{k}$ and z-projection of spin μ_s is scattered from a potential $V(\boldsymbol{r})$ which is real, and invariant under space inversion. Obtain a new symmetry of the S-matrix.

2. A particle scatters on the potential $V = f(\varrho)\, g(\varphi - z/b)$ (in cylindrical coordinates (ϱ, φ, z) with b a constant). Energy is one conserved quantity. Interpret the other conserved quantity physically. Write the $\hat{U}$ operator for the continuous symmetry.

3. Consider base functions in Exercise 2 as $\chi(\varrho)\, e^{\imath\mu\varphi}\, e^{\imath\mu z/b}\, e^{-\imath\varepsilon t/\hbar}$. What is the spectrum of μ? Show in analogy with the work in class that

$$S_{\varepsilon'\,\mu';\varepsilon\,\mu} = \tilde{S}\,\delta(\varepsilon' - \varepsilon)\,\delta_{\mu'\,\mu}. \tag{3.114}$$

What does $\tilde{S}$ depend on? What extra information is obtained from time reversal symmetry?

3.2.8 The energy-angular momentum representation

In Sec. 3.2.7 we found for spherical symmetry the form of the S-matrix in the representation with basis $|kl\mu\rangle$. As usual there must be a unitary matrix that takes us from this representation to the $|\boldsymbol{k}\rangle$ representations. Its elements will be of the form $\langle \boldsymbol{k}'|kl\mu\rangle$. What can we say about these scalar products?

We can think of the $\boldsymbol{k}'$ in $|\boldsymbol{k}'\rangle$ as given in polar form $\{k', \theta', \phi'\}$, where $k' \equiv |\boldsymbol{k}'|$ and θ' and ϕ' designate the direction of $\boldsymbol{k}'$. Now since $|kl\mu\rangle$ is an eigenstate of angular momentum and energy, its position representation wave function should contain a spherical harmonic factor $Y_{l\mu}(\theta, \phi)$. However, $\langle \boldsymbol{k}'|kl\mu\rangle$ can be regarded as belonging to the position representation of $|kl\mu\rangle$ (k' playing the role of radius vector). Thus we expect

$$\langle \boldsymbol{k}'|kl\mu\rangle = C_{kl\mu}\,\delta(k' - k)\,Y_{l\mu}(\theta', \phi') \tag{3.115}$$

where the factor $\delta(k' - k)$ is needed because both bra and ket include the eigenvalue of type k. The complex factor $C_{kl\mu}$ encompasses all features of the scalar product we have not guessed.

Let us now insert the identity operator arising from $|kl\mu\rangle$ in $\langle \boldsymbol{k}''|\boldsymbol{k}'\rangle$:

$$\sum_{l\mu} \int_0^\infty dk\, \langle \boldsymbol{k}''|kl\mu\rangle\langle kl\mu|\boldsymbol{k}'\rangle = \delta(\boldsymbol{k}'' - \boldsymbol{k}') \tag{3.116}$$

where l runs from 0 to ∞ while μ ranges from $-l$ to l. Let us express $\delta(\boldsymbol{k}'' - \boldsymbol{k}')$ in spherical polar coordinates:

$$\sum_{l\mu} \int_0^\infty dk \, \langle \boldsymbol{k}''|kl\mu\rangle\langle kl\mu|\boldsymbol{k}'\rangle = \frac{\delta(k'' - k')}{k'^2} \frac{\delta(\theta'' - \theta')}{\sin\theta'} \delta(\phi'' - \phi'). \tag{3.117}$$

The reason for dividing by $k'^2 \sin\theta'$ is that the volume element in the designated coordinates amounts to $k'^2 \sin\theta' \, dk' \, d\theta' \, d\phi'$, and we wish to get unity from integrating the 3-D delta function over all volume.

Now the delta function over the sphere figures in the completeness relation for the spherical harmonics:

$$\sum_{l\mu} Y_{l\mu}(\theta''\phi'')^* \, Y_{l\mu}(\theta'\phi') = \frac{\delta(\theta'' - \theta')}{\sin\theta'} \delta(\phi'' - \phi') \, . \tag{3.118}$$

Combining this with the previous equation gives

$$\sum_{l\mu} \int_0^\infty dk \, \langle \boldsymbol{k}''|kl\mu\rangle\langle kl\mu|\boldsymbol{k}'\rangle = \frac{\delta(k'' - k')}{k'^2} \sum_{l\mu} Y_{l\mu}(\theta''\phi'')^* \, Y_{l\mu}(\theta'\phi'), \tag{3.119}$$

which in view of the guess (3.115) tells us that all the $C_{kl\mu}$ are really C/k with a single complex constant C with $|C| = 1$. We can shift the phases of the states $|kl\mu\rangle$ such that $C = 1$. Thus

$$\langle \boldsymbol{k}'|kl\mu\rangle = \frac{\delta(k' - k)}{k} \, Y_{l\mu}(\theta', \phi') \, . \tag{3.120}$$

3.2.9 The partial waves expansion

We now wish to derive the form of the scattering amplitude (for a spherically symmetric potential), $f(k, \vartheta)$, from the result (3.104). This $f(k, \vartheta)$ was originally obtained in the early days of QT by H. Faxén and J. Holtsmark by separating the Schrödinger equation in spherical coordinates and studying the asymptotic behavior of the radial function in a potential as compared with that for the free particle—a spherical Bessel function.[12] We here take

[12] The study of the Bessel functions was systematized by Friedrich Wilhelm Bessel (1784-1846), salient German astronomer who was the first to measure the parallax of a star, and to show that Sirius has a companion. He also performed an accurate test of the universality of free fall, much more accurate than Newton's.

a shorter path, which exploits the results from spherical symmetry obtained in Sec. 3.2.7.

The scattering amplitude is another form of the transition matrix which is given in $|\boldsymbol{k}\rangle$ representation by Eq. (3.59). Let us thus derive $T_{\boldsymbol{k}'\boldsymbol{k}}$ from the $|kl\mu\rangle$ representation of the S-matrix, Eq. (3.104). We go from $|kl\mu\rangle$ representation of the S-matrix to the $|\boldsymbol{k}\rangle$ representation of the T-matrix as follows:

$$\begin{aligned}\sum_{l\mu}\int_0^\infty dk\,\langle\boldsymbol{k}''|kl\mu\rangle\,e^{2\imath\,\delta_l(k)}\,\langle kl\mu|\boldsymbol{k}'\rangle &= S_{\boldsymbol{k}''\boldsymbol{k}'}\\ &= \delta(\boldsymbol{k}''-\boldsymbol{k}') - 2\pi\imath\,T_{\boldsymbol{k}''\boldsymbol{k}'}\,\delta(\varepsilon_{\boldsymbol{k}''}-\varepsilon_{\boldsymbol{k}'})\,.\end{aligned}\tag{3.121}$$

At this point we substitute $\langle\boldsymbol{k}''|kl\mu\rangle$ and its conjugate from Eq. (3.120), and $\delta(\boldsymbol{k}''-\boldsymbol{k}')$ by its form in polar coordinates as in Eq. (3.117), and then replace in this last the angular delta function by the sum over spherical harmonics as in Eq. (3.118):

$$\begin{aligned}&\sum_{l\mu}\int_0^\infty \frac{dk}{k'k''}\,e^{2\imath\,\delta_l(k)}\delta(k''-k)\,\delta(k-k')\,Y_{l\mu}(\theta''\phi'')^*\,Y_{l\mu}(\theta'\phi')\\ -\frac{1}{k'^2}\,\delta(k''-k')&\sum_{l\mu}Y_{l\mu}(\theta''\phi'')^*\,Y_{l\mu}(\theta'\phi') = -2\pi\imath\,T_{\boldsymbol{k}''\boldsymbol{k}'}\,\delta(\varepsilon_{\boldsymbol{k}''}-\varepsilon_{\boldsymbol{k}'}).\end{aligned}\tag{3.122}$$

The k integral in the last equation collapses the product of delta functions to $\delta(k''-k')$. In the r.h.s. we have

$$\delta(\varepsilon_{\boldsymbol{k}''}-\varepsilon_{\boldsymbol{k}'}) = \frac{\delta(k''-k')}{d\varepsilon_{\boldsymbol{k}''}/dk''} = \frac{m}{\hbar^2 k'}\,\delta(k''-k')\,.\tag{3.123}$$

Hence we may cancel out from every term in Eq. (3.122) a factor $\delta(k''-k')/k'$ if we afterward put $k''=k'$ in what is left of the first and r.h.s. terms. Renaming $k'\mapsto k$ we have

$$\frac{1}{k}\sum_l\left(e^{2\imath\,\delta_l(k)}-1\right)\sum_\mu Y_{l\mu}(\theta''\phi'')^*\,Y_{l\mu}(\theta'\phi') = -\frac{2\pi\,\imath\,m}{\hbar^2}\,T_{\boldsymbol{k}''\boldsymbol{k}'}\,.\tag{3.124}$$

which, as mentioned, is to be used only when $|\boldsymbol{k}''|=|\boldsymbol{k}'|$.

We now simplify this last equation using the *addition theorem for spherical harmonics*

$$\sum_{\mu} Y_{l\mu}(\theta''\phi'')^* \, Y_{l\mu}(\theta'\phi') = \frac{2l+1}{4\pi} P_l(\cos\vartheta)\,, \tag{3.125}$$

where P_l is the usual Legendre polynomial[13] of order $l = 0, 1, 2, \cdots$ while ϑ denotes the angle between the vectors $\boldsymbol{k}''$ and $\boldsymbol{k}'$ whose directions are specified by the polar angles θ'', ϕ'' and θ', ϕ', respectively. We also replace $T_{\boldsymbol{k}''\boldsymbol{k}'}$ by its equivalent in terms of $f(\boldsymbol{k}' \to \boldsymbol{k}'')$ [see Eqs. (3.58) and (3.81)]. The final result is

$$f(\boldsymbol{k}' \to \boldsymbol{k}'') = f(k,\vartheta) = \frac{1}{2\imath k} \sum_{l=0}^{\infty} (2l+1)\,(e^{2\,\imath\,\delta_l(k)} - 1)\, P_l(\cos\vartheta)\,. \tag{3.126}$$

This is sometimes called the *partial wave expansion* of the scattering amplitude because it breaks the latter up into contributions from different angular momenta in the wave. Each partial amplitude depends on one parameter, δ_l, which itself depends only on k.

Exercises:

1. Calculate the differential scattering cross section in terms of phase-shifts. What is the condition on the δ_l as functions of l for the series to converge for small angle ϑ?

2. Calculate the total cross section in terms of the δ_l. Show that each partial wave contributes separately. What is the condition on the δ_l as functions of l for this series to converge?

3. Show rigorously that for $\vartheta \neq 0$ one can ignore the "1" in the factor $(e^{2\,\imath\,\delta_l(k)} - 1)$, and that consequently the differential scattering cross section really depends only on the differences $\delta_l - \delta_0$. Thus divergence of all the δ_l does not preclude a finite differential or total cross section.

4. Check that the optical theorem is satisfied by Eq. (3.126).

[13] named after Adrien-Marie Legendre (1752-1833), distinguished French mathematician who did a great deal of work on elliptic functions and number theory. He invented the Legendre transformations used in thermodynamics and quantum field theory as well as the least-squares method (independently of Gauss).

3.2.10 Interpretation of the $\delta_l(k)$ as phase shifts

We now show that the δ_l are phase shifts associated with the action of the potential on the scattered wave. The (time independent) Schrödinger equation for the scattering wave in the presence of a spherically symmetric potential $V(r)$ can be written as

$$-\frac{\hbar^2}{2m}\Delta u_{\boldsymbol{k}}^{(+)} + V(r)\, u_{\boldsymbol{k}}^{(+)} = E\, u_{\boldsymbol{k}}^{(+)}\,. \tag{3.127}$$

If the polar coordinate axis is chosen in the direction of $\boldsymbol{k}$, $u_{\boldsymbol{k}}^{(+)}$ depends only on r and ϑ, so that $u_{\boldsymbol{k}}^{(+)}$ can be expanded in Legendre polynomials:

$$u_{\boldsymbol{k}}^{(+)}(r,\vartheta) = \sum_{l=0}^{\infty} u_l(r)\, P_l(\cos\vartheta)\,. \tag{3.128}$$

Substituting this expansion in Eq. (3.127) and separating out the terms which contain a factor $P_l(\vartheta)$ gives the radial equation

$$\frac{d^2u_l}{dr^2} + \frac{2}{r}\frac{du_l}{dr} + \frac{l(l+1)}{r^2}u_l - \frac{2mV(r)}{\hbar^2}\,u_l + k^2\,u_l = 0\,. \tag{3.129}$$

Thus for each l the radial function u_l is determined autonomously.

When $V = 0$ the solution of Eq. (3.129) which is regular at the origin is the spherical Bessel function $j_l(kr)$. The second solution is the spherical Neumann function $n_l(kr)$. Asymptotically

$$j_l(kr) \overset{r\to\infty}{\longrightarrow} \frac{\sin(kr - l\pi/2)}{kr}; \qquad n_l(kr) \overset{r\to\infty}{\longrightarrow} -\frac{\cos(kr - l\pi/2)}{kr}\,. \tag{3.130}$$

With $V(r) \neq 0$ the solutions are, of course more complicated. But it is clear that the physical solution at radii outside the range of the potential must approach a linear combination of $j_l(kr)$ and $n_l(kr)$ with asymptotics

$$u_l \overset{r\to\infty}{\longrightarrow} \alpha_l\, \frac{\sin(kr - l\pi/2 + \gamma_l)}{kr}\,, \tag{3.131}$$

where α_l, γ_l are real constants. In view of this Eq. (3.128) gives the asymptotics

$$u_{\boldsymbol{k}}^{(+)} \overset{r\to\infty}{\longrightarrow} \sum_{l=0}^{\infty} \alpha_l \left[\frac{e^{\imath(kr - l\pi/2 + \gamma_l)}}{2\imath kr} - \frac{e^{\imath(-kr + l\pi/2 - \gamma_l)}}{2\imath kr}\right] P_l(\cos\vartheta)\,. \tag{3.132}$$

Now let us work out the asymptotics of $u_{\boldsymbol{k}}^{(+)}(\boldsymbol{r})$ by an alternative route. Recall that, with the polar axis taken along $\boldsymbol{k}$, the asymptotic form of the scattering wave $u_{\boldsymbol{k}}^{(+)}$ (normalization ignored) is

$$u_{\boldsymbol{k}}^{(+)} \sim e^{\imath kr\cos\vartheta} + \frac{f(k,\vartheta)}{r}\, e^{\imath kr}\,. \tag{3.133}$$

Substituting the *identity*

$$e^{\imath kr\cos\vartheta} = \sum_{l=0}^{\infty}(2l+1)\,\imath^l\, j_l(kr)P_l(\cos\vartheta) \tag{3.134}$$

together with the obvious expansion (appropriate for any function of ϑ)

$$f(k,\vartheta) = \sum_{l=0}^{\infty} f_l(k)\, P_l(\cos\vartheta), \tag{3.135}$$

replacing $j_l(kr)$ by its asymptotic form (3.130), and expressing the sine in terms of imaginary exponentials gives

$$u_{\boldsymbol{k}}^{(+)} \overset{r\to\infty}{\longrightarrow} \sum_{l=0}^{\infty}\left[\left(\frac{(2l+1)}{2\imath kr} + \frac{f_l}{r}\right)e^{\imath kr} - \frac{(2l+1)\,\imath^{2l}}{2\imath kr}e^{-\imath kr}\right]P_l(\cos\vartheta)\,. \tag{3.136}$$

Of course, forms (3.132) and (3.136) must agree, which means that the coefficients of the term of form $e^{\imath kr}P_l(\cos\vartheta)$ in both series must agree as must the coefficients of the term $e^{-\imath kr}P_l(\cos\vartheta)$. This tells us that

$$\alpha_l = (2l+1)\imath^l e^{\imath\,\gamma_l}\,; \qquad f_l = \frac{(2l+1)(e^{2\,\imath\,\gamma_l}-1)}{2\imath k}\,. \tag{3.137}$$

We notice that the series (3.135) with the f_l we have just obtained reproduces our older result Eq. (3.126) provided $\gamma_l = \delta_l$. We adopt this.

The scattering wave (3.132) gives us a novel way of looking at scattering which contrasts with that suggested by the form (3.133). We see an ingoing wave $e^{-\imath kr}/kr$ with phase $-\delta_l$ which is converted into an outgoing wave $e^{\imath kr}/kr$ which now carries phase δ_l. The effect of the scattering is to advance the phase of the scattered wave by $2\delta_l$, which according to Eq. (3.104), is just the lth eigenvalue of the S-matrix. We thus understand why half a S-matrix eigenvalue is called a *phase shift*.

In accordance with the results of Exercises 1 and 2 of Sec. 3.2.9, the partial wave expansions for the small angle scattering amplitude and for the total cross section converge under certain conditions on the higher order $\delta_l(k)$. Without going into derivations we can state that when the potential has a sharp or a very rapid cutoff, both series converge. If the potential falls off asymptotically as $1/r^3$ or slower, the series for $f(0)$ diverges (very strong forward scattering). If the potential falls off asymptotically as $1/r^2$ or slower, the partial wave expansion for the total cross section also diverges. Finally, if the potential falls off as 1/r or slower, the phase shifts themselves diverge. This is the case of the Coulomb potential; as shown by Exercise 3 the infinite phase shifts can be handled, and appropriate calculations show that $d\sigma/d\Omega$ is finite (except, of course, for $\vartheta = 0$), as first shown classically by Lord Rutherford.[14]

3.2.11 S-wave scattering

In classical terms if a particle has momentum $\boldsymbol{p}$ and passes a distance d from the center of the potential (the origin), it has orbital angular momentum $l = d\,p$ with respect to it. Substantial scattering will occur if d is not much larger than the potential's range b. In QT orbital angular momentum is quantized ($\hat{\boldsymbol{l}}^2 = l(l+1)\hbar^2$ with l integer). Thus from the semiclassical viewpoint scattering with wave vector k will occur in the $l = 0$ state provided $\hbar kb \ll \hbar$. Thus when $kb \ll 1$ (which means the incident particle's wavelength exceeds the range of the potential), we say that the scattering is purely S-wave scattering (in QT an $l = 0$ state is said to be an S-state).

Let us consider S-wave scattering on a spherically symmetric potential with range b. We may thus retain in $f(k, \vartheta)$, as given by Eq. (3.126), only the $l = 0$ term, namely

$$f(k) = \frac{e^{2\imath\delta_0(k)} - 1}{2\imath k} \tag{3.138}$$

[14]Ernst, 1st Baron Rutherford of Nelson (1871-1937), was a New Zealand-British experimental physicist and Nobel Laureate. He worked out the differential cross section for Coulomb scattering, on the basis of which he inferred the existence of the atomic nucleus from H. Geiger and E. Marsden's gold foil experiment. In cooperation with F. Soddy he discovered the laws of radioactive decay. He was also the first to carry out a nuclear reaction in the laboratory (in which chemical elements were transmuted). At least four of his students received Nobel prizes.

since $P_0(\cos\vartheta) = 1$. Thus S-wave scattering is always spherically symmetric. The only question is its dependence on k.

For ease of calculation we shall suppose that the potential is *strictly zero* for $r > b$. The radial eigenfunction $u_0(r)$ will have a definite value of its logarithmic derivative as $r = b$ is approached from inside (from $r < b$):

$$D_0(k) = \frac{du_0/dr}{u_0}\Big|_{r\to b_-} = \frac{d}{dr}\ln u_0\Big|_{r\to b_-} . \tag{3.139}$$

We know that for $r > b$ u_0 must be a linear combination of $j_0(kr)$ and $n_0(kr)$. It is easy to see that outside the range of the potential Eq. (3.129) for $l = 0$ has the obvious pair of solutions $\sin(kr)/kr$ and $\cos(kr)/kr$. Comparing these with the asymptotics (3.130) we realize that

$$j_0(kr) = \frac{\sin(kr)}{kr}; \qquad n_0(kr) = -\frac{\cos(kr)}{kr} . \tag{3.140}$$

The linear combination of these two with the correct asymptotics (3.131) is

$$u_0(r) = \alpha_0 \frac{\sin(kr + \delta_0)}{kr} . \tag{3.141}$$

Calculating the logarithmic derivative of this (which is insensitive to the value of α_0) at $r \to b_+$ and equating it to $D_0(k)$ (both wave function and its first derivative must be continuous) gives

$$\frac{\tan(kb + \delta_0)}{k} = \frac{b}{bD_0(k) + 1} , \tag{3.142}$$

which determines δ_0 implicitly.

Barring a coincidence the denominator $bD_0(k) + 1$ should not vanish as $k \to 0$. Thus it is plain that δ_0 must be of $\mathcal{O}(k)$, and for small kb we may replace the tangent by its argument. Replacing as well D_0 by $D(0)$ gives

$$\delta_0 = -kb \frac{bD_0(0)}{bD_0(0) + 1} + \mathcal{O}(k^2) . \tag{3.143}$$

To the same approximation we have from Eq. (3.138)

$$f = -a \equiv -b \frac{bD_0(0)}{bD_0(0) + 1} , \tag{3.144}$$

a constant! The quantity a is called Fermi's scattering length. Thus the cross section for S-wave scattering (or low energy scattering) is just $4\pi a^2$, independent of energy.

The method used here can be applied to calculate other δ_l as well.

3.2.12 The Born approximation

Let us go back to potentials which need not be spherically symmetric. The formula (3.81) for $f(\boldsymbol{k}' \to \boldsymbol{k}'')$ is not explicit because we do not *a priori* know $u_{\boldsymbol{k}}^{(+)}(\boldsymbol{r})$. This function is determined by the Lippmann-Schwinger integral equation (3.70). As usual we can solve such an equation by iteration. The first approximation is $u_{\boldsymbol{k}}^{(+)}(\boldsymbol{r}) = (2\pi)^{-3/2} \exp(\imath \boldsymbol{k} \cdot \boldsymbol{r})$. If we already use this in formula (3.81) we get Born's first approximation to the scattering amplitude:

$$f_{\mathrm{B}}(\boldsymbol{k} \to \boldsymbol{k}') = -\frac{m}{2\pi\hbar^2} \int e^{\imath(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}\, V(\boldsymbol{r})\, d^3r\,. \tag{3.145}$$

We would get Born's second approximation by substituting our first approximation for $u_{\boldsymbol{k}}^{(+)}(\boldsymbol{r})$ in the r.h.s. of the Lippman-Schwinger equation which would then give us a second order approximation for $u_{\boldsymbol{k}}^{(+)}(\boldsymbol{r})$. This in formula (3.81) would yield Born's second order approximation, and so on.

We notice from formula (3.145) that the scattering amplitude is proportional to the 3-D Fourier transform of the potential $V(\boldsymbol{r}')$ with $\boldsymbol{q} \equiv \boldsymbol{k} - \boldsymbol{k}'$ as the Fourier variable ($\hbar\boldsymbol{q}$ is called the *momentum transfer*). This is important: if the first Born approximation is accurate and the scattering amplitude can be measured accurately (including its phase) for an extensive range of momentum transfers, then inversion of the Fourier transform will give the potential doing the scattering. This has been the basis for many investigations into atomic, molecular and nuclear structure.

When the potential is spherically symmetric, Eq. (3.145) simplifies. Let us choose our z axis along the vector $\boldsymbol{q}$ and write $\boldsymbol{q} \cdot \boldsymbol{r} = qru$ with $q = |\boldsymbol{q}|$ and $u = \cos\theta$. Then

$$f_{\mathrm{B}}(\boldsymbol{k} \to \boldsymbol{k}') = -\frac{m}{\hbar^2} \int_0^\infty dr\, V(r)\, r^2 \int_{-1}^1 du\, e^{\imath qru} = -\frac{2m}{q\hbar^2} \int_0^\infty V(r)\, \sin(qr)\, r\, dr\,. \tag{3.146}$$

Finally we note that since $|\boldsymbol{k}'| = |\boldsymbol{k}|$ we have $|\boldsymbol{q}|^2 = 2k^2(1-\cos\vartheta) = 4k^2\sin^2(\vartheta/2)$ where again ϑ is the angle between $\boldsymbol{k}'$ and $\boldsymbol{k}$. Thus finally

$$f_{\mathrm{B}}(\boldsymbol{k}\to\boldsymbol{k}') = -\frac{m}{k\hbar^2\sin(\vartheta/2)}\int_0^\infty V(r)\,\sin\big(2kr\sin(\vartheta/2)\big)\,r\,dr\,, \qquad (3.147)$$

in harmony with Eq. (3.97). We note that in first Born approximation and for spherical symmetry f is always real. This results shows that the approximation is never perfect since according to the optical theorem we would expect the total cross section to be zero, yet $|f(k,\vartheta)|^2 > 0$ here.

So when is the first Born approximation—commonly called just *Born approximation*—a good approximation? That is, when is the second term on the r.h.s. of Eq. (3.70) with $u^{(+)}_{\boldsymbol{k}}(\boldsymbol{r}')$ replaced by $(2\pi)^{-3/2}\exp(\imath\boldsymbol{k}\cdot\boldsymbol{r}')$ negligible compared to $(2\pi)^{-3/2}\exp(\imath\boldsymbol{k}\cdot\boldsymbol{r})$. We make the comparison simpler if we compare just the moduli of the two terms. Further, since the second term is likely to be largest near the center of the potential, we evaluate the Green function $g^{(+)}_k(\boldsymbol{r},\boldsymbol{r}')$ in Eq. (3.78) at $\boldsymbol{r}=0$. The criterion can be put in two forms. For arbitrary potential

$$\frac{1}{2\pi}\left|\int\frac{e^{\imath kr}}{r}\,e^{\imath\boldsymbol{k}\cdot\boldsymbol{r}}\,V(\boldsymbol{r})\,d^3r\right| \ll \frac{\hbar^2}{m}\,. \qquad (3.148)$$

For spherically symmetric potential

$$\left|\int_0^\infty dr\,V(r)\,r\int_{-1}^1 du\,e^{\imath kr(1+u)}\right| = \frac{1}{k}\left|\int_0^\infty dr(e^{2\imath kr}-1)V(r)\right| \ll \frac{\hbar^2}{m}\,. \qquad (3.149)$$

It may be seen that both conditions will become satisfied for sufficiently large k (sufficiently large $\varepsilon_{\boldsymbol{k}}$). In Eq. (3.148) this happens because the exponential oscillates rapidly over most of the $\boldsymbol{r}$ domain. In Eq. (3.149) there is a term without exponential but its integral is suppressed by the k in the denominator. Thus whether the potential is spherically symmetric or not, Born approximation will become the more accurate the higher the energy of the incident particle. This is reasonable physically because, at high energies, the incident plane wave is little distorted by the much weaker potential, so that one can take $u^{(+)}_{\boldsymbol{k}}(\boldsymbol{r})$ in Eq. (3.81) to be a plane wave, as done in Born approximation.

Example: The Yukawa potential

This is a potential which played a role in Yukawa's[15] theory of the strong force by meson exchange. Whereas Coulomb's potential is the solution of Poisson's equation with a delta function source, Yukawa's potential is the corresponding solution of the von Helmholtz equation (3.68):

$$V(r) = A\,\frac{e^{-r/r_0}}{r} \tag{3.150}$$

where r_0 is called the range of the potential since $|V(r)| \ll |A|$ for $r \gg r_0$. The Yukawa potential describes approximately the force between a nucleus and an incoming neutron, as well as the screened Coulomb potential of the nucleus of a multi-electron atom felt by an incoming electron.

Application of formula (3.147) gives

$$f_{\mathrm{B}}(\boldsymbol{k} \to \boldsymbol{k}') = f_{\mathrm{B}}(k, \vartheta) = -\frac{2mA}{\hbar^2(4k^2\sin^2(\vartheta/2)) + 1/r_0{}^2)}\,. \tag{3.151}$$

Exercises:

1. Verify the result (3.151).

2. Using Eq. (3.149) work out the exact criterion for precision of formula (3.151) in terms of A, r_0 and k?

3. Calculate the *total* cross section for the Yukawa potential's f in the Born approximation.

4. Compare the total cross section for scattering from a Coulomb potential in Born approximation with Lord Rutherford's classical formula. The exact quantum-mechanical result is identical to this last. Is the Born approximation exact in this case? Explain.

[15] Hideki Yukawa (1907-1981) was the first Japanese Nobel Laureate. He devised the notion that the nuclear (strong) forces are mediated by a particle with mass of about 200 electrons; the corresponding π meson was discovered later. Yukawa's conception that a messenger particle mediates the fundamental force between elementary particles is nowadays standard in quantum field theory.

5. Set an algebraic approximate bound on the depth of $V(r)$ in terms of its range b so that the Born approximation be accurate when $1/k \gg b$. What is the bound for $1/k \ll b$?

6. For an arbitrary $V(\boldsymbol{r})$ find a symmetry of $f_{\mathrm{B}}(\boldsymbol{k} \to \boldsymbol{k}')$ different from those discussed in Sec. 3.2.7 for the exact $f(\boldsymbol{k} \to \boldsymbol{k}')$.

7. Scattering occurs in a static real potential with $V(\boldsymbol{r}) = V(-\boldsymbol{r})$. What new can you say about $f_{\mathrm{B}}(\boldsymbol{k} \to \boldsymbol{k}')$?

Chapter 4

Quantum theory and magnetic fields

Some of the conclusions we have reached so far are modified when the potential in Schrödinger's equation is supplemented by an external magnetic field. Charged particles in just such a field have their energy levels quantized in a simple way. The effects of magnetic moments must be taken into account. Effects of a topological nature appear for the first time. These novelties are closely bound up with the fact that a (electro)magnetic field is a gauge field. Some of the insights in this chapter apply to systems comprising other gauge fields.

4.1 Gauge invariance

Gauge invariance or symmetry is a dominant theme in modern theoretical physics. It is the guiding principle for formulating good theories for the elementary interaction, and has been successful in the unification of electromagnetism with the weak interaction, in the theory of the strong interaction, and even in the understanding of gravitation. Speculations about further interactions always begin from gauge invariance.

4.1.1 Gauge invariance in classical electromagnetism

Maxwell's electromagnetic equations are written in terms of electric and magnetic fields, $\boldsymbol{E}, \boldsymbol{B}$. But it is well known that the sourceless (Faraday and magnetic Gauss) equations (with $\dot{}$ meaning $\partial/\partial t$),

$$\boldsymbol{\nabla} \times \boldsymbol{E} + c^{-1}\dot{\boldsymbol{B}} = 0; \qquad \boldsymbol{\nabla} \cdot B = 0\,, \tag{4.1}$$

are identically satisfied if we write $\boldsymbol{E}, \boldsymbol{B}$ in terms of potentials $\boldsymbol{A}, \Phi$:

$$\boldsymbol{E} = -\boldsymbol{\nabla}\Phi - c^{-1}\dot{\boldsymbol{A}}; \qquad \boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}\,. \tag{4.2}$$

The choice of potential is not unique; any change of the form

$$\boldsymbol{A} \to \boldsymbol{A}' \equiv \boldsymbol{A} + \nabla\lambda; \qquad \Phi \to \Phi' \equiv \Phi - c^{-1}\dot{\lambda}\,, \tag{4.3}$$

where $\lambda(\boldsymbol{r}, t)$ is an arbitrary function, leaves $\boldsymbol{E}, \boldsymbol{B}$ invariant. This transformation is called, after Weyl, a *gauge transformation*. It is useful to regard this *gauge invariance* as an internal symmetry of electromagnetism, and pursue the consequences.

The sources of $\boldsymbol{E}, \boldsymbol{B}$ are (moving) electric charges. Hence we must consider their coupling to electromagnetism. How should we modify the usual one-particle Lagrangian $L_0 = \frac{1}{2}m\dot{\boldsymbol{r}}^2 - V(\boldsymbol{r}, t)$ to take into account this coupling (V is here regarded as representing nonelectromagnetic forces)? Obviously we must add terms containing both $\boldsymbol{r}, \dot{\boldsymbol{r}}$ as well electromagnetic variables. The unique prescription that preserves gauge invariance after the coupling is

$$L = \frac{1}{2}m\dot{\boldsymbol{r}}^2 - V(\boldsymbol{r}, t) + e(-\Phi + c^{-1}\,\dot{\boldsymbol{r}} \cdot \boldsymbol{A})\,, \tag{4.4}$$

where e is a constant, identified with the charge of the particle. Under the change (4.3) the Lagrangian changes by the addition of $(e/c)(\dot{\lambda} + \dot{\boldsymbol{r}} \cdot \nabla\lambda) = (e/c)d\lambda/dt$. Now addition of a perfect derivative to a Lagrangian does not change the equations of motion, so with the choice (4.4) the mechanics of charged particles are gauge invariant. No other choice of L will do so well.

The *canonical momentum* of the charge particle is

$$\boldsymbol{P} = \frac{\partial L}{\partial \dot{\boldsymbol{r}}} = \boldsymbol{p} + (e/c)\boldsymbol{A}\,, \tag{4.5}$$

where $\boldsymbol{p}$ denotes the *kinematic momentum* $m\dot{\boldsymbol{r}}$.

The Hamiltonian for the charged particle is

$$H = \boldsymbol{P}\cdot\dot{\boldsymbol{r}} - L = \tfrac{1}{2}m\dot{\boldsymbol{r}}^2 + \Phi\,. \tag{4.6}$$

But, of course, H must be expressed as a function of $\boldsymbol{P}$ and $\boldsymbol{r}$ so

$$H = \frac{\big[\boldsymbol{P} - (e/c)\boldsymbol{A}(\boldsymbol{r},t)\big]^2}{2m} + e\Phi(\boldsymbol{r},t)\,. \tag{4.7}$$

It may be seen that under a gauge transformation

$$\boldsymbol{P} \to \boldsymbol{P} + (e/c)\boldsymbol{\nabla}\lambda; \qquad H \to H - (e/c)\dot{\lambda}\,. \tag{4.8}$$

But although the Hamiltonian changes under time dependent gauge transformations, the particle's equation of motion is invariant in form (*covariant*) because L is essentially gauge invariant. All this is fully classical; we now turn to QT.

Exercises:

1. Derive from the Lagrangian (4.4) the classical equation of motion for a charge in the presence of $\boldsymbol{E},\boldsymbol{B}$ fields, including the Lorentz force.

4.1.2 Schrödinger's equation in a magnetic field

How to write the Schrödinger equation in the presence of a magnetic field? The rule is always the same: the equation is Eq. (1.90) but we must still work out the relevant form of $\hat{H}$. Classical physics is a good guide. We turn H in Eq. (4.7) into $\hat{H}$ by replacing the classical $\boldsymbol{r}$ by an Hermitian operator $\hat{\boldsymbol{r}}$ and replacing the classical $\boldsymbol{P}$ by the operator $(\hbar/\imath)\boldsymbol{\nabla}$. It is $\boldsymbol{P}$ rather than $\boldsymbol{p}$ that is represented by $(\hbar/\imath)\boldsymbol{\nabla}$ because in classical mechanics the components of $\boldsymbol{P}$ are canonically conjugate to the corresponding ones of $\boldsymbol{r}$, and Dirac's rule requires that $\{x, P_x\}_P = 1$ go over to $[\hat{x}, \hat{P}_x] = \imath\hbar$, which in turn requires that $\hat{P}_x = (\hbar/\imath)\,\partial/\partial x$. Thus

$$\hat{H} = \frac{\big[(\hbar/\imath)\boldsymbol{\nabla} - (e/c)\boldsymbol{A}(\hat{\boldsymbol{r}},t)\big]^2}{2m} + e\Phi(\hat{\boldsymbol{r}},t)\,. \tag{4.9}$$

The above procedure avoids a common ambiguity. Often quantization by replacing $\boldsymbol{r} \to \hat{\boldsymbol{r}}$ and $\boldsymbol{P} \to (\hbar/\imath)\boldsymbol{\nabla}$ can produce a terms like $\hat{\boldsymbol{r}}(\hbar/\imath)\boldsymbol{\nabla}$ which is not Hermitian and also is different from the alternative $(\hbar/\imath)\boldsymbol{\nabla}\,\hat{\boldsymbol{r}}$. In such cases one uses instead the symmetrized product (the arithmetic average of both options), which is Hermitian. Our classical Hamiltonian (4.7) includes the cross terms $\boldsymbol{A}(\boldsymbol{r})\boldsymbol{P} + \boldsymbol{P}\boldsymbol{A}(\boldsymbol{r})$ and upon quantization the symmetrization occurs automatically. The $\hat{H}$ is Hermitian and unambiguous.

The Schrödinger equation for a quantum charged particle in a magnetic field is thus

$$\imath\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r},t) = -\frac{\hbar^2}{2m}\big[(\boldsymbol{\nabla} - \frac{\imath e}{\hbar c}\boldsymbol{A}(\boldsymbol{r},t)\big]^2\psi(\boldsymbol{r},t) + e\Phi(\boldsymbol{r},t)\,\psi(\boldsymbol{r},t)\,. \tag{4.10}$$

Since $\boldsymbol{A}$ and Φ enter directly we must ask: is the form of this equation gauge invariant? At first sight it does not look so. But then we realize that ψ itself might change under the gauge transformation. In fact let us assume that concurrent with Eq. (4.3)

$$\psi \to \psi' \equiv e^{(\imath e\lambda/\hbar c)}\,\psi\,. \tag{4.11}$$

Now consider now the two differential operators

$$\begin{aligned}
\hat{D}_t &\equiv e^{(\imath e\lambda/\hbar c)}\left(\imath\hbar\frac{\partial}{\partial t} - e\Phi\right)e^{-(\imath e\lambda/\hbar c)} = \left(\imath\hbar\frac{\partial}{\partial t} - e\Phi + \frac{e}{c}\dot{\lambda}\right) = \left(\imath\hbar\frac{\partial}{\partial t} - e\Phi'\right);\\
\hat{D}_r &\equiv e^{(\imath e\lambda/\hbar c)}\left(\boldsymbol{\nabla} - \frac{\imath e}{\hbar c}\boldsymbol{A}\right)e^{-(\imath e\lambda/\hbar c)} = \left(\boldsymbol{\nabla} - \frac{\imath e}{\hbar c}\boldsymbol{A} - \frac{\imath e}{\hbar c}\boldsymbol{\nabla}\lambda\right) = \left(\boldsymbol{\nabla} - \frac{\imath e}{\hbar c}\boldsymbol{A}'\right).
\end{aligned} \tag{4.12}$$

If we multiply Eq. (4.10) by $e^{(\imath e\lambda/\hbar c)}$ on the left and rewrite ψ in terms of ψ' by Eq. (4.11), we can write the result as

$$\hat{D}_t\,\psi' = -\frac{\hbar^2}{2m}\hat{D}_r{}^2\,\psi'\,. \tag{4.13}$$

Now substituting in this the rightmost forms of the operators in Eqs. (4.12) gives back Schrödinger's equation but with $\Phi \mapsto \Phi', \boldsymbol{A} \mapsto \boldsymbol{A}'$ and $\psi \mapsto \psi'$. That is, Schrödinger's equation does not change its form when all quantities in it undergo a gauge transformation. In short, Schrödinger's equation is *gauge covariant*. The gauge transformation of Eqs. (4.3) and (4.11) is an internal symmetry of the Schrödinger equation.

It is obvious that the matrix element $\int \psi^* f(\hat{\boldsymbol{r}})\,\phi\, d^3r$ [or the mean value of $f(\hat{\boldsymbol{r}})$] is invariant under any gauge transformation: the phases appearing according to Eq. (4.11) cancel each other. What about $\int \psi^*\,\hat{\boldsymbol{p}}\,\phi\, d^3r$? By the quantized version of Eq. (4.5)

$$\hat{\boldsymbol{p}} = e^{-(\imath e\lambda/\hbar c)}\,\frac{\hbar}{\imath}\hat{D}_r\, e^{(\imath e\lambda/\hbar c)}\,. \tag{4.14}$$

Hence using Eqs. (4.12) again

$$\int \psi^*\,\hat{\boldsymbol{p}}\,\phi\, d^3r = \int \psi'^*\,\frac{\hbar}{\imath}\hat{D}_r\,\phi'\, d^3r = \int \psi'^*\,\frac{\hbar}{\imath}\left(\boldsymbol{\nabla} - \frac{\imath e}{\hbar c}\boldsymbol{A}'\right)\,\phi'\, d^3r\,. \tag{4.15}$$

On the r.h.s. is the matrix element, with respect to the transformed wave functions, of $\hat{\boldsymbol{p}}$ written in the new gauge. Thus any matrix element of kinematic momentum is gauge invariant. Exercise 1 shows that the same is true for any analytic $f(\hat{\boldsymbol{p}})$. The same is obviously true for any expectation value of $f(\hat{\boldsymbol{p}})$. The upshot of all this is that results of measurements and calculated transition amplitudes are all gauge invariant.

What happens to the propagator or the Green functions under a gauge transformation? Recall that the path integral is

$$K(\boldsymbol{r},t;\boldsymbol{r}_0,t_0) = \mathcal{N}\int_{\text{paths}} \mathcal{D}[\boldsymbol{r}(t)]\,\exp\left(\frac{\imath}{\hbar}\int_{t_0}^{t} L\left(\dot{\boldsymbol{r}}(t'),\boldsymbol{r}(t'),t'\right)\,dt'\right). \tag{4.16}$$

But immediately after Eq. (4.4) we found that a gauge transformation adds to the Lagrangian a contribution $(e/c)d\lambda\left(\boldsymbol{r}',t'\right)/dt'$. Thus the action changes by $(e/c)\left[\lambda(\boldsymbol{r},t) - \lambda(\boldsymbol{r}_0,t_0)\right]$, i.e. it changes by a term depending only on the common endpoints of all paths. Thus the exponential of this change can be taken outside the path integral. As a result we have the law of transformation

$$K(\boldsymbol{r},t;\boldsymbol{r}_0,t_0) \to K'(\boldsymbol{r},t;\boldsymbol{r}_0,t_0) \equiv e^{[\imath e\lambda(\boldsymbol{r},t)/\hbar c]}\,K(\boldsymbol{r},t;\boldsymbol{r}_0,t_0)\,e^{-[\imath e\lambda(\boldsymbol{r}_0,t_0)/\hbar c]}\,. \tag{4.17}$$

Therefore,

$$\begin{aligned}\psi'(\boldsymbol{r},t) &= \int K'(\boldsymbol{r},t;\boldsymbol{r}_0,t_0)\,\psi'(\boldsymbol{r}_0,t_0)\,d^3r_0 \qquad (4.18)\\ &= e^{[\imath e\lambda(\boldsymbol{r},t)/\hbar c]}\int K(\boldsymbol{r},t;\boldsymbol{r}_0,t_0)\,\psi(\boldsymbol{r}_0,t_0)\,d^3r_0 = e^{[\imath e\lambda(\boldsymbol{r},t)/\hbar c]}\,\psi(\boldsymbol{r},t)\,.\end{aligned}$$

Thus the mentioned phases make the propagation equation (2.2) consistent with the law (4.11) and hence gauge covariant. This is entirely consistent with the gauge covariance of Schrödinger' equation.

Why is gauge invariance/covariance so important? Because it represents a sort of internal symmetry of physical systems. Some quantity is changed, but this does not lead to a change in the physics of the situation. This fact imposes great restrictions on the structure of the theory: it is easier to guess the form of the equations if they are restricted by gauge covariance considerations.

Exercises:

1. If $f(x)$ is an analytic function, show that all the matrix elements of the operator $f(\hat{\boldsymbol{p}})$ for a charged particle in an electromagnetic field are gauge invariant.

4.2 Applications of gauge invariance

4.2.1 Charge in magnetic field: Landau's problem

The simplest QT problem in a magnetic field is that of a spinless electron (charge $-|e|$ and mass m) subject to no other forces than the electromagnetic one. For uniform magnetic field the problem was first solved by Landau.[1] Let us assume the field, of strength B, points in the z direction. There are various choices for $\boldsymbol{A}, \Phi$; we choose here

$$\Phi = 0; \qquad \boldsymbol{A} = (A_x, A_y, A_z) = (-By, 0, 0) \tag{4.19}$$

[1] Russian-Jewish Nobel Laureate Lev Davidovich Landau (1908-1968) is widely regarded as the salient theoretical physicist of the Soviet Union period. He developed the quantum mechanical theory of diamagnetism, invented the density matrix concept, developed (with V. Ginzburg) the phenomenological theory of superconductivity and with (E. Lifshitz) the general theory of 2nd order phase transitions. He also elucidated the eponymous damping of plasma waves, developed a theory of superfluid Helium and the quasiparticle theory of the Fermi liquid, and contributed greatly to quantum electrodynamics and to particle physics. Landau was famous as a teacher.

Consequently the Schrödinger equation is

$$\imath\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r},t) = -\frac{\hbar^2}{2m}\left[\left(\frac{\partial}{\partial x}+\frac{\imath|e|}{\hbar c}By\right)^2+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right]\psi(\boldsymbol{r},t)\,. \tag{4.20}$$

There is translational symmetry in the x and z direction, so we should find solutions which are plane waves propagating in the plane perpendicular to the z axis. In addition, the Hamiltonian here is stationary, so we can look for energy eigenfunctions. Thus

$$\psi = C\,e^{\imath(P_x\,x+P_z\,z)/\hbar}\,e^{-\imath E/\hbar}\,\chi(y), \tag{4.21}$$

where P_x and P_z are real constants. Substituting this anstz into Eq. (4.20) gives

$$E\chi = -\frac{\hbar^2}{2m}\frac{d^2\chi}{dy^2}-\frac{\hbar^2}{2m}\left(\frac{\imath P_x}{\hbar}+\frac{\imath|e|}{\hbar c}By\right)^2\chi+\frac{P_z^2}{2m}\chi\,. \tag{4.22}$$

We may introduce the notation

$$y_0 = -(cP_x/|e|B) \tag{4.23}$$

in terms of which

$$-\frac{\hbar^2}{2m}\frac{d^2\chi}{dy^2}+\tfrac{1}{2}m\left(\frac{|e|B}{mc}\right)^2(y-y_0)^2\chi = \left(E-\frac{P_z^2}{2m}\right)\chi\,. \tag{4.24}$$

This last is the Schrödinger equation for an harmonic oscillator of mass m, frequency $\omega = (|e|B/mc)$ and energy $E - P_x^2/(2m)$. In view of Eq. (2.65) we have here

$$E_n = \frac{P_z^2}{2m}+\left(n+\tfrac{1}{2}\right)\frac{|e|\hbar B}{mc};\qquad n=0,1,2,\cdots \tag{4.25}$$

which are called the *Landau levels*. And of course the y depending factor of the eigenfunction in the magnetic field is $\chi_n(y)$, the n-th level energy eigenfunction of the harmonic oscillator with $\omega = (|e|B/mc)$. The full eigenfunction is

$$\psi(x,y,z,t) = Ae^{\imath(P_x\,x+P_z\,z)/\hbar}\,e^{-\imath E_n(P_z)\,t/\hbar}\,\chi_n(y)\,. \tag{4.26}$$

We observe here a large degeneracy: for fixed n and P_z we have one energy level, but an infinite number of eigenfunctions distinguished by the value of P_x. We can understand this by correspondence with the classical picture. Classically a charge moves in a circular spiral wound around the direction of the magnetic field. Its conserved energy determines the radius of the spiral, and its P_z the pitch. For a given energy there are many orbits depending where in a plane normal to the field we locate the axis of the spiral. This multiplicity is the classical analogue of the mentioned quantum degeneracy.

Example: Landau's problem in symmetric gauge

Suppose we choose instead the "symmetric" gauge

$$\Phi = 0; \qquad \boldsymbol{A} = \tfrac{1}{2}\boldsymbol{B} \times \boldsymbol{r} = \Big(-\tfrac{1}{2}By, \tfrac{1}{2}Bx, 0 \Big) . \tag{4.27}$$

The Schrödinger equation now takes the form

$$\imath\hbar \frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\left[\left(\frac{\partial}{\partial x} + \frac{\imath|e|}{2\hbar c}By \right)^2 + \left(\frac{\partial}{\partial y} - \frac{\imath|e|}{2\hbar c}Bx \right)^2 + \frac{\partial^2}{\partial z^2} \right] \psi . \tag{4.28}$$

We can rewrite this as

$$\imath\hbar \frac{\partial}{\partial t}\psi = \left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} + \tfrac{1}{2}m\tilde{\omega}^2(x^2+y^2) \right) - \frac{|e|B}{2mc}\,\hat{l}_z \right] \psi \tag{4.29}$$

where $\hat{\boldsymbol{l}} = \hat{\boldsymbol{r}} \times \hat{\boldsymbol{P}}$ and $\tilde{\omega} = (|e|B/2mc) \neq \omega$. It may easily be seen that $\hat{l}_z = \hat{x}\hat{P}_y - \hat{y}\hat{P}_x$.

This Schrödinger equation describes a 2-D isotropic harmonic oscillator with frequency $\tilde{\omega}$ in the x-y plane which has a certain coupling to the magnetic field through its orbital angular momentum. The oscillator's C.M. is free to move in the z direction. Of course $\hat{l}_z$ is the rotation operator in the x-y plane and it is clear that such rotation leaves x^2+y^2 and $\partial_x^2 + \partial_y^2$ invariant. Thus $\hat{l}_z$ commutes with the harmonic oscillator's (partial) Hamiltonian and, of course, also with ∂_z^2. We may thus look for joint eigenfunctions of $\hat{H}, \hat{l}_z$ and $\hat{P}_z$ of the form

$$\psi = \tilde{C}\, e^{\imath P_z z/\hbar}\, e^{\imath\mu\phi} e^{-\imath Et/\hbar}\, \eta(r) . \tag{4.30}$$

where P_z and E are real constants, and $\mu = 0, 1, 2, \cdots$ is the azimuthal quantum number (the eigenvalue of $\hat{L}_z/\hbar$), and $r \equiv \sqrt{x^2 + y^2}$. We write the additional factor as a function of radius in the plane because in cylindrical coordinates r is orthogonal to z and ϕ.

Substituting this ansatz into Eq. (4.29) yields

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \tfrac{1}{2}m\tilde{\omega}^2(x^2 + y^2)\right]\eta = \left(E - \frac{P_z^2}{2m} + \frac{e\hbar B}{2mc}\mu\right)\eta \quad (4.31)$$

We have here the energy eigenvalue problem for two *uncoupled* harmonic oscillators with common frequency $\tilde{\omega}$. We know that each must have an energy spectrum of form $(n + \frac{1}{2})\hbar\tilde{\omega}$ with some nonnegative integer n. The eigenvalue in the r.h.s. must thus be $(n_1 + n_2 + 1)\hbar\tilde{\omega}$. Thus we conclude that

$$E = \frac{P_z^2}{2m} + (n_1 + n_2 + 1 - \mu)\left(\frac{|e|\hbar B}{2mc}\right) . \quad (4.32)$$

Exercises:

1. If the uniform magnetic field points in the z direction, and is obviously cylindrically symmetric, how is it that in gauge (4.19) the degeneracy is with respect to P_x but not P_y, and why is the y dependence of the wave function complicated, but not the x dependence?

2. Reconciliate the form of the spectrum in Eq. (4.32) with that in Eq. (4.25) by discussing the form of the eigenfunctions associated with the symmetric gauge.

4.2.2 Pauli's equation

All that was said in Sec. 4.2.1 referred to a spinless charged particle. As already mentioned in Sec. 1.1.2, electrons have spin $\frac{1}{2}$, that is $\boldsymbol{s} = \frac{1}{2}\hbar\boldsymbol{\sigma}$ with

the Pauli matrices σ_i given by Eq. (1.12). Experiment shows that an electron is endowed with an intrinsic magnetic moment related to its spin by

$$\boldsymbol{\mu} = -(|e|/mc)\boldsymbol{s} \tag{4.33}$$

(here we think of spin as an ordinary vector). We say that the *gyromagnetic ratio* of the electron spin is $-(|e|/mc)$. Now in classical electromagnetism a rotating object carrying charge q has a magnetic moment related to its orbital angular momentum by

$$\boldsymbol{\mu} = (q/2mc)\boldsymbol{l}\,. \tag{4.34}$$

In view of the factor of two difference between the two, we see that the spin gyromagnetic factor of the electron is *anomalous*.

Recall that when placed in a magnetic field $\boldsymbol{B}$, a magnetic moment $\boldsymbol{\mu}$ has energy $-\boldsymbol{\mu}\cdot\boldsymbol{B}$. To take this point into account Pauli added to the Schrödinger Hamiltonian the term $-\boldsymbol{\mu}\cdot\boldsymbol{B}$, and proposed the following modified Schrödinger equation, now called the Pauli equation, for an electron in a magnetic field:

$$\imath\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r},t) = -\frac{\hbar^2}{2m}\Big(\boldsymbol{\nabla} + \frac{\imath|e|}{\hbar c}\boldsymbol{A}(\boldsymbol{r},t)\Big)^2\psi(\boldsymbol{r},t) + \frac{|e|\hbar}{2mc}\boldsymbol{\sigma}\cdot\boldsymbol{B}\,\psi(\boldsymbol{r},t)\,. \tag{4.35}$$

Pauli's equation is heuristic; in particular it provides no explanation for why the gyromagnetic ratio of the electron is anomalous; it just accepts it.

Since $\boldsymbol{\sigma}$ is a vector of 2×2 matrices, the wave function in the context of the Pauli equation must be a 2-spinor:

$$\psi = \begin{pmatrix}\psi_\uparrow(\boldsymbol{r},t)\\ \psi_\downarrow(\boldsymbol{r},t)\end{pmatrix}\,, \tag{4.36}$$

that is, we deal with two partial differential equations, possibly coupled through the spin term. Thus terms in the Hamiltonian without a $\boldsymbol{\sigma}$ must have as a factor the 2×2 unit matrix I; however, we shall cavalierly ignore such a factor whenever this cannot lead to misunderstanding.

We can see graphically how Pauli's equation reflects the anomalous magnetic moment as follows. Expanding the square in Eq. (4.35) gives us for the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta - \frac{\imath|e|\hbar}{2mc}\big(\boldsymbol{A}\cdot\boldsymbol{\nabla} + \boldsymbol{\nabla}\cdot\boldsymbol{A}\big) + \frac{e^2}{2mc^2}\boldsymbol{A}^2 + \frac{|e|\hbar}{2mc}\boldsymbol{\sigma}\cdot\boldsymbol{B}\,. \tag{4.37}$$

We now write $\boldsymbol{A}$ in the symmetric gauge. It is clear from Eq. (4.27) that in this gauge $\boldsymbol{\nabla}\cdot\boldsymbol{A}=0$. Hence, $\boldsymbol{\nabla}\cdot\boldsymbol{A}\,\psi=\boldsymbol{A}\cdot\boldsymbol{\nabla}\psi$. Further

$$\boldsymbol{A}\cdot\boldsymbol{\nabla}=\tfrac{1}{2}\boldsymbol{B}\times\boldsymbol{r}\cdot\boldsymbol{\nabla}=\tfrac{1}{2}\boldsymbol{B}\cdot(\boldsymbol{r}\times\boldsymbol{\nabla})\,, \tag{4.38}$$

so that

$$\hat{H}=-\frac{\hbar^2}{2m}\Delta+\frac{|e|}{2mc}\boldsymbol{B}\cdot(\hat{\boldsymbol{l}}+2\boldsymbol{s})+\frac{e^2}{8mc^2}(\boldsymbol{B}\times\hat{\boldsymbol{r}})^2\,. \tag{4.39}$$

We observe immediately that spin couples to magnetic field twice as strongly as does orbital angular momentum. That is to say, the electron's spin has an anomalously large gyromagnetic ratio—by a factor of two, just as required experimentally.

Let us discuss the various terms in the Hamiltonian (4.39). After the kinetic energy comes the paramagnetic term, so called because it is responsible for the *paramagnetism* of many substances. Ignoring thermal effects what determines the equilibrium state of an electron in the material is the requirement of minimum mean energy. Clearly the paramagnetic term contributes $(|e|/2mc)\boldsymbol{B}\cdot\langle\hat{\boldsymbol{l}}+2\boldsymbol{s}\rangle$ to the mean energy, and this contribution is minimized if $\langle\hat{\boldsymbol{l}}+2\boldsymbol{s}\rangle$ becomes antialigned with $\boldsymbol{B}$. In view of Eqs. (4.33) and (4.34), the electron (charge $-|e|$) will contribute magnetic moment aligned with $\boldsymbol{B}$. In other words, the electronic magnetic susceptibility of the material will be positive, which means it will be paramagnetic.

The above ignores the effect of the third term in Eq. (4.39), called the diamagnetic term. It contributes mean energy $(e^2/8mc^2)\langle(\boldsymbol{B}\times\hat{\boldsymbol{r}})^2\rangle$ for each electron. This can be minimized by the system moving into the regions of weaker $\boldsymbol{B}$. This amounts to the field repelling the system, a characteristic of *diamagnetism*. If this effect dominates the former one, the material will be diamagnetic. The effect is called *Landau diamagnetism*; it is a purely quantum effect since in classical physics diamagnetism is forbidden (van Leuwen's theorem).

The prevalent opinion in theoretical physics is that the explanation of the anomalous gyromagnetic ratio lies in relativistic theory; it indeed comes out of Dirac's equation for the electron, as we shall see in the second part of this course. However, there is a nonrelatvistic argument by Feynman that will yield the factor of two anomaly. It goes as follows.

Since we know that the electron has spin $\frac{1}{2}$, its Hamiltonian with arbitrary

potential $V(\boldsymbol{r})$, but still without magnetic field, must be a 2×2 matrix of operators so that it can operate on wave functions of the form (4.36). Out of the operators at hand, $\hat{\boldsymbol{r}}, \hat{\boldsymbol{p}}$ and $V(\hat{\boldsymbol{r}})$ the only such matrix we can build is

$$\hat{H} = I \left[\frac{\hat{\boldsymbol{p}}^2}{2m} + V(\hat{\boldsymbol{r}}) \right]. \tag{4.40}$$

There is a significant way to rewrite the unit 2×2 matrix I. It is based on the identity

$$(\boldsymbol{\sigma} \cdot \hat{\boldsymbol{a}})(\boldsymbol{\sigma} \cdot \hat{\boldsymbol{b}}) = \hat{\boldsymbol{a}} \cdot \hat{\boldsymbol{b}}\, I + \imath\, \boldsymbol{\sigma} \cdot \hat{\boldsymbol{a}} \times \hat{\boldsymbol{b}}\,, \tag{4.41}$$

valid for any operators $\hat{\boldsymbol{a}}, \hat{\boldsymbol{b}}$ (either of or both $\hat{\boldsymbol{a}}$ and $\hat{\boldsymbol{b}}$ can also be plain vectors). Thus Eq. (4.40) can be put in the form

$$\hat{H} = \frac{(\boldsymbol{\sigma} \cdot \hat{\boldsymbol{p}})^2}{2m} + V(\hat{\boldsymbol{r}}). \tag{4.42}$$

Imagine that now the magnetic field is turned on. In analogy with the passage from Eq. (4.7) to Eq. (4.9) we will now have for an electron (with charge $-|e|$)

$$\hat{H} = \frac{1}{2m} \left(\boldsymbol{\sigma} \cdot \left(\frac{\hbar}{\imath} \boldsymbol{\nabla} + \frac{|e|}{c} \boldsymbol{A} \right) \right)^2 + V(\hat{\boldsymbol{r}}). \tag{4.43}$$

In accordance with identity (4.41)

$$\left(\boldsymbol{\sigma} \cdot \left(\frac{\hbar}{\imath} \boldsymbol{\nabla} + \frac{|e|}{c} \boldsymbol{A} \right) \right)^2 = \left(\frac{\hbar}{\imath} \boldsymbol{\nabla} + \frac{|e|}{c} \boldsymbol{A} \right)^2 + \frac{|e|\hbar}{c} \boldsymbol{\sigma} \cdot (\boldsymbol{\nabla} \times \boldsymbol{A} + \boldsymbol{A} \times \boldsymbol{\nabla}) \tag{4.44}$$

where we have dropped the vanishing operators $\boldsymbol{\nabla} \times \boldsymbol{\nabla}$ and $\boldsymbol{A} \times \boldsymbol{A}$. It should be remembered that every term here acts on the wave function to the right. Thus $\boldsymbol{\nabla} \times \boldsymbol{A} = -\boldsymbol{A} \times \boldsymbol{\nabla} + \boldsymbol{B}$ (exchanging arguments of a crossproduct introduces a negative sign). Therefore

$$\hat{H} = \frac{1}{2m} \left(\frac{\hbar}{\imath} \boldsymbol{\nabla} + \frac{|e|}{c} \boldsymbol{A} \right)^2 + \frac{|e|\hbar}{2mc} \boldsymbol{B} \cdot \boldsymbol{\sigma} + V(\hat{\boldsymbol{r}})\,. \tag{4.45}$$

Comparison with Eq. (4.35) shows that we have recovered Pauli's Hamiltonian, including the correct gyromagnetic factor associated with spin.

We notice that $\hat{H}$ here is not time-reversal even. First of all the single $\imath$ inside the brackets makes the Hamiltonian not real. Second, the term linear

in $\boldsymbol{\sigma}$ *anticommutes* with $\hat{\tau} = -\imath\sigma_2\hat{K}$ because its σ_2 part is pure imaginary. The conditions for operation of Kramers' theorem are thus not met, and the Kramers' degeneracy is not compulsory. However, using the tools developed to prove the theorem we can obtain a useful result along the same line.

Time reversal as implemented by $\hat{\tau} = -\imath\sigma_2\hat{K}$ refers to the electron only; the magnetic field $\boldsymbol{B}$ is assumed fixed. However, we can imagine including the exterior field and its sources in the time reversal. What happens then? Of course the external currents generating $\boldsymbol{B}$ switch sign under time reversal; so must $\boldsymbol{B}$ and $\boldsymbol{A}$. Let us define a new time reversal operator: $\hat{\tau} = -\imath\sigma_2\hat{K}\tau_{\mathrm{B}}$ where $\hat{\tau}_{\mathrm{B}}$ is the operator that inverts the external currents while commuting with the electron variables. Then it is obvious that the new $\hat{\tau}$ *commutes* with the Hamiltonian (4.45).

We can now formally repeat the proof of Kramers' theorem and show that when the system includes an odd number of spin $\frac{1}{2}$ particles, the state $\hat{\tau}|E\rangle$ is different from $|E\rangle$. But obviously both correspond to energy E. Therefore we have a degeneracy again. But it is not a degeneracy between pairs of states of the same system, but rather between corresponding states of the system placed in field $\boldsymbol{B}$ and the same system placed in field $-\boldsymbol{B}$. We can write this as

$$E_i(\boldsymbol{B}) = E_{-i}(-\boldsymbol{B})\,. \tag{4.46}$$

A simple example can be given for an H atom in a magnetic field. We would label its states with Bohr's quantum number n, the total angular momentum j and its z-projection (azimuthal quantum number) μ. Thus

$$E_{n,j,\mu}(\boldsymbol{B}) = E_{n,j,-\mu}(-\boldsymbol{B})\,. \tag{4.47}$$

Exercises:

1. Prove the identity (4.41) for two operators $\hat{\boldsymbol{a}}, \hat{\boldsymbol{b}}$ that *may not commute*. Do not use specific forms of Pauli's matrices but instead the defining relation (3.33).

2. Work out the Landau levels for a spinning electron using the Pauli Hamiltonian with a uniform $\boldsymbol{B}$. How will the energy eigenvectors look?

4.2.3 The Aharonov-Bohm effect

In electromagnetism whenever the magnetic field vanishes everywhere, it is permitted to take $\boldsymbol{A} = 0$. However, if $\boldsymbol{B}$ exists somewhere in space, then in general $\boldsymbol{A}$ cannot be chosen zero in regions free of $\boldsymbol{B}$. For example consider an infinitely long solenoid with current activating it. The magnetic field is totally confined inside the solenoid (Fig. 4.1). If we daw a closed contour $\mathcal{C}$ that encloses the solenoid once, then by Stokes' theorem

$$\oint_{\mathcal{C}} \boldsymbol{A} \cdot d\boldsymbol{r} = \int_{\Sigma} \boldsymbol{B} \cdot d\boldsymbol{S} \tag{4.48}$$

where the surface Σ with area element $d\boldsymbol{S}$ spans $\mathcal{C}$. But the flux passing through the solenoid is nonzero. Thus $\boldsymbol{A}$ cannot be chosen zero on any $\mathcal{C}$ which spans a surface that cuts $\boldsymbol{B}$ lines. Neither can we choose $\boldsymbol{A} = \boldsymbol{\nabla}\lambda$ with λ a single-valued function throughout the exterior of the solenoid because the first integral in Eq. (4.48) would still vanish. However, it is possible to do this if λ is a *multiple-valued* function, so that the first integral is nonvanishing.

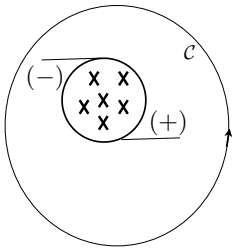

Figure 4.1: **Solenoid pictured along its axis carries some magnetic flux into the paper. The line integral of $\boldsymbol{A}$ along the shown contour $\mathcal{C}$ equals that flux.**

Consider now the celebrated two slit experiment. A source of electrons is separated from an electron detector by a plane screen opaque to electrons in which two parallel slits have been cut. If electrons are emitted singly, we can calculate the probability that a particular electron will be detected using the Feynman propagator. It is the sum of two parts. One is $K_{\mathrm{f}}^{(1)}(\boldsymbol{r}_1, t_1; \boldsymbol{r}_0, t_0)$, is the sum over paths for a free electron from the source event $(\boldsymbol{r}_0, t_0)$ to the

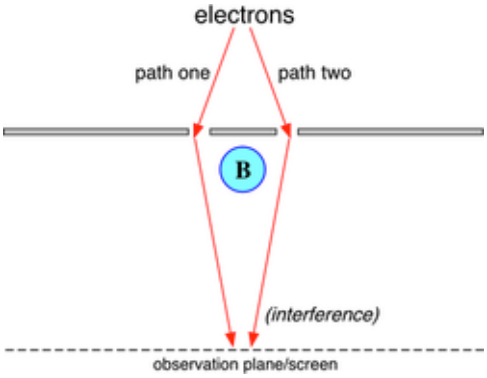

Figure 4.2: **The two slit experiment with electrons assisted by the influence of a magnetic flux carrying solenoid.**

detection event $(\boldsymbol{r}_1, t_1)$ through slit 1, and the second, $K_{\rm f}^{(2)}(\boldsymbol{r}_1, t_1; \boldsymbol{r}_0, t_0)$, is the sum of paths from emission to detection passing through slit 2. Paths that bump into the screen are not included. There is also a contribution to each propagator from paths that make multiple passes through one or both slits; we shall not try to correct for these; they contribute little to the path integral, being so different from the uniform path.

Now suppose that immediately behind and parallel to the screen we align a long solenoid between the slits (Fig. 4.2). When the current flows through it a $\boldsymbol{B}$ field appears inside it, but if the solenoid is enclosed in a sheet of material opaque to electrons, the electron paths that enter into the propagator are not influenced by the magnetic field. What changes in $K_{\rm f}^{(1)}$ once the solenoid is active? According to Eq. (4.4) we have to add to the free action of the electron the term $-(|e|/c)\int \boldsymbol{A}\cdot\dot{\boldsymbol{r}}\,dt = -(|e|/c)\int \boldsymbol{A}\cdot d\boldsymbol{r}$. Since the paths contributing to $K^{(1)}$ do not penetrate into the magnetic field, the integral here is path independent [see Eq. (4.48)]. The same is true for $K^{(2)}$. Thus we can write

$$K_{\rm tot} = K_{\rm f}^{(1)} e^{-\imath(|e|/\hbar c)\int_1 \boldsymbol{A}\cdot d\boldsymbol{r}} + K_{\rm f}^{(2)} e^{-\imath(|e|/\hbar c)\int_2 \boldsymbol{A}\cdot d\boldsymbol{r}} \tag{4.49}$$

where the subscripts in the integrals refer to whether the paths summed over lie on one side of the solenoid, or on the other.

The probability to detect the electron at $(\boldsymbol{r}, t)$ is

$$\begin{aligned} |K_{\rm tot}|^2 &= |K_{\rm f}^{(1)}|^2 + |K_{\rm f}^{(1)}|^2 \\ &+ K_{\rm f}^{(1)} K_{\rm f}^{(2)*} e^{\imath(|e|/\hbar c)(\int_2 - \int_1)\boldsymbol{A}\cdot d\boldsymbol{r}} + K_{\rm f}^{(1)*} K_{\rm f}^{(2)} e^{\imath(|e|/\hbar c)(\int_1 - \int_2)\boldsymbol{A}\cdot d\boldsymbol{r}} \\ &= |K_{\rm f}^{(1)}|^2 + |K_{\rm f}^{(1)}|^2 \qquad (4.50) \\ &+ 2\mathcal{R}(K_{\rm f}^{(1)} K_{\rm f}^{(2)*}) \cos\varphi - 2\mathcal{I}(K_{\rm f}^{(1)} K_{\rm f}^{(2)*}) \sin\varphi\,, \qquad (4.51) \end{aligned}$$

where

$$\varphi = \frac{|e|}{\hbar c}\left(\int_1 - \int_2\right) \boldsymbol{A}\cdot d\boldsymbol{r} = \frac{|e|}{\hbar c}\oint \boldsymbol{A}\cdot d\boldsymbol{r} = \frac{|e|}{\hbar c}\phi \qquad (4.52)$$

with the closed integral performed on a contour which surrounds the solenoid, and ϕ is the magnetic flux through the solenoid.

We see that the probability involves interference between the two slits, just as in the case of no magnetic field. However, with the solenoid active, the interference pattern is modulated by the amount of flux. Whenever the flux ϕ is an integral multiple of the basic unit

$$\phi_{\rm AB} \equiv \frac{2\pi\hbar c}{|e|} = 4.14 \times 10^{-7}\,\text{Maxwell (gauss cm}^2\text{)}\,, \qquad (4.53)$$

the interference pattern is the same as when there is no magnetic flux at all. For intermediate values of ϕ, $|K_{\rm tot}|^2$ as a function of position of the detector depends on the amount of flux through the solenoid, modulo ϕ_0. And, of course, this dependence *is not due* to direct interaction of the charges with the magnetic field.

The Aharonov[2]-Bohm[3] effect is a well tested effect. It is yet another example (following Berry's phase) of a topological quantum effect. It is

[2]Israeli theoretical physicist Yakir Aharonov (1932-) is at Tel-Aviv University. He discovered the Aharonov-Bohm effect while a Ph. D. student of Bohm's. He has made many other contributions to conceptual issues in QT. We owe to him elucidation of the Aharonov-Casher effect, the theory of weak measurement in QT and the Aharonov-Bergmann-Leibowitz formula.

[3]David Joseph Bohm (1917-1992) was an American-Jewish theoretical physicist and philosopher. He spent a large part of his life in England after being forced to leave America during the McCarty era. Apart from the Aharonov-Bohm effect we owe him a deterministic formulation of QT (de Broglie-Bohm theory) which is to all appearances experimentally equivalent to standard QT. Bohm also made important contributions to plasma physics.

topological because it owes its existence to the fact that the manifold in which Feynman's paths extend is not simply connected: there is an interior region (that occupied by the solenoid) which is not part of the manifold.

Exercises:

1. Aharonov and Bohm's solenoid is replaced by a capacitor whose voltage difference $V(t)$ is time dependent. Suppose a wavepacket state of an electron is split in two with one part passing near the right plate while the other passes near the left plate. Discuss the electric analog of the Aharonov and Bohm *gedanken* experiment. How does phase difference between the two sub-wavepackets change during flight?

4.2.4 The quantization of magnetic flux

This curious effect takes place with the help of superconductors. In an ordinary metal electrons are free to move, but collide occasionally with defects and distortions of the lattice, or with impurities; thus the metal exhibits electrical resistance. In superconductors the electrons are able to pair up (Cooper pairs) with help of their mutual interaction via the lattice which helps to overcome the Coulomb repulsion. These pairs, of charge $-2|e|$ are bosons. At the low temperatures which permit superconductivity the gas of pairs undergoes Bose condensation to a unified macroscopic state. An energy gap prevents the electrons for jumping out of the *condensate*. As a result, the charge moves without impediment, and the electrical resistance of the superconductor is exactly zero.

An essential property of the type-I (hard) superconductors is that they do not permit magnetic flux to pass through them (*Meissner-Ochsenfeld effect*[4]). If the precursor metal is magnetized, and is then cooled to below the superconducting tresshold T_C, it will expel any magnetic field in its interior (Fig. 4.3) provided the field is not so strong that it destroys the superconductivity. And if the superconductor is exposed to exterior magnetic fields, they will not penetrate its interior past a thin skin.

[4]Fritz Walther Meissner (1882 -1974), a German technical physicist, was an expert on low temperature physics. Robert Ochsenfeld (1901-1993) was a German physicist.

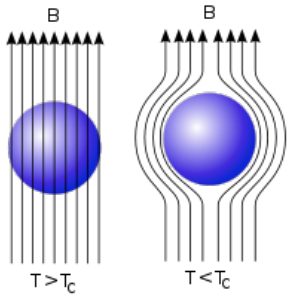

Figure 4.3: **A conducting sphere in a magnetic field expels any magnetic field from its interior once it is brought below the critical T_C and becomes superconducting.**

With this in mind consider a ring made of material that can become a type-1 superconductor. Let it be exposed to magnetic field which threads the hole of the ring but also passes through the metal. Now suppose the temperature is lowered until the ring becomes superconducting. The metal will expel all magnetic flux. But being unable to pass through the ring, whatever flux threaded the hole together with flux expelled will remain trapped by the ring. Let us denote the trapped magnetic flux by ϕ.

In a microscopic description of electromagnets the magnetic field is described by the Ampere-Maxwell equation

$$\boldsymbol{\nabla} \times \boldsymbol{B} = (4\pi/c)\boldsymbol{J} + (1/c)\,\partial_t \boldsymbol{E} \tag{4.54}$$

where $\boldsymbol{J}$ is the microscopic current carried by the Cooper pairs. If we imagine that the situation has become stationary, the $\dot{\boldsymbol{E}} = 0$. Further inside the ring $\boldsymbol{B} = 0$ by the Meissner-Ochsenfeld effect. Therefore in the ring material we must have $\boldsymbol{J} = 0$. What is the expression for $\boldsymbol{J}$?

We know that that in Schrödinger theory the *probability density* is $\psi\psi^*$. Inside a superconductor ψ must be interpreted as the wave function of the condensate (ψ is often called the *order parameter*). We therefore should write for the charge density here $\varrho = -2|e|\psi\psi^*$. As already mentioned in Sec. 3.2.5, the *probability current* associated with ψ is

$$\boldsymbol{j} = \frac{\hbar}{2mi}(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*)\,. \tag{4.55}$$

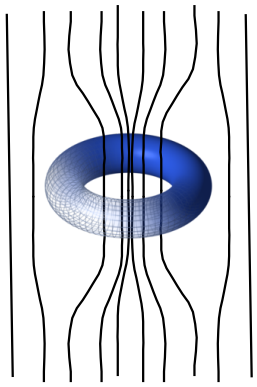

Figure 4.4: **Lines of magnetic field are expelled from the superconductor material, some into the hole of the ring (leading to high flux), and some to the exterior of it.**

But we cannot write $\boldsymbol{J} = -2|e|(\hbar/2m\imath)(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*)$. Unlike the proposed expression for ρ, this last expression is not gauge-invariant in the presence of an electromagnetic field!

We can make $\boldsymbol{J}$ gauge invariant by replacing $\boldsymbol{\nabla} \mapsto \boldsymbol{\nabla} + (2\imath|e|/\hbar c)\boldsymbol{A}$ in the last proposals, cf. Eq. (4.10). Thus

$$\begin{aligned} \boldsymbol{J} &= \frac{|e|\hbar}{m\imath}\left(\psi^*\Big[\boldsymbol{\nabla} + (2\imath|e|/\hbar c)\boldsymbol{A}\Big]\psi - \psi\Big[\boldsymbol{\nabla} - (2\imath|e|/\hbar c)\boldsymbol{A}\Big]\psi^*\right) && (4.56)\\ &= \frac{|e|\hbar}{m\imath}(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*) + (4e^2/mc)\boldsymbol{A}\psi^*\psi\,. && (4.57)\end{aligned}$$

The first version is particularly useful here. We write the wave function in polar form

$$\psi(\boldsymbol{r}) = \sqrt{\frac{\varrho(\boldsymbol{r})}{-2|e|}}\, e^{\imath\theta(\boldsymbol{r})} \tag{4.58}$$

which when substituted in Eq. (4.56) gives

$$\boldsymbol{J} = -\frac{\hbar\varrho}{m}\left[\boldsymbol{\nabla}\theta + \frac{2|e|}{\hbar c}\boldsymbol{A}\right]\,. \tag{4.59}$$

This vanishes when

$$\boldsymbol{\nabla}\theta = -(2|e|/\hbar c)\boldsymbol{A} \tag{4.60}$$

This result is in harmony with the fact that $\boldsymbol{B} = 0$; so $\boldsymbol{A}$ should be a gradient.

Let us now draw a contour following the great central circle of the torus; $\mathcal{C}$ circles inside the torus once and then closes upon itself. We now integrate $\boldsymbol{\nabla}\theta$ along it:

$$\Delta\theta = \oint_{\mathcal{C}} \boldsymbol{\nabla}\theta \cdot d\boldsymbol{r} = -\frac{2|e|}{\hbar c} \oint_{\mathcal{C}} \boldsymbol{A} \cdot d\boldsymbol{r} = -\frac{2|e|}{\hbar c}\phi \tag{4.61}$$

Here we have used Eq. (4.48) in the last equality. Of course $\Delta\theta$, the change in θ all around $\mathcal{C}$ must be an integral multiple of 2π; otherwise ψ will not be single-valued. We thus conclude that

$$\phi = \phi_0\, n; \quad n = 0, \mp 1, \mp 2, \cdots \quad \text{with} \quad \phi_0 \equiv \frac{\pi\hbar c}{|e|} = 2.07{\times}10^{-7}\,\text{Maxwell} \tag{4.62}$$

This is the quantization of magnetic flux. The basic unit, ϕ_0, called the *fluxon*, is half of the Aharonov-Bohm critical flux ϕ_{AB}.

The phenomenon of flux quantization is even more visible in type-II (soft) superconductors. Such a material does admit magnetic fields through it, but the flux is forced into narrow threads of magnetic field called *magnetic vortices*. The same argument we have given shows that a magnetic vortex contains flux equal to $n\phi_0$. Mostly only vortices with $n = 1$ are stable. The structures mentioned are called "vortices" because there is an analog phenomenon in a rotating vat filled with *superfluid* He^4 in which the whole vorticity which should accompany the rotation is confined to thin threads where the superfluid rotates like in a water vortex. There is also an analogous quantum of fluid circulation.

Exercises:

1. Do ρ and $\boldsymbol{J}$ in a superconductor obey the continuity equation? Work it out!

2. Discuss the quantization of magnetic flux using the propagator for a spinless charged particle.

4.2.5 Bosons, fermions and anyons

So far we have applied QT to a single particle. When several particles are present, and they are of the same kind, we must take into account that they are totally identical, and cannot be told one from another. The upshot of this is that the Hamiltonian governing, say, two identical particles subject to some forces must be symmetric under particle interchange so that the dynamics shall not be able to distinguish between the particles. Thus

$$\hat{H} = -\frac{\hbar^2}{2m}(\Delta_1 + \Delta_2) + V(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2); \qquad V(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2) = V(\hat{\boldsymbol{r}}_2, \hat{\boldsymbol{r}}_1)\,. \tag{4.63}$$

As usual in QT, the operation of interchange or permutation is performed by a unitary operator $\hat{P}_{1,2}$ (P for *p*ermute):

$$\hat{P}_{1,2}\,\hat{H}(1,2)\,\hat{P}_{1,2}^{\dagger} \equiv \hat{H}(2,1) = \hat{H}(1,2)\,. \tag{4.64}$$

Another requirement is that the probability density associated with the two particles shall not change when they are permuted (since they are identical). Thus

$$\hat{P}_{1,2}\,\psi(1,2) \equiv \psi(2,1) = \omega\,\psi(1,2); \qquad |\omega| = 1. \tag{4.65}$$

What do we take for ω? It used to be argued that since permuting twice brings each particle to itself, so that ${\hat{P}_{1,2}}^2 = 1$, we must take $\omega = \pm 1$. This gave rise to two distinct kinds of particles: 1) bosons with $\omega = +1$ such as the photon, pion, kaon, He^4 nucleus, H atom, $\cdots$, and 2) fermions with $\omega = -1$ such as the electron, muon, the quarks, the Li^7 nucleus, the deuterium atom, $\cdots$. Fierz[5] and Pauli's spin-statistics theorem within quantum field theory shows that any particle or composite with total integral spin must be a boson while any particle or composite with half integral spin must be a fermion.

In the 1980's Leinaas and Myrheim[6]s pointed out that in 2-D the statement ${\hat{P}_{1,2}}^2 = 1$ cannot be accepted for topological reasons. Instead of just

[5]Markus Eduard Fierz (1912-2006) was a Swiss physicist, who first formulated the spin-statistics theorem (later proved rigorously by Pauli); he also contributed to statistical mechanics, particle physics and (with Pauli) to the quantum field theory of spin-2 particles (gravitons).

[6]Jon Magne Leinaas (1946-) and Jan Myrheim (1948-) are two Norwegian theoretical physicists specializing in quantum theory issues.

exchanging the particles we can imagine that they are gradually transported each to its neighbor's location. As shown in Fig. 4.5 when this transport is extended to bring the particles back to their original locations, it looks, from the point of view of one particle, as if the second one is circling it. In 2-D this "circle" cannot be shrunk to a point (being obstructed by the first particle), so that two interchanges do not amount to the identity. (Of course in 3-D this is not true and conventional wisdom prevails.

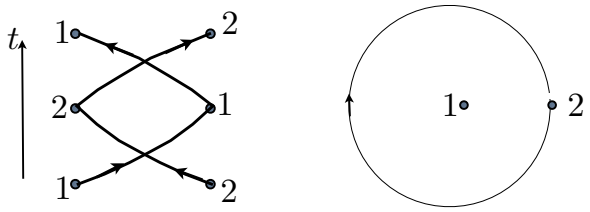

Figure 4.5: **Left panel: the double permutation of particles 1 and 2 as a process occurring over time from the point of view of the laboratory. Right panel: the same process as seen by particle 1.**

The above discussion was augmented by Wilczek[7] who named the new kind of particles any-ons (today spelled anyons). It is clear that without the $\hat{P}_{1,2}{}^2 = 1$ constraint one can only say that ω is a *unimodular* (of unit absolute magnitude) complex number. It follows that there are an infinite number of classes of anyons, distinguished one from the other by the value of ω.

Let us construct an anyon! In a soft superconductor placed in an exterior magnetic field there will be magnetic vortices crossing the material in the direction of the field. As mentioned, usually such vortices are stable only if they comprise one fluxon. Now suppose each vortex captures an electron. We then have a collection of charged magnetized electrons. But the vortices can move only parallel to themselves, so the system is a 2-D one.

Let $K_0(\boldsymbol{r}, t; \boldsymbol{r}_0, t_0)$ be the propagator for a magnetized electron *all by itself* in the superconductor. Let us now consider what happens as vortex X is transported all the way around vortex Y. There is now a contribution

[7]Nobel laureate Frank Anthony Wilczek (1951-) is an American theoretical physicist of Jewish origin who proved (with D. Gross and independently of D. Politzer) that according to quantum chromodynamics—the modern gauge theory of the strong interaction—there is asymptotic freedom: the interaction gets weaker at higher energies. He also originated (with S. Weinberg) the notion of axion—a very weakly interacting particle.

from $\boldsymbol{A}$ (which cannot vanish identically since there are magnetic fields in the vortex cores) to the classical action in the exponent of the path integral. As we take X *half way* around Y, X's propagator will acquire a phase originating from $\int_1 \boldsymbol{A}\cdot d\boldsymbol{r}$. As explained in Sec. 4.2.3 in connection with the Aharonov-Bohm effect, this is common to all paths. Thus in the first leg of the circumnavigation, X's propagator just gets multiplied by a phase.

On the second half of the tour, the contribution $\int_2 \boldsymbol{A}\cdot d\boldsymbol{r}$ is again common to all paths. X's picks up an extra phase from this. The total change of phase, following Eq. (4.52), is $\Delta\varphi = (|e|/\hbar c)\phi_0$ because our vortices carry a fluxon each. But as explained above, the tour of X around Y is equivalent to a double exchange of X and Y which should generate a factor ω^2. Using Eq. (4.62) to calculate $\Delta\varphi$ we see that the phase acquired by the fluxon wave function upon exchange is $\omega^2 = e^{\imath\pi} = -1$. Thus $\omega = e^{\imath\pi/2} = \imath$. Thus a magnetized electron is neither a boson nor a fermion, but something in between.

Anyons are seen in nature. For example, the quasiparticle excitations observed in the quantum Hall effect are anyons. It is also suspected that excitations in the cuprate high temperature superconductors, in which layers play an important role, are anyons.

Exercises:

1. Could $\hat{P}_{1,2}$ be antiunitary? Explain.

2. Why must ω be unimodular?

3. Prove that it is impossible for ω to be $+1$ for one state of a system and -1 for another.

4. Is ω a conserved quantum number? Explain.

5. Show that $\{\hat{P}_{1,2}, \hat{I}\}$ comprise the same group Z_2 we met in connection with spatial inversion. If N particles are permuted, one can define $\hat{P}_{a,b,c,\cdots}$ as a permutation of particles $1, 2, 3, \cdots$ so that they take up the order $a, b, c, \cdots$. Show that the group made up by all $\hat{P}_{a,b,c,\cdots}$ (the permutation group S_N) is nonabelian.

4.2.6 The magnetic monopole and quantum theory

Maxwell's equations (4.1), (4.54) and the Gauss electric equation, in the absence of sources ρ and $\boldsymbol{J}$, are symmetric under the interchange $\boldsymbol{E} \mapsto \boldsymbol{B}$ and $\boldsymbol{B} \mapsto -\boldsymbol{E}$. The symmetry in question is named *duality*. However, the presence of the sources breaks the symmetry, i.e. Gauss' electric equation has a source but Gauss' magnetic equation does not.

One can speculate on new physics where one restores the duality symmetry by generalizing the equations as follows:

$$\begin{aligned} \boldsymbol{\nabla} \times \boldsymbol{E} + c^{-1}\dot{\boldsymbol{B}} &= 4\pi c^{-1}\boldsymbol{J}_M\,, \qquad \boldsymbol{\nabla}\cdot\boldsymbol{B} = 4\pi\varrho_M\,; \\ \boldsymbol{\nabla} \times \boldsymbol{B} - c^{-1}\dot{\boldsymbol{E}} &= 4\pi c^{-1}\boldsymbol{J}\,, \qquad \boldsymbol{\nabla}\cdot\boldsymbol{E} = 4\pi\varrho\,; \end{aligned} \tag{4.66}$$

where ϱ_M and $\boldsymbol{J}_M$ are magnetic and current charge densities which are easily proved to comply with a law of continuity, just like their electric analogues. There is now duality symmetry under the duality transformation

$$\boldsymbol{E} \mapsto \boldsymbol{B}, \quad \boldsymbol{B} \mapsto -\boldsymbol{E}\,; \tag{4.67}$$

$$\rho \mapsto \varrho_M, \quad \varrho_M \mapsto -\varrho, \qquad \boldsymbol{J}_M \mapsto \boldsymbol{J}, \quad \boldsymbol{J} \mapsto -\boldsymbol{J}_M\,. \tag{4.68}$$

The set of equations (4.66) has more symmetry than the conventional Maxwell equations; this is the reason for taking them seriously, even though no genuine case of a magnetic charge has ever been seen.

From the QT point of view a problem looms immediately. To write Schrödinger's equation we need the vector potential $\boldsymbol{A}$. Of course if we assume, as usual, that $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$, we must have $\boldsymbol{\nabla}\cdot\boldsymbol{B} = 0$ which by the second of Eqs. (4.66) would force the magnetic charge density to vanish everywhere. It would seem that quantum considerations rule out magnetic charge! However, in 1931 Dirac pointed out that by allowing $\boldsymbol{A}$ to have certain singularities, one opens the way for at least pointlike magnetic charges to be allowed. Since then these charges have been termed *magnetic monopoles*.

Here is an example of a potential suitable for a magnetic monopole written in spherical polar coordinates (r, ϑ, φ):

$$\boldsymbol{A} = (A_r, A_\vartheta, A_\varphi) = \left(0, 0, \frac{g}{r}\frac{1-\cos\vartheta}{\sin\vartheta}\right)\,; \tag{4.69}$$

Here g is a real constant. Obviously this $\boldsymbol{A}$ is singular along the negative z axis, $\vartheta = \pi$. We take the curl of $\boldsymbol{A}$; because there are no A_r, A_ϑ components we must have $B_\varphi = 0$. And because rA_φ is independent of r there is no B_ϑ. Further

$$B_r = (\boldsymbol{\nabla} \times \boldsymbol{A})_r = \frac{1}{r^2 \sin\vartheta}\Big[\partial_\vartheta(r\sin\vartheta A_\varphi) - \partial_\varphi(rA_\vartheta)\Big] \tag{4.70}$$

$$= \begin{cases} g/r^2; & 0 \le \vartheta < \pi \\ \infty, & \vartheta = \pi\,. \end{cases} \tag{4.71}$$

Thus for $\vartheta \neq \pi$ the potential (4.69) generates a radial $1/r^2$ magnetic field, just what would be expected from the Gauss magnetic equation with a point magnetic source $\rho_M = g\,\delta(\boldsymbol{r})$. Thus g is the strength of the magnetic monopole.

The line singularity in Eq. (4.71), referred to as *Dirac's string*, is the price paid for being able to describe the monopole's field by a potential. This singularity need not be rectilinear; it could twist and turn so long as it extends to infinity, and so long as it satisfies the condition

$$\oint \boldsymbol{A}\cdot d\boldsymbol{r} = 4\pi g\,, \tag{4.72}$$

with the contour circling the singularity once. For example, with Eq. (4.69)

$$\oint \boldsymbol{A}\cdot d\boldsymbol{r} = 2\pi r\sin\vartheta A_\varphi|_{\vartheta=\pi} = 2\pi g(1-\cos\vartheta)|_{\vartheta=\pi} = 4\pi g. \tag{4.73}$$

By Eq. (4.48) this tells us that the flux entering the monopole along the singularity equals the flux that escapes from the monopole as a radial spherically symmetric field. In other words, despite the appearances, the magnetic field here is consistent with the traditional notion that magnetic lines have no sources: $\boldsymbol{\nabla}\cdot\boldsymbol{B} = 0$. This description when smoothed over small scales can be summarized with the first of Eqs. (4.66).

We can reinterpret the above setup within the standard Maxwell framework as a very thin solenoid coming from infinity and channeling magnetic flux $4\pi g$ which then escapes from its end at $\boldsymbol{r} = 0$. The solenoid being thin, the outward flux is essentially radial, giving the appearance of a monopole of strength g. $\boldsymbol{\nabla}\cdot\boldsymbol{B} = 0$ is obeyed everywhere. We can thus construct a magnetic monopole without invoking new physics. In both of the above cases

it would seem that due to the thinness of the Dirac string/solenoid we just see an isolated magnetic monopole.

However, this is not so: the Aharonov-Bohm effect allows discovery of an arbitrarily thin string/solenoid via the interference of electrons it gives rise to. It would seem that we cannot manufacture a true isolated monopole. However, we must recall that whenever the flux $4\pi g$ along the string/solenoid is a whole multiple of $\phi_{\rm AB}$ in Eq. (4.53), the interference pattern is identical to that produced in the absence of any magnetic flux. Thus the fact that the field does not come from a true monopole cannot be discovered when the following *Dirac quantization condition* is satisfied:

$$g = \frac{n\hbar c}{2|e|} = \frac{n|e|}{2\alpha}; \qquad n = \pm 1, \pm 2, \cdots , \tag{4.74}$$

Here $\alpha = e^2/(\hbar c) \approx 1/137$ is the fine structure constant. Actually Dirac used a different argument (the Aharonov-Bohm effect was still unknown) to arrive at the conclusion that any magnetic monopoles in nature will comply with this quantization condition. It may be seen that the unit of magnetic charge is much larger than the unit charge $|e|$.

The opposite side of the coin is just as interesting. We solve the first equality in (4.74) equation to get

$$|e| = \frac{n\hbar c}{2g}; \qquad n = \pm 1, \pm 2, \cdots . \tag{4.75}$$

One can then argue that if in some place in the universe there exits even a single magnetic monopole (strength g_*), then electric charges everywhere must be whole multiples of the unit charge $\frac{1}{2}\hbar c/g_*$. It is a fact that all charges in nature are, with extremely high precision, integer multiples of the d quark charge (a third of the electron's). There are few other ways to understand this quantization; this gives Dirac's hypothesis great weight, and monopoles are looked for whenever a new technique is introduced or new physical theory explored.

Chapter 5

Second quantization

Apart from the mention we made in Sec. 4.2.5 of two particle systems, we have dealt with the QT of single particles only (even when discussing scattering we used the effective particle approach). When the quantum system contains a number of particles of the same species, a totally new approach is required. Why? First of all we know that in 3-D quantum particles are either bosons or fermions. The wave funcion of several bosons must be symmetric under every exchange of them; that of several fermions must be antisymmetric under each pair exchange. We need a formalism that produces symmetric or antisymmetric wave functions. Further, in relativistic quantum systems (and in some nonrelativistic ones), particle number is not conserved: particles can be created or destroyed. The QT as presented up to know is powerless in confronting such processes in which probability is not conserved.

The formalism of second quantization provides an automatic way to produce symmetric or antisymmetric wave functions, and a way to deal with systems where the number of particles changes so that probability of a single particle is not conserved. In this chapter we shall only deal with nonrelativistic systems, and leave the question of particle creation and annihilation to later chapters.

5.1 Second quantization for bosons

5.1.1 Symmetrizing and antisymmetrizing by brute force

A system of N identical particles interacting among themselves must, in nonrelativistic QT, be described by an Hamiltonian of the form

$$\hat{H} = \sum_a^N \left[\frac{\hat{\boldsymbol{p}}_a^2}{2m} + U(\hat{\boldsymbol{r}}_a) \right] + V(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2, \cdots) \tag{5.1}$$

where U is the common external potential and V is the mutual interaction potential; it must be invariant under any reordering of its arguments,. This $\hat{H}$, by being symmetric under any exchange of particles, cannot discriminate between one particle and another, as appropriate when dealing with identical particles.

Suppose we manage to find a multiparticle solution of Schrödinger's equation $\phi(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2, \cdots, t)$ (there could also be spin; we mention it later). This is not automatically the physical wave function. If the system is bosonic, we must make it into a totally symmetric wave function. Using the permutation operator $\hat{P}_{a,b,c,\cdots}$ introduced in Sec. 4.2.5 we could find the correct wave function as follows:

$$\psi(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2, \cdots, t) = \sum_{\text{perm}} \hat{P}_{a,b,c,\cdots}\ \phi(\hat{\boldsymbol{r}}_a, \hat{\boldsymbol{r}}_b, \cdots, t) \tag{5.2}$$

where the sum goes over all permutations of $(a, b, c \cdots)$. This ψ obviously satisfies the Schrödinger equation, and is completely symmetric under any exchange of its arguments.

If the system is fermionic, it necessarily consists of particles with spin (we shall always take the spin to be $\frac{1}{2}$). We first find a solution of the Schrödinger equation of the form $\phi(\hat{\boldsymbol{r}}_1, \mu_1; \hat{\boldsymbol{r}}_2, \mu_2; \cdots, t)$ with the $\mu = \pm\frac{1}{2}$. Then we form

$$\psi(\hat{\boldsymbol{r}}_1, \mu_1; \hat{\boldsymbol{r}}_2, \mu_2; \cdots, t) = \sum_{\text{perm}} (-1)^\sigma \hat{P}_{a,b,c,\cdots}\ \phi(\hat{\boldsymbol{r}}_a, \mu_a; \hat{\boldsymbol{r}}_b, \mu_b; \cdots, t) \tag{5.3}$$

where $\sigma = 0$ for an even permutation of $a, b, \cdots$ and $\sigma = 1$ for an odd one. Obvioulsy ψ satisfies the Schrödinger equation and is completely antisymmetric (flips sign under exchange of neighboring particles). The labor in

symmetrizing or antisymmetrizing in this brute force way grows very rapidly with N. That is why one opts for second quantization. We first explain this later method for spinless particles; esxtensions will follow.

5.1.2 Fock space

The first requirement in second quantization is a basis of one-particle functions. If the potential V in Eq. (5.1) is the real constant $\mathcal{K}$, this is easy to construct. We find the set of eigenfunctions $\{u_i(\boldsymbol{r})\}$ of the one-particle Hamiltonian

$$\hat{H}_1 = \frac{\hat{\boldsymbol{p}}^2}{2m} + U(\hat{\boldsymbol{r}}) + \frac{\mathcal{K}}{N}\,. \tag{5.4}$$

And if $V \neq$ const., it may be possible to go over to normal coordinates in which the Hamiltonian becomes a sum of parts, each depending on only one coordinate; the procedure is analogous to the diagonalization of the Hamiltonian of a vibrational system in classical mechanics. In the following discussion we shall focus on just one of these (possibly different) one-particle Hamiltonians. The situation is thus analogous to that dealing with Eq. (5.4).

When diagonalization is not be feasible, or is too messy, it may be appropriate to ignore the interaction V at the start, and try to deal with it later on by perturbation theory. In all three cases, the u_i of $\hat{H}_1$ are called the *mode functions*; each is obviously associated with an energy eigenvalue ε_i.

Given the modes we can represent a special kind of many-particle state by the *occupation vector* $|n_1, n_2, \cdots\rangle$ with $n_1, n_2, \cdots$ nonnegative integers. This says that n_1 bosons are in mode 1, n_2 in mode 2, etc. The n_i are called occupation numbers. Of course $\sum_i n_i = N$. This way of stating things is called the *occupation number representation* or *Fock representation*. If $|\psi, t\rangle$ is the abstract state of the system, we can write its wave function in the occupation number representation as

$$\chi(n_1, n_2, \cdots; t) = \langle n_1, n_2, \cdots | \psi, t\rangle\,. \tag{5.5}$$

Of course χ is the probability amplitude to find n_1 bosons in the mode 1, etc.

In the occupation vector the arguments must be nonnegative integers; we would like to consider them eigenvalues of suitable observables. We recall that

in the theory of the harmonic oscillator one deals with raising and lowering operators $\hat{a}^\dagger$ and $\hat{a}$ which obey the algebra $[\hat{a}, \hat{a}^\dagger] = 1$. Then the observable $\hat{N} = \hat{a}^\dagger \hat{a}$ has the spectrum $(0, 1, 2, \cdots)$. Therefore we shall imagine that each of our modes u_i is equipped with a pair of operators $\hat{a}_i^\dagger$ and $\hat{a}_i$, and that in general

$$[\hat{a}_i, \hat{a}_j] = 0; \qquad [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0; \qquad [\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij} \,. \tag{5.6}$$

Thus the algebras of operators of distinct modes are disjoint. We may now define a Hermitian *number operator* for each mode:

$$\hat{N}_i = \hat{a}_i \, \hat{a}_i^\dagger \,. \tag{5.7}$$

We then have

$$[\hat{N}_i, a_j^\dagger] = [\hat{a}_i^\dagger \, \hat{a}_i, a_j^\dagger] = \hat{a}_i^\dagger \, [\hat{a}_i, a_j^\dagger] + [a_j^\dagger, a_j^\dagger] \, a_i = \hat{a}_j^\dagger \, \delta_{ij}, \tag{5.8}$$

By induction one can prove for any integral n that

$$[\hat{N}_i, a_j^{\dagger n}] = n \, a_j^{\dagger n} \, \delta_{ij} \,. \tag{5.9}$$

Let us now define the special state $|\upsilon\rangle$; it is the state which is annulled by any one of the $\hat{a}_j$ or equivalently by any of the $\hat{N}_i$: $\hat{N}_i|\upsilon\rangle = 0$. We normalize it so that $\langle\upsilon|\upsilon\rangle = 1$. We now ask what is the nature of the state $a_j^{\dagger n}|\upsilon\rangle$? From Eq. (5.9) we have

$$\hat{N}_i \, a_j^{\dagger n}|\upsilon\rangle = [\hat{N}_i, a_j^{\dagger n}] \, |\upsilon\rangle + \hat{a}_j^{\dagger n} \, \hat{N}_i|\upsilon\rangle = n \, \delta_{ij} \, a_j^{\dagger n}|\upsilon\rangle \,. \tag{5.10}$$

Thus our state is proportional to $|0, 0, \cdots, n, 0, \cdots\rangle$ with n in the j-th slot. From this and Eq. (5.6) is also obvious that

$$a_j^{\dagger n_j} \, a_k^{\dagger \, n_k} \cdots |\upsilon\rangle \propto |0, 0, \cdots, n_j, \cdots, n_k, \cdots\rangle \,. \tag{5.11}$$

Obviously $\hat{a}_j^\dagger$ increases the number of particles in the j-th mode (eigenvalue of $\hat{N}_j$) by one without changing the numbers in other modes. It is thus called a *creation operator*. In light of Eqs. (5.6)-(5.7) consider

$$\langle 0, 0, \cdots, n_j, \cdots, n_k, \cdots | \hat{a}_j \, \hat{a}_j^\dagger | 0, 0, \cdots, n_j, \cdots, n_k, \cdots \rangle \tag{5.12}$$

$$= \langle 0, 0, \cdots, n_j, \cdots, n_k, \cdots | \hat{N}_j | 0, 0, \cdots, n_j, \cdots, n_k, \cdots \rangle \tag{5.13}$$

$$+ \langle 0, 0, \cdots, n_j, \cdots, n_k, \cdots | 0, 0, \cdots, n_j, \cdots, n_k, \cdots \rangle \,. \tag{5.14}$$

The $\hat{N}_j$ brings out a factor n_j; thus

$$\hat{a}_j^\dagger|\cdots,n_j,\cdots,n_k,\cdots\rangle = \sqrt{n_j+1}|\cdots,n_j+1,\cdots,n_k,\cdots\rangle\,. \tag{5.15}$$

Proceeding by induction from the *normalized* state $|\upsilon\rangle$ we see that the properly normalized state with n_j particles in mode j, etc. is

$$|\cdots,n_j,\cdots,n_k,\cdots\rangle = \frac{1}{\sqrt{n_j!}}\cdots\frac{1}{\sqrt{n_k!}}\cdots a_j^{\dagger n_j}\cdots a_k^{\dagger n_k}|\upsilon\rangle \tag{5.16}$$

The states of this form for all possible sets of occupation numbers form an orthonormal basis for *Fock space*, the space of states characterized by the numbers of particles in the various modes. States (5.16) form a complete basis as we now show. First operating on a particular state with any $\hat{N}_j$ or any $\hat{a}_j^\dagger$ does not give states not of type (5.16). Second we shall show that operating with any $\hat{a}_j$ does not either.

We do this with the *annihilation operator* $\hat{a}_j$. Consider the hermitian conjugate of Eq. (5.8):

$$[\hat{N}_i, a_j] = -\hat{a}_j\delta_{ij}\,. \tag{5.17}$$

It follows from it that

$$\hat{N}_j\,\hat{a}_j\,|0,0,n_j,\cdots,n_k,\cdots\rangle = (n_j-1)\,\hat{a}_j\,|0,0,n_j-1,\cdots,n_k,\cdots\rangle\,, \tag{5.18}$$

so that $\hat{a}_j$ reduces the eigenvalue of $\hat{N}_j$ by one, except for the case that n_j is already zero, when $\hat{a}_j$ annihilates the state. It is obvious that $\hat{a}_j$ changes a state of type (5.16) into another state of the same type, or else annihilates it. Thus the space spanned by the vectors (5.16) is closed under the operation of $\hat{a}_j$, $\hat{a}_j^\dagger$ and $\hat{N}_j$.

Since the mean of $\hat{N}_j = \hat{a}_j^\dagger\,\hat{a}_j$ in $|0,0,n_j,\cdots,n_k,\cdots\rangle$ is n_j, it follows that

$$\hat{a}_j|\cdots,n_j,\cdots,n_k,\cdots\rangle = \sqrt{n_j}\,|\cdots,n_j-1,\cdots,n_k,\cdots\rangle\,, \tag{5.19}$$

which complements Eq. (5.15) and includes the case that $\hat{a}_j$ annihilates the state with $n_j = 0$.

Now consider the following state in Fock space (the $\alpha_{n_1,n_2,\cdots}$ are complex constants):

$$|N\rangle = \sum_{\sum_j n_j = N} \alpha_{n_1,n_2,\cdots}\,|n_1,n_2,\cdots\rangle\,. \tag{5.20}$$

By the constraint in the summation, there are N particles in each state in the sum. Thus $|N\rangle$ is an eigenstate of $\sum_k \hat{a}_k^\dagger \hat{a}_k$, namely it is a generic state with N particles; these are distributed in some way over the modes.

Note that the above formalism is specific for bosons. Start with $|\upsilon\rangle$ and operate on it with $\hat{a}_j^{\dagger n_j} \hat{a}_k^{\dagger n_k}$ to first create n_k particles in mode k and then n_j particles in mode j. The result is the same as operating with $\hat{a}_k^{\dagger n_k} \hat{a}_j^{\dagger n_j}$ in which the particles appear in opposite order. Thus the states (5.16) are symmetric under exchange of the particles (more on this below).

Exercises:

1. Prove that the basis states of Fock space (5.16) are orthonormal.

2. Show that

$$e^{\beta \hat{a}^\dagger \hat{a}} = \sum_{n=0}^{\infty} \frac{(e^\beta - 1)^n}{n!} \hat{a}^{\dagger n} \hat{a}^n \tag{5.21}$$

   where β is a real number.

5.1.3 The field operator

Suppose we can solve the eigenvalue problem of the one-particle Hamiltonian (5.4). From the mode eigenfunctions $u_i(\boldsymbol{r})$ we can form

$$\hat{\psi}(\boldsymbol{r}) = \sum_i \hat{a}_i \, u_i(\boldsymbol{r}) \,, \tag{5.22}$$

which is called the *field operator* because it is an operator which varies in space ($\hat{\psi}(\boldsymbol{r})$ exists both in real space and in Fock space). What does $\hat{\psi}(\boldsymbol{r})$ do?

Let us form a generic *one-particle* state

$$|\Phi\rangle = \sum_j \alpha_j \, \hat{a}_j^\dagger \, |\upsilon\rangle \,. \tag{5.23}$$

In this state the particle is in mode j with amplitude α_j. We may suppose that $\sum_j |\alpha_j|^2 = 1$. Now by exploiting Eq. (5.6) we get

$$\hat{\psi}(\boldsymbol{r})|\Phi\rangle = \sum_j \sum_i \alpha_j \left(\hat{a}_j{}^\dagger \hat{a}_i + \delta_{ij}\right)|v\rangle\, u_i(\boldsymbol{r}) = \sum_i \alpha_i\, u_i(\boldsymbol{r})|v\rangle\,. \tag{5.24}$$

The state is thus the vacuum multiplied by the function $\sum_i \alpha_i\, u_i(\boldsymbol{r})$. Thus $\hat{\psi}(\boldsymbol{r})$ annihilates one particle, not in a particular mode, but rather at $\boldsymbol{r}$.

The function $\sum_i \alpha_i\, u_i(\boldsymbol{r})$ may be regarded as the wave function of the state $|\Phi\rangle$. We can write this more formally:

$$\phi(\boldsymbol{r}) \equiv \langle \boldsymbol{r}|\Phi\rangle = \langle v|\hat{\psi}(\boldsymbol{r})|\Phi\rangle \tag{5.25}$$

Is this wave function normalized? Yes, provided only that $|\Phi\rangle$ is. Let us start with

$$\int |\phi(\boldsymbol{r})|^2\, d^3r = \langle\Phi|\hat{\psi}(\boldsymbol{r})^\dagger|v\rangle\langle v|\hat{\psi}(\boldsymbol{r})|\Phi\rangle\, d^3r \tag{5.26}$$

$$= \int \sum_{n_1=0,\cdots}^{\infty} \langle\Phi|\hat{\psi}(\boldsymbol{r})^\dagger|n_1, n_2, \cdots\rangle\langle n_1, n_2, \cdots|\hat{\psi}(\boldsymbol{r})|\Phi\rangle\, d^3r\,. \tag{5.27}$$

We replaced $|v\rangle\langle v|$ by the sum of projectors $\sum |n_1, n_2, \cdots\rangle\langle n_1, n_2, \cdots|$ because $\hat{\psi}|\Phi\rangle$ is proportional to the vacuum, which is orthogonal to every basis vector save for itself. The sum in Eq. (5.27) is over all basis vectors in Fock space, Eq. (5.16). By completeness of Fock space the sum of projectors is just $\hat{I}$. Therefore,

$$\int |\phi(\boldsymbol{r})|^2\, d^3r = \langle\Phi| \int \hat{\psi}(\boldsymbol{r})^\dagger \hat{\psi}(\boldsymbol{r})\; d^3r|\Phi\rangle\,. \tag{5.28}$$

Using Eq. (5.22) and the orthogonality of the u_i we get

$$\int \hat{\psi}(\boldsymbol{r})^\dagger \hat{\psi}(\boldsymbol{r})\, d^3r = \sum_i \hat{a}_i^\dagger\, \hat{a}_i = \sum_i \hat{N}_i = \hat{N}\,. \tag{5.29}$$

which defines the total particle number observable $\hat{N}$. Since $|\Phi\rangle$ is a one-particle state, $\hat{N}\,|\Phi\rangle = |\Phi\rangle$, and so the integral in Eq. (5.28) is unity, as promised.

Eq. (5.25) connects field theory (or QT of many-particle systems) to one-particle quantum mechanics: the state-vacuum matrix element of the field operator equals the one-particle wave function. We can use the idea to construct the many-particle wave function $\phi_N(\boldsymbol{r}_1, \boldsymbol{r}_2 \cdots)$ for N bosons. Just operate with the product $\hat{\psi}(\boldsymbol{r}_1)\,\hat{\psi}(\boldsymbol{r}_2)\,\cdots$ on the state (of type $|N\rangle$ as shown in Eq. (5.20)), and take a scalar product of the result with the vacuum state. By Eqs. (5.6) and (5.22) $\hat{\psi}$'s at various locations commute. Thus the resulting wave function (which has still to be normalized—see Exercise 2) is automatically symmetric under exchange of particles.

Exercises:

1. Prove explicitly that $\hat{\psi}(\boldsymbol{r}_0)^\dagger|v\rangle$ is a one-particle state with the particle localized at $\boldsymbol{r} = \boldsymbol{r}_0$.
2. Prove that $[\hat{\psi}(\boldsymbol{r})^\dagger, \hat{N}] = -\hat{\psi}(\boldsymbol{r})^\dagger$ and use the result to normalize the many-particle wave function $\phi_N(\boldsymbol{r}_1, \boldsymbol{r}_2 \cdots) \propto \langle v|\hat{\psi}(\boldsymbol{r}_1)\,\hat{\psi}(\boldsymbol{r}_2)\,\cdots|N\rangle$.
3. It is possible to use the eigenfunctions $u_i(\boldsymbol{r})$ of any observable, not just the Hamiltonian, to form the expansion (5.22). Of course the $\hat{a}_i$ depend on the choice of observable. Prove that the formula $\hat{N} = \sum_i \hat{a}_i^\dagger\,\hat{a}_i$ is invariant in form regardless of which basis is used.
4. Use second quantization methods to construct the wave function for a system of 3 bosons, one in the ground state, one in level #2 and one in level #3.

5.1.4 Observables in second quantization

We have dealt with many-particle states and the operators used to construct them. We still have to specify how to define observables in second quantization. Eq. (5.29) specifies that $\hat{N}$, the sum of mode occupation number operators, can be calculated as

$$\hat{N} = \int \hat{\psi}(\boldsymbol{r})^\dagger \hat{\psi}(\boldsymbol{r})\, d^3r\,. \tag{5.30}$$

In crude language we could say that the total number operator is like the average of the identity taken with respect to the "wave function" $\hat{\psi}$.

Let us try this sort of idea for building many-particle observables on the Hamiltonian. As our base functions we use the $u_i(\boldsymbol{r})$ of the one-particle Hamiltonian $\hat{H}_1$ of Eq. (5.4); each is associated with a certain eigenvalue ε_i. Obviously the energy observable for the whole system will be $\sum_i \hat{N}_i\,\varepsilon_i$, which we can identify with the total Hamiltonian $\hat{\mathcal{H}}$. Of course

$$\begin{aligned}\hat{\mathcal{H}} &= \sum_i \varepsilon_i\, a_i^\dagger\, a_i = \sum_{ij} \varepsilon_i\, a_i^\dagger\, a_j \underbrace{\int u_i^*(\boldsymbol{r})\, u_j(\boldsymbol{r})\, d^3r}_{\delta ij} \\ &= \int \hat{\psi}(\boldsymbol{r})^\dagger \hat{H}_1\, \hat{\psi}(\boldsymbol{r})\, d^3r\,. \end{aligned} \tag{5.31}$$

The total Hamiltonian indeed equals the "average" of the one-particle Hamiltonian taken with respect to the field operator.

We thus adopt the following rule. Given a one-particle observable $\hat{O}$, its many-particle form is taken to be

$$\hat{\mathcal{O}} = \int \psi(\boldsymbol{r})^\dagger \hat{O}\, \psi(\boldsymbol{r})\, d^3r\,. \tag{5.32}$$

Thus, for example, the angular momentum observable for a collection of identical bosons is

$$\hat{\mathcal{L}} = \int \hat{\psi}(\boldsymbol{r})^\dagger\, \boldsymbol{r} \times \frac{\hbar}{i}\boldsymbol{\nabla}\, \hat{\psi}(\boldsymbol{r})\, d^3r\,. \tag{5.33}$$

Because we pass here from a differential (or similar) operator which was already a step to QT, and we average it over a quantum field, this procedure, as well as the use of creation and annihilation operators, is called *second quantization*.

So far we have dealt with observables which can be regarded as one-particle observables before doing the averaging required by second quantization. Occasionally we deal with two-body operators to start with. Consider the last term on the r.h.s. of Eq. (5.1). Suppose that it consists of the sum of all possible terms of the form $V(\hat{\boldsymbol{r}}_i, \hat{\boldsymbol{r}}_j)$, each involving a pair of particles in the system. How to second quantize this system?

Thus far the second quantized observables Eqs. (5.30)-(5.33) have the form of a one-particle operator acting on the "density of particles" $\hat{\psi}^\dagger\,\hat{\psi}$.

Now that we focus on a two-particle operator we should recall the example of electrostatic energy of a density distribution $n(\boldsymbol{r})$ of charges q:

$$V = \tfrac{1}{2} q^2 \int \frac{n(\boldsymbol{r})\, n(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|}\, d^3r\, d^3r' \,. \tag{5.34}$$

By analogy we should construct the following second quantized operator for our problem

$$\hat{\mathcal{V}} = \frac{1}{2} \int \hat{\psi}(\boldsymbol{r}_1)^\dagger \hat{\psi}(\boldsymbol{r}_1)\, V(\boldsymbol{r}_1, \boldsymbol{r}_2)\, \hat{\psi}(\boldsymbol{r}_2)^\dagger \hat{\psi}(\boldsymbol{r}_2)\, d^3r_1\, d^3r_2 \,. \tag{5.35}$$

In the last equations the factor $\frac{1}{2}$ guards against double counting of interactions. Of course there is another way of ordering the operators whereby the two $\hat{\psi}^\dagger$s precede the $\hat{\psi}$ (see Exercise 2), but the difference is not important.

Exercises:

1. Show that the second-quantized operator $\hat{\mathcal{O}} = \int \hat{\psi}(\boldsymbol{r})^\dagger\, \hat{O}\, \hat{\psi}(\boldsymbol{r})\, d^3r$ (where $\hat{O}$ is a one-particle operator in position representation) commutes with $\hat{N}$.

2. Show that for a system with a definite total number of particles, the difference between Eq. (5.35) and that with an alternative operator ordering is just a constant number, not an operator.

5.1.5 Exchange energy

Suppose we have a system of identical bosons with a two-particle potential $V(\boldsymbol{r}_1, \boldsymbol{r}_2)$. We define its state $|n_1, n_2, \cdots\rangle$ according to the modes deriving from $\hat{H}_1$). What is the mean energy in that state? That is, what is the expectation value of the total Hamiltonian?

We take $\hat{H}_1$ as in Eq. (5.4). Then by Eqs. (5.31) and (5.35) we write

$$\hat{\mathcal{H}} = \int \hat{\psi}(\boldsymbol{r})^\dagger \hat{H}_1\, \hat{\psi}(\boldsymbol{r})\, d^3r + \frac{1}{2} \int \hat{\psi}(\boldsymbol{r}_1)^\dagger \hat{\psi}(\boldsymbol{r}_1)\, V(\boldsymbol{r}_1, \boldsymbol{r}_2)\, \hat{\psi}(\boldsymbol{r}_2)^\dagger \hat{\psi}(\boldsymbol{r}_2)\, d^3r_1\, d^3r_2 \,. \tag{5.36}$$

Substituting Eq. (5.22) with the $\hat{H}_1$ eigenfunctions as basis into the second term here gives us

$$\hat{\mathcal{H}} = \sum_i \varepsilon_i \, a_i^\dagger \, a_i + \frac{1}{2} \sum_{ijkl} \hat{a}_i^\dagger \, \hat{a}_j \, \hat{a}_k^\dagger \, \hat{a}_l \, V_{ijkl} \, ; \tag{5.37}$$

$$V_{ijkl} \equiv \int u_i(\boldsymbol{r}_1)^* \, u_j(\boldsymbol{r}_1) V(\boldsymbol{r}_1, \boldsymbol{r}_2) \, u_k(\boldsymbol{r}_1)^* \, u_l(\boldsymbol{r}_1) \, d^3 r_1 \, d^3 r_2 \, . \tag{5.38}$$

The interaction term has two annihilation operators and two creation operators in each term; it is obvious that if $\hat{\mathcal{H}}$ acts on any state, it produces another state with the same number of particles. The Hamiltonian in Eq. (5.37) can be summarized diagrammatically as in Fig. 5.1.

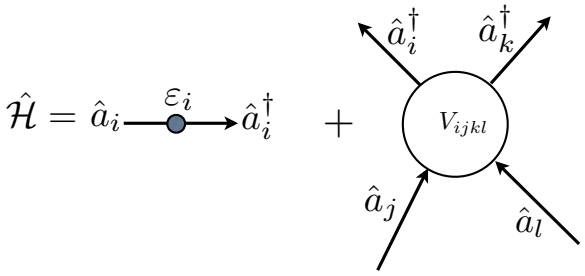

Figure 5.1: **Diagrammatic representation of the Hamiltonian (5.37).**

Now we look at $\langle \hat{\mathcal{H}} \rangle \equiv \langle n_1, n_2, \cdots | \hat{\mathcal{H}} | n_1, n_2, \cdots \rangle$. The contribution of the first term in $\mathcal{H}$ is obviously $\sum_i n_i \varepsilon_i$. The orthogonality of the $|n_1, n_2, \cdots\rangle$ means that the expectation value of the potential term in Eq. (5.37) will vanish unless the two modes in which particles are created are the same modes in which particles are annihilated; but it is, of course, possible for a single mode to be involved.

The term with $i = j = k = l$ is

$$\tfrac{1}{2} V_{iiii} \, \langle n_1, n_2, \cdots | \hat{a}_i^\dagger \, \hat{a}_i \, \hat{a}_i^\dagger \, \hat{a}_i | n_1, n_2, \cdots \rangle = \tfrac{1}{2} V_{iiii} \, n_i(n_i - 1) + \cdots \tag{5.39}$$

In the calculation we replace $\hat{a}_i^\dagger \, \hat{a}_i \, \hat{a}_i^\dagger \, \hat{a}_i$ by $\hat{a}_i^\dagger \, \hat{a}_i^\dagger \, \hat{a}_i \, \hat{a}_i + \hat{a}_i^\dagger \, \hat{a}_i$. We discard the second term (see below). The expectation value of the quartic term is just

the norm of the state $(\hat{a}_i)^2\,|n_1, n_2, \cdots\rangle$. Using Eq. (5.19) twice discloses that the said norm is $n_i(n_i - 1)$ assuming $|n_1, n_2, \cdots\rangle$ is normalized.

We now look at the case $i = j \neq k = l$:

$$\frac{1}{2}\,V_{iijj}\,\langle n_1, n_2, \cdots|\hat{a}_i^\dagger\,\hat{a}_i\,\hat{a}_k^\dagger\,\hat{a}_k|n_1, n_2, \cdots\rangle = \frac{1}{2}\,V_{iikk}\,n_i\,n_k\,. \tag{5.40}$$

Here we have just applied $\hat{N}_k$ and then $\hat{N}_i$ to the state.

Similarly for $i = l \neq j = k$ we have

$$\frac{1}{2}\,V_{ijji}\,\langle n_1, n_2, \cdots|\hat{a}_i^\dagger\,\hat{a}_j\,\hat{a}_j^\dagger\,\hat{a}_i|n_1, n_2, \cdots\rangle = \frac{1}{2}\,V_{ijji}\,n_i\,n_j\,. \tag{5.41}$$

We have replaced $\hat{a}_i^\dagger\,\hat{a}_j\,\hat{a}_j^\dagger\,\hat{a}_i$ by $\hat{a}_j^\dagger\,\hat{a}_j\,\hat{a}_i^\dagger\,\hat{a}_i + \hat{a}_i^\dagger\,\hat{a}_i$. We again discard the second term. These extra terms of the form $\hat{a}_i^\dagger\,\hat{a}_i$ have to do with the particular operator ordering assumed in Eq. (5.35), and would disappear for an alternative ordering. Another reason for ignoring them is that together they have the form $\sum_{i,j} V_{ijji}\,n_i$, and so can be absorbed into the first term in Eq. (5.42) below by redefining the ε_i.

Putting all these together gives

$$\langle\hat{\mathcal{H}}\rangle = \sum_i n_i\varepsilon_i + \frac{1}{2}\sum_i V_{iiii}\,n_i(n_i - 1) + \frac{1}{2}\sum_{i\neq j} V_{iijj}\,n_i\,n_j\; + \frac{1}{2}\sum_{i\neq j} V_{ijji}n_i\,n_j. \tag{5.42}$$

The first term in the r.h.s. has obvious significance. The second term says that the $\frac{1}{2}\,n_i(n_i - 1)$ pairs of particles in mode i each contribute

$$V_{iiii} = \int\int |u_i(\boldsymbol{r}_1)|^2\,V(\boldsymbol{r}_1, \boldsymbol{r}_2)\,|u_i(\boldsymbol{r}_2)|^2\,d^3r_1\,d^3r_2 \tag{5.43}$$

to the mean energy. This is reasonable on classical grounds since $|u_i(\boldsymbol{r}_1)|^2$ is density of probability. The next term shows that n_in_j pairs, one particle in mode i and one in j, contribute each

$$V_{iijj} = \frac{1}{2}\int\int |u_i(\boldsymbol{r}_1)|^2\,V(\boldsymbol{r}_1, \boldsymbol{r}_2)\,|u_j(\boldsymbol{r}_2)|^{\,2}\,d^3r_1\,d^3r_2\,. \tag{5.44}$$

This is also reasonable on analogy with the classical expression (5.34).

But the last term in Eq. (5.42) is strange. It has each of $n_i n_j$ pairs contributing energy

$$V_{ijji} = \frac{1}{2}\int\int u_i(\boldsymbol{r}_1)^*\, u_j(\boldsymbol{r}_1)\, V(\boldsymbol{r}_2,\boldsymbol{r}_2)\, u_j(\boldsymbol{r}_2)^*\, u_i(\boldsymbol{r}_2)\, d^3r_1\, d^3r_2\,. \tag{5.45}$$

Here we do not identify any density of probability! The extra term is a purely quantum phenomenon, a so called *exchange effect*. Its roots are in the identity of bosons of the same type. For let us imagine the wave function of a *pair* of particles, one in mode i and one in j. Using the recipe (5.2) we have

$$w(\boldsymbol{r}_1,\boldsymbol{r}_2) = \frac{u_i(\boldsymbol{r}_1)\, u_j(\boldsymbol{r}_2) + u_i(\boldsymbol{r}_2)\, u_j(\boldsymbol{r}_1)}{\sqrt{2}} \tag{5.46}$$

The $\sqrt{2}$ is for normalization assuming the u_i are normalized. Calculating the mean value of $V(\boldsymbol{r}_1,\boldsymbol{r}_2)$ in this state (again cf. Eq. (5.34)) gives

$$\frac{1}{2}\int\int |w(\boldsymbol{r}_1,\boldsymbol{r}_2)|^2\, V(\boldsymbol{r}_1,\boldsymbol{r}_2)\, d^3r_1\, d^3r_2 = \frac{1}{2}V_{iijj} + \frac{1}{2}V_{ijji}\,. \tag{5.47}$$

Obviously we have recovered the troublesome term in Eq. (5.42) along with its companion two-mode contribution. It may be seen that the second quantization formalism has taken care of symmetrizing wave functions behind the scene.

The exchange effect has important consequences for any collection of bosons. When the two particles in $w(\boldsymbol{r}_1,\boldsymbol{r}_2)$ are near each other, $|w^2|$ approaches $2|u_i(\boldsymbol{r}_1)|^2\,|u_j(\boldsymbol{r}_1)|^2$, which is twice what intuition would suggest. Thus if V is negative (attractive forces) the exchange effect favors bringing a boson closer to its fellows than in a random distribution since this helps to lower the system's energy. Of course if V describes a repulsion, the exchange energy is positive and tends to keep bosons as far apart as possible. The density correlation function for a boson gas or liquid is thus affected by this phenomenon. The energy of a bosonic system receives a contribution from the exchange effect and thus we speak of *exchange energy*.

5.1.6 Dynamics of systems of identical particles

Thus far we have discussed identical particle systems at a fixed time. How do they change? We answer this question here in Heisenberg picture. We assume that the fundamental operator, the field operator, obeys an Heisenberg

equation:

$$\imath\hbar\,\frac{\partial\hat{\psi}(\boldsymbol{r},t)}{\partial t}=[\hat{\psi}(\boldsymbol{r},t),\hat{\mathcal{H}}]\,. \tag{5.48}$$

This, of course, makes $\hat{\psi}$ time dependent; in expanding it in basis function as in Eq. (5.22) we must now regard the $\hat{a}_i$ as time dependent.

For a first exploration we take $\hat{H}$ as in Eq. (5.31). And we use the obvious result (see Exercises)

$$[\hat{\psi}(\boldsymbol{r},t),\hat{\psi}(\boldsymbol{r}',t)^\dagger]=\delta(\boldsymbol{r}-\boldsymbol{r}')\,. \tag{5.49}$$

Then, in view of the rule

$$[\hat{A},\hat{B}\,\hat{C}]=[\hat{A},\hat{B}]\,\hat{C}+\hat{B}\,[\hat{A},\hat{C}] \tag{5.50}$$

we have

$$[\hat{\psi}(\boldsymbol{r},t),\hat{\mathcal{H}}]=\int[\hat{\psi}(\boldsymbol{r},t),\hat{\psi}(\boldsymbol{r}',t)^\dagger]\,\hat{H}_1'\,\hat{\psi}(\boldsymbol{r}',t)\,d^3r'=\hat{H}_1\,\hat{\psi}(\boldsymbol{r},t)\,, \tag{5.51}$$

from which follows that

$$\imath\hbar\,\frac{\partial\hat{\psi}(\boldsymbol{r},t)}{\partial t}=\hat{H}_1\,\hat{\psi}(\boldsymbol{r},t)\,. \tag{5.52}$$

In other words, when there are no two-particle interactions, the field operator obeys Schrödinger's equation. An immediate consequence is that Eq. (5.22) may now be written in terms of the eigenfunctions and eigenvalues of $\hat{H}_1$ as

$$\hat{\psi}(\boldsymbol{r},t)=\sum_i\hat{a}_i(0)\,e^{-\imath\varepsilon_i t/\hbar}\,u_i(\boldsymbol{r})\,. \tag{5.53}$$

This is analogous to the fact that in the expansion of a wave function in energy eigenfunctions, the term with energy ε_i varies as $e^{-\imath\varepsilon_i t/\hbar}$.

Now we consider the full Hamiltonian (5.36); we may concentrate on the commutator

$$[\hat{\psi}(\boldsymbol{r},t),\hat{\psi}(\boldsymbol{r}_1,t)^\dagger\,\hat{\psi}(\boldsymbol{r}_1,t)\,\hat{\psi}(\boldsymbol{r}_2,t)^\dagger\,\hat{\psi}(\boldsymbol{r}_2,t)]\,, \tag{5.54}$$

which after employing Eq. (5.50) repeatedly we cast into the form

$$\delta(\boldsymbol{r}-\boldsymbol{r}_1)\hat{\psi}(\boldsymbol{r}_1,t)\,\hat{\psi}(\boldsymbol{r}_2,t)^\dagger\,\hat{\psi}(\boldsymbol{r}_2,t)+\delta(\boldsymbol{r}-\boldsymbol{r}_2)\hat{\psi}(\boldsymbol{r}_1,t)^\dagger\,\hat{\psi}(\boldsymbol{r}_1,t)\,\hat{\psi}(\boldsymbol{r}_2,t)\,. \tag{5.55}$$

If we now substitute this into $[\hat{\psi}(\boldsymbol{r},t),\mathcal{V}]$ with $\mathcal{V}$ from Eq. (5.35) and construct the Heisenberg equation we get

$$\imath\hbar\,\frac{\partial\hat{\psi}(\boldsymbol{r},t)}{\partial t} = \hat{H}_1\,\hat{\psi}(\boldsymbol{r},t) + \frac{1}{2}\left\{\int \hat{\psi}(\boldsymbol{r}',t)^\dagger\,V(\boldsymbol{r},\boldsymbol{r}')\,\hat{\psi}(\boldsymbol{r}',t)\,d^3r\,,\;\hat{\psi}(\boldsymbol{r},t)\right\} \tag{5.56}$$

where we have used the symmetry $V(\boldsymbol{r}',\boldsymbol{r}) = V(\boldsymbol{r},\boldsymbol{r}')$ and introduced the anticommutator $\{\cdots\}$. (The anticommutator of $\hat{A}$ and $\hat{B}$ is defined as $\{\hat{A}\,,\hat{B}\} \equiv \hat{A}\,\hat{B} + \hat{B}\,\hat{A}$. This symbol is distinguished from a Poisson bracket by the lack the P subscript.)

This equation of motion (*field equation*) for $\hat{\psi}(\boldsymbol{r},t)$ is actually a *nonlinear, nonlocal* integrodifferential equation. It is nonlocal because values of $\hat{\psi}$ at places other than $\boldsymbol{r}$ influence the rate of change of $\hat{\psi}(\boldsymbol{r},t)$. The physical reason is that the potential $V(\boldsymbol{r}',\boldsymbol{r})$ connects particles far apart. The equation is nonlinear because the interaction term in the Hamiltonian involves four field operators. The physical reason is that when particles scatter each other, there are two ingoing and two outgoing particles—requiring four field factors. The nonlocality and nonlinearity make it difficult to solve Eq. (5.56).

Let us consider a simplification. Assume that

$$V(\boldsymbol{r}',\boldsymbol{r}) = \lambda\,\delta(\boldsymbol{r}'-\boldsymbol{r}) \tag{5.57}$$

with λ a real constant. This means the force between two particles is a contact force (acts only at zero range) of constant strength. Substituting Eq. (5.57) in Eq. (5.56) we get

$$\imath\hbar\,\frac{\partial\hat{\psi}(\boldsymbol{r},t)}{\partial t} = \left[\hat{H}_1 + \lambda\,\hat{\psi}(\boldsymbol{r},t)^\dagger\,\hat{\psi}(\boldsymbol{r},t)\right]\hat{\psi}(\boldsymbol{r},t)\,. \tag{5.58}$$

This local but still nonlinear, partial differential equation is called the *nonlinear Schrödinger equation*, first employed by E. P. Gross and L. P. Pitaevskii as a model of a superfluid. An earlier variant of it—the Ginzburg[1]-Landau equation—has been important in superconductivity theory. A relativistic version of it—the Higgs equation—is central in modern gauge theory of particles. The equation is also used in quantum and nonlinear optics.

[1]Nobel Laureate Vitaly Lazarevich Ginzburg (1916-2009) was a prolific Russian-Jewish theoretical physicist. He made crucial contributions to the theories of superconductivity, propagation of electromagnetic waves in plasmas, cosmic rays acceleration and collapsed astrophysical objects.

As might be expected from the graphic representation of the Hamiltonian (5.36), the total number of particles, $\hat{N}$, is conserved in this theory. The proof is as follows. First $\hat{N}$ commutes with the first term in (5.36) by virtue of Exercise 1, Sec. 5.1.4. This can also be seen by observing that the $\hat{N}_i$ commute among themselves.

Next we commute $\hat{N}$ with the group of field operators in the integrand of Eq. (5.35). We use Exercise 3 of Sec. 5.1.3 together with its Hermitian conjugate $[\hat{\psi}(\boldsymbol{r},t),\hat{N}] = \hat{\psi}(\boldsymbol{r},t)$. In condensed notation

$$\begin{aligned}
&\hat{N}\hat{\psi}_1^\dagger\hat{\psi}_1\hat{\psi}_2^\dagger\hat{\psi}_2 = \hat{\psi}_1^\dagger\hat{N}\hat{\psi}_1\hat{\psi}_2^\dagger\hat{\psi}_2 + \hat{\psi}_1^\dagger\hat{\psi}_1\hat{\psi}_2^\dagger\hat{\psi}_2 \\
&= \hat{\psi}_1^\dagger\hat{\psi}_1\hat{N}\hat{\psi}_2^\dagger\hat{\psi}_2 - \hat{\psi}_1^\dagger\hat{\psi}_1\hat{\psi}_2^\dagger\hat{\psi}_2 + \hat{\psi}_1^\dagger\hat{\psi}_1\hat{\psi}_2^\dagger\hat{\psi}_2 = \hat{\psi}_1^\dagger\hat{\psi}_1\hat{N}\hat{\psi}_2^\dagger\hat{\psi}_2 \\
&= \hat{\psi}_1^\dagger\hat{\psi}_1\hat{\psi}_2^\dagger\hat{N}\hat{\psi}_2 + \hat{\psi}_1^\dagger\hat{\psi}_1\hat{\psi}_2^\dagger\hat{\psi}_2 = \hat{\psi}_1^\dagger\hat{\psi}_1\hat{\psi}_2^\dagger\hat{\psi}_2\hat{N} - \hat{\psi}_1^\dagger\hat{\psi}_1\hat{\psi}_2^\dagger\hat{\psi}_2 + \hat{\psi}_1^\dagger\hat{\psi}_1\hat{\psi}_2^\dagger\hat{\psi}_2 \\
&= \hat{\psi}_1^\dagger\hat{\psi}_1\hat{\psi}_2^\dagger\hat{\psi}_2\hat{N}
\end{aligned} \tag{5.59}$$

Thus $\hat{N}$ commutes with the interaction part of the Hamiltonian (5.36) as well as with its "free part". It follows from Heisenberg's equation that $\hat{N}$ is a conserved observable.

Exercises:

1. Prove Eq. (5.49) assuming the $\hat{a}_i(t)$ and $\hat{a}_i(t)^\dagger$ obey the usual commutation relations at any given time.

2. Work out from Eq. (5.52) the equation of motion for $\hat{a}_i(t)$ when the Hamiltonian is (5.36). Does $\hat{a}_i$ vary harmonically? Why? Verify Eq. (5.53) when the interaction term (5.35) vanishes.

5.2 Second quantization for fermions

The second quantization for bosons is Dirac's creation. The use of commutators like those in Eqs. (5.6) and (5.49) runs into trouble when applied to fermions. The formalism allows states with any number of particles in a mode, something which Pauli's exclusion principle forbids for fermions. The

formalism must thus be adapted for for fermions. This was done by Wigner and Jordan.[2]

5.2.1 Anticommutators and multi-fermion states

Wigner and Jordan required creation and annihilation operators for various modes of fermonic particles to obey anticommutator relations:

$$\{\hat{a}_i, \hat{a}_j\} = 0; \qquad \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0; \qquad \{\hat{a}_i, \hat{a}_j^\dagger\} = \delta_{ij}\,. \tag{5.60}$$

From the elementary operators one forms number operators:

$$\hat{N}_i = \hat{a}_i^\dagger\, \hat{a}_i\,. \tag{5.61}$$

We now consider

$$\hat{N}_i{}^2 = \hat{a}_i^\dagger\, (-\hat{a}_i^\dagger\, \hat{a}_i + 1)\, \hat{a}_i \;= \hat{a}_i^\dagger\, \hat{a}_i \;= \hat{N}_i\,, \tag{5.62}$$

where the term $(a_i^\dagger)^2\, (\hat{a}_i)^2$ drops out because, according to Eq. (5.60), the square of a creation or an annihilation operator is zero! The result tells us that eigenvalues of $\hat{N}_i$ obey ${n_i}^2 = n_i$. Hence

$$n_i = 0, 1\,. \tag{5.63}$$

This fits in with the Pauli exclusion principle.

We now remark that all $\hat{N}_i$ commute with each other. We use the identities in the Exercises to transform $[\hat{N}_i, \hat{N}_j]$:

$$[N_i, N_j] = [\hat{a}_i^\dagger\, \hat{a}_i, \hat{a}_j^\dagger\, \hat{a}_j] = \hat{a}_i^\dagger [\hat{a}_i, \hat{a}_j^\dagger\, \hat{a}_j] + [\hat{a}_i^\dagger, \hat{a}_j^\dagger\, \hat{a}_j]\hat{a}_i \tag{5.64}$$

$$= \hat{a}_i^\dagger \{\hat{a}_i, \hat{a}_j^\dagger\}\hat{a}_j - \hat{a}_i^\dagger\, \hat{a}_j^\dagger \{\hat{a}_i, \hat{a}_j\} + \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\}\hat{a}_j\, \hat{a}_i - \hat{a}_j^\dagger \{\hat{a}_i^\dagger, \hat{a}_j\}\hat{a}_i \tag{5.65}$$

$$= \hat{a}_i^\dagger\, \hat{a}_j\, \delta_{ij} - \hat{a}_j^\dagger \hat{a}_i\, \delta_{ij} = 0 \tag{5.66}$$

Thus mutual eigentstates of the several $\hat{N}_i$ are possible.

[2] Pascual Jordan (1902-1980) was a German theoretical and mathematical physicist who devised (with Born and Heisenberg) the matrix formalism of quantum mechanics, contributed to quantum field theory and to gravitational theory (anticipating the Brans-Dicke scalar tensor theory). Jordan was a Nazi party member for some time.

We build the mutual eigenstates in analogy with the boson case. First we define the vacuum state $|\upsilon\rangle$; it is the state annihilated by every $\hat{a}_i$. Then to form the state $|\chi\rangle$ with one fermion in each of modes $i, j, k \cdots$ we operate on $|\upsilon\rangle$ with $\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k^\dagger \cdots$. Obviously $|\chi\rangle$ is still annihilated by every $\hat{a}_n$ with $n \neq i, n \neq j, \cdots$ because if we operate on it with $\hat{a}_n$, we can permute $\hat{a}_n$ stepwise with every creation operator preceding $|\upsilon\rangle$ and eventually annihilate it. Thus $|\chi\rangle$ has no particles in modes other than modes $i, j, k \cdots$.

Let us now look at

$$\hat{N}_j \, \hat{a}_i^\dagger \, \hat{a}_j^\dagger \, \hat{a}_k^\dagger \cdots |\upsilon\rangle \, . \tag{5.67}$$

We can commute $\hat{N}_j$ with the various $\hat{a}_i^\dagger$ with $i \neq j$ which precede $\hat{a}_j^\dagger$ because each such operation involves two anticommutations between operators for distinct modes. Thus the string of operators is unchanged. When we reach $\hat{a}_j^\dagger$ we have

$$\hat{N}_j \, \hat{a}_j^\dagger = \hat{a}_j^\dagger \, \hat{a}_j \hat{a}_j^\dagger = (-\hat{a}_j \, \hat{a}_j^\dagger + 1) \, \hat{a}_j^\dagger = \hat{a}_j^\dagger \, , \tag{5.68}$$

so that

$$\hat{N}_j |\chi\rangle = |\chi\rangle \, . \tag{5.69}$$

We may conclude that indeed $|\chi\rangle$, as formed above, contains one particle in mode i, one in mode $j, \cdots$ and no particles in the other modes.

We remark that interchanging two particles (interchanging the corresponding $\hat{a}_i^\dagger$ and $\hat{a}_j^\dagger$) in $|\chi\rangle$ changes the sign of the state. This is because the interchange is carried out by permuting, say, $\hat{a}_i^\dagger$ with every creation operator on the way to $\hat{a}_j^\dagger$ and then permutting $\hat{a}_j\dagger$ back to the original place of $\hat{a}_i\dagger$. It is easily seen that this involves an odd number of sign changes. Thus the formalism automatically builds states antisymmetric under exchange of particles, as required for fermions.

We also remark that the collection of states of the form shown in Eq. (5.67) is a complete set. Trying to build extra states by operating on $|\upsilon\rangle$ twice with a creation operator will kill the state since $\hat{a}_i^{\dagger 2} = 0$. Thus Fock space for fermions is spanned exclusively by the basis whose vectors are of the form displayed in Eq. (5.67).

Exercises:

1. Prove the following *identities* for any operators:

$$[\hat{A}, \hat{B}\,\hat{C}] = \{\hat{A}, \hat{B}\}\,\hat{C} - \hat{B}\,\{\hat{A}, \hat{C}\}\,, \tag{5.70}$$
$$]\hat{A}\,\hat{B}, \hat{C}] = \hat{A}\,\{\hat{B}, \hat{C}\} - \{\hat{A}, \hat{C}\}\,\hat{B}\,. \tag{5.71}$$

5.2.2 The field operator for fermions

Fermions are always spinning particles. Thus the basis functions u_i we need to form the field operator are not scalar functions but spinorial functions. We here restrict attention to spin $\frac{1}{2}$ particles. The basis functions are then labeled as $u_{j\sigma_j}(\boldsymbol{r})$ where

$$u_{j\uparrow}(\boldsymbol{r}) = \begin{pmatrix} u_{\uparrow}^{(j)}(\boldsymbol{r}) \\ 0 \end{pmatrix}; \qquad u_{j\downarrow}(\boldsymbol{r}) = \begin{pmatrix} 0 \\ u_{\downarrow}^{(j)}(\boldsymbol{r}) \end{pmatrix} \tag{5.72}$$

are two separate functions for each spatial mode.

We can now write the field operator as a spinorial operator with space dependence:

$$\hat{\psi}(\boldsymbol{r}) = \sum_j \sum_{\sigma_j} \hat{a}_{j\sigma_j}\, u_{j\sigma_j}(\boldsymbol{r})\,. \tag{5.73}$$

Obviously $\hat{\psi}(\boldsymbol{r})$ commutes with $\hat{\psi}(\boldsymbol{r}')$ and $\hat{\psi}(\boldsymbol{r})^\dagger$ with $\hat{\psi}(\boldsymbol{r}')^\dagger$. In addition

$$\{\hat{\psi}(\boldsymbol{r}), \hat{\psi}(\boldsymbol{r}')^\dagger\} = \sum_{ij} \sum_{\sigma_i\sigma_j} \{\hat{a}_{i\sigma_i}, \hat{a}_{j\sigma_j}^\dagger\}\, u_{i\sigma_i}(\boldsymbol{r})\, u_{j\sigma_j}(\boldsymbol{r}')^\dagger \tag{5.74}$$
$$\sum_{ij} \sum_{\sigma_i\sigma_j} \delta_{ij}\, \delta_{\sigma_i\sigma_j} u_{i\sigma_i}(\boldsymbol{r})\, u_{j\sigma_j}(\boldsymbol{r}')^\dagger = \sum_i \sum_{\sigma_i} u_{i\sigma_i}(\boldsymbol{r})\, u_{i\sigma_i}(\boldsymbol{r}')^\dagger\,.$$

For the moment let us concentrate on a problem whose one-particle Hamiltonian $\hat{H}_1$ does not depend on spin, e.g. let us us exclude the Pauli spin term in Eq. (4.35). Then obviously for all j, $u_{\uparrow}^{(j)}(\boldsymbol{r}) = u_{\downarrow}^{(j)}(\boldsymbol{r}) = u_j(\boldsymbol{r})$. Therefore,

$$\sum_i \sum_{\sigma_i} u_{i\sigma_i}(\boldsymbol{r})\, u_{i\sigma_i}(\boldsymbol{r}')^{*T} = \sum_i u_i(\boldsymbol{r})\, u_i(\boldsymbol{r})^* \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} (1 \quad 0) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} (0 \quad 1) \right]$$

We have thus shown that when no spin enters $\hat{H}_1$

$$\{\hat{\psi}(\boldsymbol{r}), \hat{\psi}(\boldsymbol{r}')^\dagger\} = \delta(\boldsymbol{r} - \boldsymbol{r}') \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{5.75}$$

This must actually be true in the more general case too.

As with bosons, $\hat{\psi}(\boldsymbol{r}_0)$ here annihilates a particle at $\boldsymbol{r} = \boldsymbol{r}_0$ and $\hat{\psi}(\boldsymbol{r}_0)^\dagger$ creates a particle at that point. Thus we may again build wave functions for one and several fermions by the same method as we did for bosons. In particular,

$$\phi(\boldsymbol{r}_1, \cdots \boldsymbol{r}_N) \propto \langle v | \, \hat{\psi}(\boldsymbol{r}_1) \cdots \hat{\psi}(\boldsymbol{r}_N) \underbrace{\hat{a}_i^\dagger \cdots \hat{a}_j^\dagger}_{N \text{ operators}} | v \rangle \,. \tag{5.76}$$

By the argument at the end of Sec. 5.2.1 we may see that this wave function is antisymmetric in any two arguments. Since we build it to be continuous this means that ϕ tends to zero when two arguments approach each other. This means one does not find identical fermions close together (just the opposite from bosons—see end of Sec. 5.1.5), another manifestation of Pauli's exclusion principle, which is seen to be encompassed by the formalism.

It is obvious that one can write the operator for total number of fermions as $\hat{N} = \int \hat{\psi}(\boldsymbol{r}_1)^\dagger \, \hat{\psi}(\boldsymbol{r}) \, d^3r$.

Exercises:

1. For fermions prove that $[\hat{N}, \psi(\boldsymbol{r})] = -\psi(\boldsymbol{r})$.
2. Show that one must divide the expression (5.76) by $\sqrt{N!}$ in order to normalize it.

5.2.3 Wavefunctions for the Helium atom

The Helium atom has atomic number $Z = 2$ and two electrons. The one-particle Hamiltonian is

$$\hat{H}_1 = -\frac{\hbar^2}{2m}\Delta - \frac{2e^2}{r} \tag{5.77}$$

where m is the electron's effective mass. We would like to know the wave functions of this atom in the ground state, and in some simple excited state. In this section we neglect the electron-elecron interaction. The eigenfunctions of $\hat{H}_1$ are hydrogenic energy eigenfunctions, but with $Z = 2$. We write them in the format (5.72); the electron's field operator has the form (5.73).

The ground state of He is

$$|\phi_g\rangle = \hat{a}^\dagger_{1\uparrow}\,\hat{a}^\dagger_{1\downarrow}\,|v\rangle. \tag{5.78}$$

where "1" refers to the first Bohr orbital level. Of course, since $\hat{a}_i^2 = 0$, we cannot have both spins aligned. The norm of $|\phi_g\rangle$ is

$$\langle\phi_g|\phi_g\rangle = \langle v|\,\hat{a}_{1\downarrow}\,\hat{a}_{1\uparrow}\,\hat{a}^\dagger_{1\uparrow}\,\hat{a}^\dagger_{1\downarrow}|v\rangle = \langle v|\,\hat{a}_{1\uparrow}\,\hat{a}^\dagger_{1\uparrow}\,\hat{a}_{1\downarrow}\,\hat{a}^\dagger_{1\downarrow}\,|v\rangle\,. \tag{5.79}$$

We have here permuted the leftmost operator *two* sites to the right [this does not require sign change by Eq. (5.60)]. By the commutation rules we have $\hat{a}_{1\uparrow}\,\hat{a}^\dagger_{1\uparrow}\,\hat{a}_{1\downarrow}\,\hat{a}^\dagger_{1\downarrow} = (1 - \hat{a}^\dagger_{1\uparrow}\,\hat{a}_{1\uparrow})(1 - \hat{a}^\dagger_{1\downarrow}\,\hat{a}_{1\downarrow})$. Since the $\hat{a}_\downarrow$ operators annihilate $|v\rangle$, we have simply $\langle\phi_g|\phi_g\rangle = \langle v|1|v\rangle = 1$.

To form the wave function we use the pattern of Eq. (5.76). But in writing the $\hat{\psi}$ operators we need retain from the series (5.73) only the terms which will annihilate particles actually present in $|\phi_g\rangle$; the rest of the terms will simply give zero. Therefore,

$$\phi_g(\boldsymbol{r}_a, s_b; \boldsymbol{r}_b, s_b) = \frac{u_1(\boldsymbol{r}_a)u_1(\boldsymbol{r}_b)}{\sqrt{2}}\langle v|\big(|\uparrow\rangle_a\,\hat{a}_{1\uparrow} + |\downarrow\rangle_a\,\hat{a}_{1\downarrow}\big)\big(|\uparrow\rangle_b\,\hat{a}_{1\uparrow} + |\downarrow\rangle_b\,\hat{a}_{1\downarrow}\big)|\phi_g\rangle\,. \tag{5.80}$$

Here a, b label the electrons, while "1" labels the orbit (mode). The spinors $|\uparrow\rangle$ and $|\downarrow\rangle$ are defined in Eq. (1.13). Obviously the terms $\hat{a}_{1\uparrow}|\uparrow\rangle_a\,\hat{a}_{1\uparrow}|\uparrow\rangle_b$ and $\hat{a}_{1\downarrow}|\downarrow\rangle_a\,\hat{a}_{1\downarrow}|\downarrow\rangle_b$ in the scalar product do not contribute because ${\hat{a}_i}^2 = 0$.

We are left with

$$\begin{aligned}
\phi_g(\boldsymbol{r}_a, s_a; \boldsymbol{r}_b, s_b) &= \frac{u_1(\boldsymbol{r}_a)u_1(\boldsymbol{r}_b)}{\sqrt{2}}\langle v|\Big(|\uparrow\rangle_a|\downarrow\rangle_b\,\hat{a}_{1\uparrow}\hat{a}_{1\downarrow} + |\downarrow\rangle_a|\uparrow\rangle_b\,\hat{a}_{1\downarrow}\hat{a}_{1\uparrow}\Big)|\phi_g\rangle \\
&= u_1(\boldsymbol{r}_a)u_1(\boldsymbol{r}_b)\frac{\Big(|\uparrow\rangle_a|\downarrow\rangle_b - |\downarrow\rangle_a|\uparrow\rangle_b\Big)}{\sqrt{2}}\,\langle v|\hat{a}_{1\uparrow}\,\hat{a}_{1\downarrow}|\phi_g\rangle \\
&= u_1(\boldsymbol{r}_a)u_1(\boldsymbol{r}_b)\,\frac{|\uparrow\rangle_a|\downarrow\rangle_b - |\downarrow\rangle_a|\uparrow\rangle_b}{\sqrt{2}}\,,
\end{aligned} \tag{5.81}$$

where we took recourse to Eq. (5.78) and made multiple use of Eq. (5.60). The resulting wave function factors into spin and spatial parts; the spin part is antisymmetric under exchange of particles whereas the spatial part is symmetric. Overall the ground wave function is antisymmetric as it should. We see further that the spin state is necessarily a *singlet* state, the one corresponding to total spin $S = 0$. Since the two electrons are in the same spatial state, but in opposite spin states, the situation concurs with Pauli's exclusion principle.

We now consider the excited state

$$|\phi_{+1}\rangle \equiv \hat{a}^\dagger_{2\uparrow}\,\hat{a}^\dagger_{1\uparrow}|v\rangle\,. \tag{5.82}$$

Here "2" labels the Bohr $n = 2$ energy level with $l = 0$. The $+1$ refers to the $S_z = +1$ spin projection. Of course there are other spin states that go together with this spatial state; they will be dealt with below. We now have

$$\begin{aligned}\phi_{+1}(\boldsymbol{r}_a, s_b; \boldsymbol{r}_b, s_b) &= \frac{|\uparrow\rangle_a|\uparrow\rangle_b}{\sqrt{2}}\langle v|\big(\hat{a}_1 u_1(\boldsymbol{r}_a) + \hat{a}_2 u_2(\boldsymbol{r}_a)\big)\big(\hat{a}_1 u_1(\boldsymbol{r}_b) + \hat{a}_2 u_2(\boldsymbol{r}_b)\big)|\phi_{+1}\rangle \\ &= \frac{|\uparrow\rangle_a|\uparrow\rangle_b}{\sqrt{2}}\langle v|\big(\hat{a}_1 u_1(\boldsymbol{r}_a)\hat{a}_2 u_2(\boldsymbol{r}_b) + \hat{a}_2 u_2(\boldsymbol{r}_a)\hat{a}_1 u_1(\boldsymbol{r}_b)\big)|\phi_{+1}\rangle \\ &= \frac{|\uparrow\rangle_a|\uparrow\rangle_b}{\sqrt{2}}\big(u_1(\boldsymbol{r}_a)u_2(\boldsymbol{r}_b) - u_2(\boldsymbol{r}_a)u_1(\boldsymbol{r}_b)\big)\langle v|\hat{a}_1\,\hat{a}_2|\phi_{+1}\rangle\,. \end{aligned} \tag{5.83}$$

Since the matrix element here is just the norm of the state $|v\rangle$, which is unity, we find

$$\phi_{+1}(\boldsymbol{r}_a, s_b; \boldsymbol{r}_b, s_b) = \frac{\big(u_1(\boldsymbol{r}_a)u_2(\boldsymbol{r}_b) - u_2(\boldsymbol{r}_a)u_1(\boldsymbol{r}_b)\big)}{\sqrt{2}}|\uparrow\rangle_a|\uparrow\rangle_b\,. \tag{5.84}$$

We see that in $|\phi_{+1}\rangle$ it is the spatial wave function which is antisymmetric. Because the spin wave function is symmetric, we have a total antisymmetric wave function.

It is obvious that the state $|\phi_{-1}\rangle \equiv \hat{a}^\dagger_{2\downarrow}\,\hat{a}^\dagger_{1\downarrow}|v\rangle$ is a $S_z = -1$ state, whose wave function will differ from that in Eq. (5.84) only by having the spin factor $|\downarrow\rangle_a|\downarrow\rangle_b$. Both these states belong to the triplet with $S = 1$. Excited Helium in one of the triplet spin states with antisymmetric spatial wave function is called *orthohelium*.

We now look simultaneously at two $S_z = 0$ states:

$$|\phi_\pm\rangle \equiv \frac{1}{\sqrt{2}}\big(\hat{a}^\dagger_{1\uparrow}\,\hat{a}^\dagger_{2\downarrow} \pm \hat{a}^\dagger_{1\downarrow}\,\hat{a}^\dagger_{2\uparrow}\big)\,|v\rangle\,. \tag{5.85}$$

These states are normalized. We proceed to form their wave functions:

$$\begin{aligned}&\phi_+(\boldsymbol{r}_a, s_a; \boldsymbol{r}_b, s_b)\\ &= \frac{1}{2}\langle v|\big(\hat{a}_{1\uparrow}u_1(\boldsymbol{r}_a)|\uparrow\rangle_a + \hat{a}_{2\downarrow}u_2(\boldsymbol{r}_a)|\downarrow\rangle_a + \hat{a}_{1\downarrow}u_1(\boldsymbol{r}_a)|\downarrow\rangle_a + \hat{a}_{2\uparrow}u_2(\boldsymbol{r}_a)|\uparrow\rangle_a\big)\times\\ &\big(\hat{a}_{1\uparrow}u_1(\boldsymbol{r}_b)|\uparrow\rangle_b + \hat{a}_{2\downarrow}u_2(\boldsymbol{r}_b)|\downarrow\rangle_b + \hat{a}_{1\downarrow}u_1(\boldsymbol{r}_b)|\downarrow\rangle_b + \hat{a}_{2\uparrow}u_2(\boldsymbol{r}_b)|\uparrow\rangle_b\big)\,.\end{aligned} \tag{5.86}$$

Again all squares of the same $\hat{a}$ disappear; in addition a product of $\hat{a}$'s that does not balance a pair of $\hat{a}^\dagger$ in Eq. (5.85) will annihilate the vacuum state, so all these can be dropped. We are left with

$$\begin{aligned}&u_1(\boldsymbol{r}_a)u_2(\boldsymbol{r}_b)\big(\hat{a}_{1\uparrow}\,\hat{a}_{2\downarrow}|\uparrow\rangle_a|\downarrow\rangle_b + \hat{a}_{1\downarrow}\,\hat{a}_{2\uparrow}|\downarrow\rangle_a|\uparrow\rangle_b\big)\\ &+u_1(\boldsymbol{r}_b)u_2(\boldsymbol{r}_a)\big(\hat{a}_{2\downarrow}\,\hat{a}_{1\uparrow}|\downarrow\rangle_a|\uparrow\rangle_b + \hat{a}_{2\uparrow}\,\hat{a}_{1\downarrow}|\uparrow\rangle_a|\downarrow\rangle_b\big)\,.\end{aligned} \tag{5.87}$$

A tedious calculation shows that the matrix element of this expression between $|\phi_+\rangle$ and $\langle v|$ is

$$\phi_+(\boldsymbol{r}_a, s_b; \boldsymbol{r}_b, s_b) = \frac{u_1(\boldsymbol{r}_b)u_2(\boldsymbol{r}_a) - u_2(\boldsymbol{r}_b)u_1(\boldsymbol{r}_a)}{\sqrt{2}}\,\frac{|\uparrow\rangle_a|\downarrow\rangle_b + |\downarrow\rangle_a|\uparrow\rangle_b}{\sqrt{2}} \tag{5.88}$$

This wave function's spatial part is antisymmetric while the spin part is symmetric; the total wave function is antisymmetric as required. These symmetry properties are precisely analogous to those of states $|\phi_{+1}\rangle$ and $|\phi_{-1}\rangle$, and show $|\phi_+\rangle$ to belong with them in the triplet state with $S = 1$, and to form part of orthohelium's complement of states.

The matrix elements of expression (5.87) between $|\phi_-\rangle$ and $\langle v|$ gives

$$\phi_-(\boldsymbol{r}_a, s_b; \boldsymbol{r}_b, s_b) = \frac{\big(u_1(\boldsymbol{r}_b)u_2(\boldsymbol{r}_a) + u_2(\boldsymbol{r}_b)u_1(\boldsymbol{r}_a)\big)}{\sqrt{2}}\,\frac{|\downarrow\rangle_a|\uparrow\rangle_b - |\uparrow\rangle_a|\downarrow\rangle_b}{\sqrt{2}} \tag{5.89}$$

Here it is the spin wave function which is antisymmetric (singlet state—$S = 0$), while the spatial wave function is symmetric. Helium in such an excited state is called *parahelium*.

Some of the above wave function exhibit *entanglement*, which Schrödinger was first to identify as one of the defining characteristics of the quantum world. The spin wave functions of $|\phi_g\rangle$, $|\phi_-\rangle$, $|\phi_+\rangle$ and the spatial wave functions of all parahelium and orthohelium states are both entangled in the sense that they cannot be factored into wave functions for this and that particle. The states of the particles are thus correlated independently of the forces between them. If one determines the state of one particle in an entangled pair, one actually learns about the state of the other without looking at it.

5.2.4 Many particle observables for fermions

The prescription for turning a one-particle operator $\hat{O}$ into a many-particle fermion operator is similar to that for bosons:

$$\begin{aligned}\hat{\mathcal{O}} &= \int \psi(\boldsymbol{r})^\dagger \hat{O}\, \psi(\boldsymbol{r})\, d^3r \qquad (5.90)\\ &= \int d^3r \sum_j \left(\hat{a}^\dagger_{j\uparrow} u_{j\uparrow}(\boldsymbol{r})^\dagger + \hat{a}^\dagger_{j\downarrow} u_{j\downarrow}(\boldsymbol{r})^\dagger\right) \hat{O} \sum_i \left(\hat{a}_{i\uparrow} u_{i\uparrow}(\boldsymbol{r}) + \hat{a}_{i\downarrow} u_{i\downarrow}(\boldsymbol{r})\right).\end{aligned}$$

The (normalized) spinors are defined as in Eq. (5.72). If $\hat{O}$ does not depend on spin, e.g. momentum, orbital angular momentum, etc. and the u_j are eigenfunction of $\hat{O}$, one can immediately carry out the multiplication of the spin parts of the $u_{j\sigma_j}$ as well as the integration:

$$\hat{\mathcal{O}} = \sum_j \left(\hat{a}^\dagger_{j\uparrow}\, a_{j\uparrow} + a^\dagger_{j\downarrow}\, a_{j\downarrow}\right) o_j = \sum_{j\sigma_j} \hat{a}^\dagger_{j\sigma_j}\, a_{j\sigma_j}\, o_j\,. \qquad (5.91)$$

We second quantize a two-particle operator like $V(\boldsymbol{r}_1, s_1; \boldsymbol{r}_2, s_2)$ as in Eq. (5.35). The full Hamiltonian with interactions, Eq. (5.36), takes the form

$$\begin{aligned}\hat{\mathcal{H}} &= \sum_i \varepsilon_i\, a^\dagger_i\, a_i + \frac{1}{2} \sum_{ijkl} \sum_{\sigma_i\sigma_j\sigma_k\sigma_l} \hat{a}^\dagger_{i\sigma_i}\, \hat{a}_{j\sigma_j}\, \hat{a}^\dagger_{k\sigma_k}\, \hat{a}_{l\sigma_l}\, V_{i\sigma_i;j\sigma_j;k\sigma_k;l\sigma_l}\,, \qquad (5.92)\\ V_{i\sigma_i;j\sigma_j;k\sigma_k;l\sigma_l} &\equiv \int\int u_{i\sigma_i}(\boldsymbol{r}_1)^\dagger\, u_{j\sigma_j}(\boldsymbol{r}_1)\, V(\boldsymbol{r}_1, s_1; \boldsymbol{r}_2, s_2)\, u_{k\sigma_k}(\boldsymbol{r}_2)^\dagger\, u_{l\sigma_l}(\boldsymbol{r}_2)\, d^3r_1\, d^3r_2\,.\end{aligned}$$

In this general form the terms with $(i, \sigma_i) = (k, \sigma_k)$ or $(j, \sigma_j) = (l, \sigma_l)$ must vanish because $\hat{a}_i^2 = (\hat{a}_i^\dagger)^2 = 0$. Further, the orthogonality of the spinors

(5.72) kills the components of the $V_{i\sigma_i;j\sigma_i;k\sigma_k;l\sigma_k}$ with $\sigma_i \neq \sigma_j$ or $\sigma_k \neq \sigma_l$. In addition, the symmetry under exchange of the potential tells us that

$$V_{i\sigma_i;j\sigma_i;k\sigma_k;l\sigma_k} = V_{k\sigma_k;l\sigma_k;i\sigma_i;j\sigma_i} \,. \tag{5.93}$$

In the example that follows the two-particle potential is the Coulomb one; it does not depend on spin, so that we may drop the spin indices in the $V_{i\sigma_i;j\sigma_i;k\sigma_k;l\sigma_k}$.

Example: Energies of orthohelium and parahelium

To zeroth order orthohelium and parahelium are degenerate in energy. But the perturbation due to the Coulomb potential between the electrons removes the degeneracy. What are the energies of parahelium and orthohelium (relative to a Bohr model of the atom) in perturbation theory?

Obviously in He the nonvanishing matrix elements of the potential are

$$V_{ijkl} = \int\int u_i(\boldsymbol{r}_a)^*\, u_j(\boldsymbol{r}_a)\, \frac{e^2}{|\boldsymbol{r}_a - \boldsymbol{r}_b|}\, u_k(\boldsymbol{r}_b)^*\, u_l(\boldsymbol{r}_b)\, d^3r_a\, d^3r_b \,, \tag{5.94}$$

where all mention of spins has disappeared, so we use conjugate rather than Hermitian conjugate eigenfunctions. Because of rotational invariance of V, the three states in the orthohelium triplet must remain degenerate, so we need only calculate

$$\tfrac{1}{2} V_{ijkl}\, \langle \phi_\pm |\, \hat{a}^\dagger_{i\sigma_i}\, \hat{a}_{j\sigma_i}\, \hat{a}^\dagger_{k\sigma_k}\, \hat{a}_{l\sigma_k}\, | \phi_\pm \rangle \,. \tag{5.95}$$

Using the form (5.85) for $|\phi_\pm\rangle$ and remembering the constraints inferred following Eq. (5.92), we see that we get a nonzero contribution only for the following combinations of quantum numbers (always $\sigma_i = \sigma_j$ and $\sigma_k = \sigma_l$)

i	j	k	l	σ_i	σ_k
1	1	2	2	1/2	− 1/2
1	2	2	1	1/2	− 1/2
2	1	1	2	1/2	− 1/2
2	2	1	1	1/2	− 1/2

(5.96)

as well as for the four analogous cases with σ_i and σ_k interchanged. Each of the latter four cases contributes to Eq. (5.95) the same as the corresponding case in the list since the potential is spin-independent. Further, because of Eq. (5.93) the first and fourth cases contribute the same, and the second and third contribute the same. We should thus calculate the contributions from the first two cases in the table, multiply them by four and add them.

For the first case in the table the mean value in Eq. (5.95) gives as its only surviving term

$$\frac{1}{2}\langle \upsilon |\, \hat{a}_{2\downarrow}\, \hat{a}_{1\uparrow} \cdot \hat{a}^\dagger_{1\uparrow}\, \hat{a}_{1\uparrow}\, \hat{a}^\dagger_{2\downarrow}\, \hat{a}_{2\downarrow} \cdot \hat{a}^\dagger_{1\uparrow}\, \hat{a}^\dagger_{2\downarrow} | \upsilon \rangle \,, \tag{5.97}$$

which is nothing but the mean value of $\hat{N}_{1\uparrow}\, \hat{N}_{2\uparrow}$ in the state with one up-spin particle in level 1 and one in level 2. This mean value is, of course, unity.

For the second case in the list the surviving term is a cross term:

$$\begin{aligned} &\pm \frac{1}{2}\langle \upsilon |\, \hat{a}_{2\downarrow}\, \hat{a}_{1\uparrow} \cdot \hat{a}^\dagger_{1\uparrow}\, \hat{a}_{2\uparrow}\, \hat{a}^\dagger_{2\downarrow}\, \hat{a}_{1\downarrow} \cdot \hat{a}^\dagger_{1\downarrow}\, \hat{a}^\dagger_{2\uparrow} | \upsilon \rangle \\ &= \mp \frac{1}{2}\langle \upsilon |\, \hat{a}_{2\downarrow}\, \hat{a}_{1\uparrow}\, \hat{a}^\dagger_{1\uparrow}\, \hat{a}^\dagger_{2\downarrow}\, \hat{a}_{1\downarrow}\, \hat{a}^\dagger_{1\downarrow}\, \hat{a}_{2\uparrow}\, \hat{a}^\dagger_{2\uparrow} | \upsilon \rangle \\ &= \mp \frac{1}{2}\langle \upsilon |\, \hat{a}_{2\downarrow}\, \hat{a}^\dagger_{2\downarrow}\, \hat{a}_{1\uparrow}\, \hat{a}^\dagger_{1\uparrow}\, \hat{a}_{1\downarrow}\, \hat{a}^\dagger_{1\downarrow}\, \hat{a}_{2\uparrow}\, \hat{a}^\dagger_{2\uparrow} | \upsilon \rangle \end{aligned} \tag{5.98}$$

where we have permuted the order of operators, paying one minus sign at each such step. We have here the mean value in vacuum of the product of four different operators of the form $\hat{a}\,\hat{a}^\dagger$. These can all be written as $1 - \hat{a}^\dagger\,\hat{a} = 1 - \hat{N}^\dagger$. But any $\hat{N}$ annihilates the vacuum. Hence the mean comes out to be ∓ 1.

Putting together all the above we have

$$\langle \upsilon | \hat{\mathcal{H}} | \upsilon \rangle = \varepsilon_1 + \varepsilon_2 + V_{1122} \mp V_{1221}; \tag{5.99}$$

$$V_{1122} = \int\int |u_1(\boldsymbol{r}_a)|^2 \, \frac{e^2}{|\boldsymbol{r}_a - \boldsymbol{r}_b|} \, |u_2(\boldsymbol{r}_b)|^2 \, d^3 r_a \, d^3 r_b \tag{5.100}$$

$$V_{1221} = \int\int u_1(\boldsymbol{r}_a)^* \, u_2(\boldsymbol{r}_a) \, \frac{e^2}{|\boldsymbol{r}_a - \boldsymbol{r}_b|} \, u_2(\boldsymbol{r}_b)^* \, u_1(\boldsymbol{r}_b) \, d^3 r_a \, d^3 r_b$$

Thus orthohelium and parahelium are split in energy. Whereas V_{1122} is obviously positive, the sign of the *exchange integral* V_{1221} is unclear. How do we know which of the two He states is higher in energy?

This can be found out from the two-particle wave functions (5.88)-(5.89); they lead to a result identical to the added term in Eq. (5.99):

$$\frac{1}{2}\int\int \phi_\pm(\boldsymbol{r}_a,\boldsymbol{r}_b)^\dagger \frac{e^2}{|\boldsymbol{r}_a-\boldsymbol{r}_b|}\phi_\pm(\boldsymbol{r}_a,\boldsymbol{r}_b)\,d^3r_a\,d^3r_b = V_{1122}\mp V_{1221}\,. \qquad (5.101)$$

Now the ϕ_- wave function of parahelium, Eq. (5.89), has a symmetric spatial factor which is particularly large when the two particles are together. By contrast ϕ_+ of orthohelium. Eq. (5.88), is spatially antisymmetric, and thus small when the particles are close. This means the integral (5.101), which is obviously positive, is bigger for parahelium than for orthohelium. Obviously, then, the V_{1221} integral is positive. The energy split between parahelium or ortohelium is $2V_{1221}$ with ortohelium the more stable (lower energy) state. The positivity of the integral (5.101) shows that $V_{1221} < V_{1122}$, which puts an upper bound on the splitting. It must be reiterated that all these are first-order perturbation theory results.

As remarked by Heisenberg, the phenomenon of ferromagnetism finds part of its explanation in the exchange integral. As in the above example, the Coulomb repulsion, aided by the exchange phenomenon, favors energetically $S = 1$ states of electron pairs (with spins aligned) over $S = 0$ states. An electron has a magnetic moment operator antialigned with its spin. So thanks to the exchange force all the magnetic moments in a piece of a suitable metal line up parallel to each other. A macroscopic magnetization consequently appears spontaneously, and we get ferromagnetism.

Exercises:

1. Show that $\hat{N}$ is conserved for a fermion system with two-particle interactions.

2. Show that even though fermion fields are anticommuting, a *fermion* field operator representing noninteracting particles still obeys Schrödinger's equation (despite the fact that Heisenberg's equation involves a commutator).

3. If $f(x)$ is an analytic function and $\hat{a}_i$ is a fermion annihilation operator, show that $f(\hat{a}_i\,, \hat{a}_j\,, \cdots)$ is a *linear* function of its argument.

4. A system contains both bosons (operators $\hat{a}$ and $\hat{a}^\dagger$) and fermions (operators $\hat{b}$ and $\hat{b}^\dagger$). Show that the new commutation rules

$$[\hat{a}, \hat{b}] = [\hat{a}^\dagger, \hat{b}^\dagger] = [\hat{a}^\dagger, \hat{b}] = [\hat{a}, \hat{b}^\dagger] = 0\,. \tag{5.102}$$

   are consistent with other commutation relations.

5. Build the spin operator $\hat{\mathcal{S}}$ for a many-fermion system using the eigenfunctions (5.72).

Chapter 6

Relativistic wave equations

All that we have seen up to now refers to nonrelativistic circumstances. The need for a relativistic wave equation arises, among other things, because a simple estimate shows that velocities of the electron in an hydrogen atom in the lower Bohr energy levels is not totally negligible compared to c. Of course, in accelerator experiments one meets ver relativistic situations where it is simply inadequate to start from nonrelativistic QT and make relativistic corrections. But combining relativity with QT is a tricky undertaking. There are certain incompatibilities between the two theories. Relativity regards time on equal footing with spatial coordinates. QT regards time as an evolution parameter that enters Schrödinger's equation in a manner different from the spatial variables.

The total reconciliation of relativistic and quantum ideas occurs only at the level of quantum field theory. However, there are some parts of the structure that can be obtained at the level of QT. One of them is the relativistic wave equations. Unlike in nonrelativistic QT where one wave equations is good for spinning or nonspinning particles, fermions, bosons or anyone, etc., in relativistic theory each spin requires its particular wave equation.

6.1 Klein-Gordon equation

6.1.1 Origins of the Klein-Gordon equation

One way to obtain the Schrödinger equation is to start with the nonrelativistic classical energy-momentum relation:

$$E = \frac{\boldsymbol{p}^2}{2m}\,, \tag{6.1}$$

replace in it

$$\boldsymbol{p} \mapsto \frac{\hbar}{\imath}\boldsymbol{\nabla}; \qquad E \mapsto \imath\hbar\frac{\partial}{\partial t}\,, \tag{6.2}$$

and regard the resulting differential operator relation as operating on the actual wave function.

Originally Schrödinger tried this procedure with the relativistic classical energy-momentum relation

$$E^2 = c^2\boldsymbol{p}^2 + m^2c^4 \tag{6.3}$$

and obtained the *relativistic Schrödinger wave equation*

$$-\hbar^2\frac{\partial^2}{\partial t^2}\psi = -c^2\hbar^2\Delta\psi + m^2c^4\psi\,. \tag{6.4}$$

This has the obvious solution

$$\psi = Ae^{\imath(\boldsymbol{p}\cdot\boldsymbol{r}-Et)/\hbar} \tag{6.5}$$

where the $\boldsymbol{p}$ and E obey Eq. (6.3), and so can be interpreted as momentum and energy of the particle. Then Schrödinger added a potential to Eq. (6.4); this gave a correct account of the Bohr levels of hydrogen, but got the fine structure of the levels (then already regarded as reflecting relativistic corrections) wrong. Schrödinger gave up on his relativistic equation and proceeded to start with Eq. (6.1). Later Klein,[1] Gordon,[2] Fock and others rediscovered and applied Eq. (6.4); it is nowadays called the free Klein-Gordon equation.

[1] Swedish-Jewish theoretical physicist Oskar Benjamin Klein (1894-1977) was the son of the Chief Rabbi of Stockholm. Apart from his eponymous wave equation we owe him the formulation of the Klein paradox, the Kaluza-Klein theory of elementary forces as a reflection of many dimensions, and the Klein-Nishina formula for Compton scattering.

[2] Walter Gordon (1893-1939) was a German-Jewish theoretical physicist. He is known for the Klein-Gordon equation, the exact solution of the Dirac equation for the Hydrogen atom, and the Gordon decomposition of the Dirac current.

6.1.2 Properties of the Klein-Gordon equation

What particle obeys the Klein-Gordon equation? Recall that relation (6.3) is relativistically covariant (looks the same in any Lorentz[3] frame). Since the substitution (6.2) is consistent with relativity, the operator in Eq. (6.4),

$$\frac{\partial^2}{\partial t^2} - c^2\Delta + m^2c^4/\hbar^2\,, \tag{6.6}$$

must be a scalar (invariant) operator in the relativistic sense. In fact with it we can write the Klein-Gordon equation in the manifestly covariant form

$$\eta^{\alpha\beta}\partial_\alpha\,\partial_\beta\,\psi - (m^2c^2/\hbar^2)\psi = 0\,, \tag{6.7}$$

where here and henceforth the Einstein summation convention is in force, $\eta^{\alpha\beta} = \mathrm{diag}\{-1,1,1,1\}$ is the (contravariant) Minkowski metric, and

$$\partial_\alpha = \{c^{-1}\partial/\partial t, \partial/\partial x, \partial/\partial y, \partial/\partial z\}\,.$$

Now if ψ is really a single component wave function, then covariance of the Klein-Gordon equation (6.7) follows from the assumption that ψ is a scalar (Lorentz invariant) function. But a relativistic scalar is automatically a scalar under rotations (because a rotation can be viewed as the composition of two Lorentz transformations in suitable directions). We conclude that the Klein-Gordon equation as written here is the wave equation for spin-0 particles (also called scalar particles). In nature a number of mesons $(\pi^0, \pi^+, K^0, \bar{K}^0, K^+, \cdots)$ have spin-0 and are thought to be well described by the Klein-Gordon equation provided their energies are low enough to make disruption of these composite objects unlikely.

Does ψ have probability interpretation? Let us adopt the Schrödinger nonrelativistic probability current of Eq. (4.55), or

$$\boldsymbol{j} = \frac{\hbar}{2mi}(\psi^*\,\boldsymbol{\nabla}\psi - \psi\,\boldsymbol{\nabla}\psi^*)\,. \tag{6.8}$$

[3]named for the prominent Dutch theoretical physicist Hendrik Antoon Lorentz (1853-1928), a Nobel laureate. Lorentz developed the electromagnetic theory of matter, identified the electromagnetic Lorentz force, invented (independently of Larmor) the Lorentz transformations, and remarked on the Lorentz-FitzGerald contraction. The Lorentz-Lorenz formula—the relation of index of refraction and molecule polarizability—is also named after him.

The usual form for the probability density, $\rho = \psi^* \psi$ does not look similar to $\boldsymbol{j}$, so that it would break covariance; neither will it lead to a continuity equation. With an eye on covariance, let us promote (6.8) to a 4-vector current:

$$j^\alpha = \frac{\hbar}{2m\imath}\eta^{\alpha\beta}(\psi^* \, \partial_\beta\psi - \psi \, \partial_\beta\psi^*) \, . \tag{6.9}$$

We now consider

$$\partial_\alpha j^\alpha = \frac{\hbar}{2m\imath}\eta^{\alpha\beta}(\partial_\alpha\psi^* \, \partial_\beta\psi - \partial_\alpha\psi \, \partial_\beta\psi^* + \psi^* \, \partial_\alpha\partial_\beta\psi - \psi \, \partial_\alpha\partial_\beta\psi^*) \, . \tag{6.10}$$

The first two terms cancel by virtue of the symmetry of $\eta^{\alpha\beta}$ and the last two by virtue of Eq. (6.7). Thus considerations of relativistic covariance have led us to a conserved 4-current.

Since we expect the continuity equation to take on the usual form

$$\partial_\alpha j^\alpha = \partial_t\rho + \boldsymbol{\nabla} \cdot \boldsymbol{j} = 0 \, , \tag{6.11}$$

we must identify charge density ρ with j^t/c. Hence

$$\rho = -\frac{\hbar}{2m\imath c^2}(\psi^* \, \partial_t\psi - \psi \, \partial_t\psi^*) \, . \tag{6.12}$$

To check this let us consider the solution

$$\psi = F(\boldsymbol{r})e^{-\imath Et/\hbar} \tag{6.13}$$

of the Klein-Gordon equation which represents a stationary state. The F must obey a von Helmholtz equation. We find

$$\rho = \frac{E}{mc^2}|F|^2 = \frac{E}{mc^2}|\psi|^2 \, . \tag{6.14}$$

Thus in the nonrelativistic limit ($E \approx mc^2$) we have $\rho \approx |\psi|^2$ which is the correct result for probability density. But ρ in Eq. (6.12) could easily become negative if the time dependence is not that of a stationary state. This rules out our j^α as a generic expression for probability 4-current. Further developments have shown that it is really a charge 4-current. For this later interpretation to make sense, ψ must be complex (otherwise $j^\alpha = 0$) and one must multiply the above expression for j^α by the elementary charge e.

Exercises:

1. Find the exact spherically symmetric and asymptotically bounded stationary solution of the free Klein-Gordon equation with $E < mc^2$. What is the role of the Compton wavelength[4] $\lambda_{\rm C} = \hbar/(mc)$ in it?

2. Write the solution to the free Klein-Gordon equation as $\psi = \chi(\boldsymbol{r}, t)e^{-\imath Et/\hbar}$ and show that for $E \ll mc^2$, χ obeys the usual time dependent free Schrödinger equation.

6.1.3 The Klein paradox

Thus far we have dealt with the free Klein-Gordon equation; let us now generalize it to describe a charged particle in an electromagnetic field described by the potential $\boldsymbol{A}$ and Φ. As in forming the electromagnetic coupled Schrödinger equation (4.10), we now replace $\partial_t \mapsto \partial_t + (\imath e/\hbar c)\Phi$ and $\boldsymbol{\nabla} \mapsto \boldsymbol{\nabla} - (\imath e/\hbar c)\boldsymbol{A}$ in Eq. (6.4):

$$-\hbar^2\big[\partial_t + (\imath e/\hbar)\Phi\big]^2\psi = -c^2\hbar^2\big[\boldsymbol{\nabla} - (\imath e/\hbar c)\boldsymbol{A}\big]^2\psi + m^2c^4\psi \tag{6.15}$$

The same type of argument as used in Sec. 4.1.2 shows that the proposed equation is covariant under the substitutions (4.3) and (4.11). The electromagnetically coupled Klein-Gordon equation can also be cast in manifestly relativistically covariant form:

$$\eta^{\alpha\beta} D_\alpha\, D_\beta\, \psi - (m^2c^2/\hbar^2)\psi = 0\,, \tag{6.16}$$

where $D_\alpha \equiv \partial_\alpha - (\imath e/\hbar c)A_\alpha$ and $A_\alpha = \{-c\Phi, \boldsymbol{A}\}$ is the well known electromagnetic 4-potential. D_α is called the (gauge) covariant derivative.

From now one we consider only the case $\boldsymbol{A} = 0$. Eq. (6.15) takes the form

$$\Delta\psi - \frac{1}{c^2}\big[\partial_t + (\imath e/\hbar)\Phi\big]^2\psi - (m^2c^2/\hbar^2)\psi = 0\,, \tag{6.17}$$

[4]named after Arthur Holly Compton (1892-1962), an American experimental physicist and Nobel laureate known for studies of X-ray scattering by matter during which he discovered his eponymous effect. Compton played a crucial role in the Manhattan project.

which is appropriate for any problem involving only an electric field. We shall look in particular at the one dimensional potential plotted in Fig. 6.1. In any region where the potential is constant the solution of Eq. (6.17) can be assumed to be of the form

$$\psi = C\, e^{\imath(px-Et)/\hbar}\,. \tag{6.18}$$

Substituting this ansatz in Eq. (6.17) gives

$$p^2 = \frac{1}{c^2}(E - e\Phi - mc^2)(E - e\Phi + mc^2)\,. \tag{6.19}$$

In region A we have $E > e\Phi + mc^2$ so that $p^2 > 0$. Thus p is real and we have ordinary wave propagation; if $p > 0$ the wave propagates to the right into the rising potential. In region B we have $E < e\Phi + mc^2$ but obviously $E > e\Phi - mc^2$ so that $p^2 < 0$ and p is imaginary. In this region the solution is a combination of rising and decreasing exponentials $e^{\pm|p|x}$. The situation is like the behavior in nonrelativistic quantum mechanics of a wave function inside a high potential barrier where the potential prevents propagation. Tunneling can then occur if the wave meets a region where the barrier disappears. But here we have a further rise of potential into the region C where obviously $E < e\Phi \pm mc^2$. Instead of this further impeding propagation we find that now $p^2 > 0$ and we again have propagation.

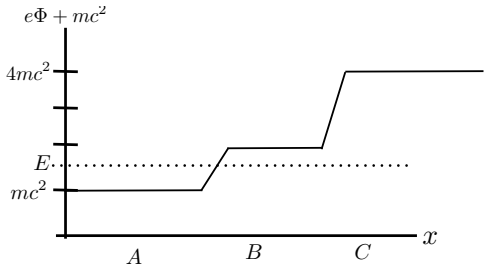

Figure 6.1: **The solid broken line is the potential $\Phi(x)$ discussed in connection with the Klein paradox. The dotted line marks the energy of the particle under discussion.**

We confirm these conclusions by calculating for ψ in Eq. (6.18) the current (6.8) (it does not require an electromagnetic part since $\boldsymbol{A} = 0$):

$$j^x = \frac{\hbar}{2m\imath}(\psi^*\partial_x\psi - \psi\partial_x\psi^*) = \frac{p + p^*}{2m}\psi^*\,\psi \tag{6.20}$$

Thus in regions A and C where p is real there is a current, but the current vanishes in region B where p is imaginary. The flow in region C is classically forbidden; this phenomenon goes beyond the familiar tunneling.

Let us rearrange Eq. (6.19) as

$$(E - e\Phi)^2 = c^2p^2 + m^2c^4 \tag{6.21}$$

and solve it for E:

$$E = \pm\sqrt{m^2c^4 + c^2p^2} + e\Phi\,. \tag{6.22}$$

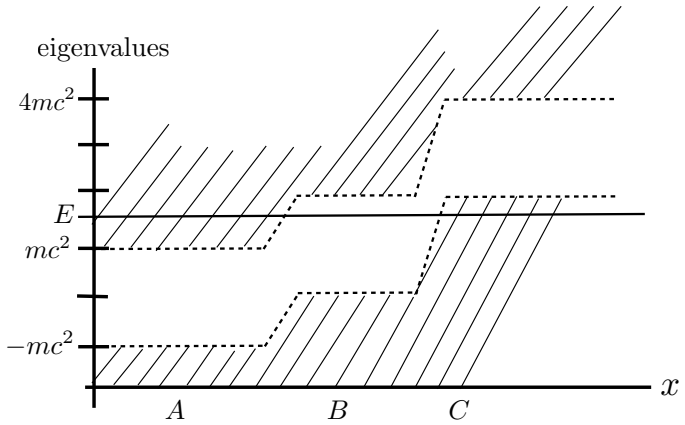

Figure 6.2: **The Klein-Gordon energy eigenvalues of propagating particles, in both positive and negative energy bands, for the potential shown in Fig. 6.1. The energy E is the one specified there. Note that a Klein-Gordon particle can tunnel from the upper band to the lower band at fixed energy.**

Fig. 6.2 shows (dashed) the energy levels of the Klein-Gordon particle with real p as a function of x with the same potential as in Fig. 6.1; the allowed eigenvalues cover full bands because p can have any real value. We notice there is a gap separating the two bands of eigenvalues. For the specified energy E, the particle when in A is in the allowed upper band; in region B it is in the gap and thus the particle cannot be propagating there. Finally in region C the particle's energy is again in an allowed band, this time the lower one. If there were no potential (Eq. (6.3)) the lower band would correspond to states with energy lying below $-mc^2$. If we take such states seriously,

then the reason for the flow in region C, which seems classically forbidden, is that the particle tunnels (through region B) from a positive energy state to a "negative energy state".

We have resolved the Klein paradox at the cost of taking the "negative energy" band seriously. But this produces a deeper paradox. If a particle can jump into a negative energy state, what is to prevent all particles in the world from taking that jump and so liberating energy. Note that the "negative energy" eigenvalues are unbounded from below. The Klein paradox thus seems to hint at a deep instability of the world. But in actuality the world is more or less stable. This inconsistency can only be solved within quantum field theory, to which we shall come in the second part of this course.

Exercises:

1. Demonstrate the gauge covariance of Eq. (6.7).

2. Write down the electric current associated with the electromagnetically coupled Klein-Gordon equation and its corresponding charge density. Show that both are gauge covariant.

3. Rewrite the electric current and density of the previous exercise together in relativistically covariant form, and show that the 4-electric current is subject to a continuity equation even in the presence of an electromagnetic field.

4. Ignore the magnetic field as you repeat Exercise 1 of Sec. 6.1.2 for a particle in an electric potential; show that for $|e\Phi|, E \ll mc^2$, the χ satisfies the Schrödinger equation with an electric potential.

5. Solve the Landau problem for the Klein-Gordon equation in the gauge (4.19).

6.2 Dirac equation

Historically Dirac invented his equation to solve the problems posed by the Klein-Gordon equation. It was not originally appreciated that the two equa-

tions deal with different kinds of particles. So the Dirac equation was first understood as an improvement over the Klein-Gordon equation.

6.2.1 Problems with the Klein-Gordon equation

The original problems were the absence of a positive probability density, and the existence of negative energy levels. From a more modern perspective we can add a third problem: the Klein-Gordon equation cannot describe real electrons which carry spin. The problem of negative energy states cannot be solved in the QT context; its resolution requires quantum field theory and leads to the notion of antiparticles (which actually exist). It is not really a problem, only a misunderstanding. But the lack of a probability density hinders development of relativistic QT in analogy with the nonrelativistic theory.

Dirac identified this lack as coming from the second-order in time character of the Klein-Gordon equation. In Schrödinger theory the density is $\psi^*\psi$. When we calculate $\partial_t(\psi^*\psi)$ we can get $\partial_t\psi$ and $\partial_t\psi^*$ from the Schrödinger equation, which is first-order in time, and thus get a continuity equation. For the Klein-Gordon equation it is natural that the density is of form (6.12); a partial time derivative of this, after suitable cancellation, leads to a linear combination of ${\partial_t}^2\psi$ and ${\partial_t}^2\psi^*$ which can be calculated with Klein-Gordon's equation and leads to a continuity equation, as we saw. But form (6.12) is not positive definite. Alternative expressions such as $|\psi|^2$ or $|\partial_t\psi|^2$ are positive, but their time derivatives cannot be reduced reduced to space derivatives only, as required in order to form a continuity equation.

From all this Dirac concluded that one needs the wave equation to be first-order in time. Relativity then dictates that it must also be first-order is space derivatives. How to get a wave equation of this form? How to "take the square root" of Klein-Gordon's equation? Suppose we make the replacements (6.2) in Eq. (6.22) and operate with the resulting operator equality on the wave function. We do get a first-order in time wave equation, but it has its second spatial derivative operators under the square root. If we expand the square root we get a partial differential equation which is of infinite-order in space, a feature which brings in all kinds of instabilities.

6.2.2 Constructing the Dirac equation

Dirac opted to take the square root using matrices. We follow here a slightly different path than his. In view of Eq. (4.41) we may write the energy-momentum relation (6.3) as

$$(E - c\boldsymbol{\sigma}\cdot\boldsymbol{p})(E + c\boldsymbol{\sigma}\cdot\boldsymbol{p}) = m^2c^4\,. \tag{6.23}$$

Making the replacements (6.2) leads to the wave equation

$$(\imath\hbar\partial_t + \imath c\hbar\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})\,(\imath\hbar\partial_t - \imath c\hbar\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})\,\phi_L = m^2c^4\,\phi_L\,, \tag{6.24}$$

where $\phi_L(\boldsymbol{r},t)$ is the wave function, a 2-spinor. Now define a second 2-spinor

$$\phi_R(\boldsymbol{r},t) = \frac{1}{mc^2}(\imath\hbar\partial_t - \imath c\hbar\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})\,\phi_L\,. \tag{6.25}$$

Obviously the equation for ϕ_R is

$$(\imath\hbar\partial_t + \imath c\hbar\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})\phi_R = mc^2\phi_L\,. \tag{6.26}$$

Instead of the Klein-Gordon equation we have two first order coupled equations, Eqs. (6.25)-(6.26), for the 2-spinor wave functions ϕ_L and ϕ_R.

We can unify these pair of equations if we define the 4×4 matrix of operators (I stands for the 2×2 identity matrix)

$$\hat{H}_D = c\boldsymbol{\alpha}\cdot\frac{\hbar}{\imath}\boldsymbol{\nabla} + mc^2\beta = c\begin{pmatrix}\boldsymbol{\sigma} & 0\\ 0 & -\boldsymbol{\sigma}\end{pmatrix}\cdot\frac{\hbar}{\imath}\boldsymbol{\nabla} + mc^2\begin{pmatrix}0 & I\\ I & 0\end{pmatrix} \tag{6.27}$$

and the 4-spinor

$$\phi = \begin{pmatrix}\phi_R\\ \phi_L\end{pmatrix}. \tag{6.28}$$

Then Eqs. (6.25)-(6.26) together read

$$\imath\hbar\,\partial_t\phi = \hat{H}_D\,\phi\,. \tag{6.29}$$

This is the free Dirac equation in 3-D space. It is a Schrödinger-type equation for a 4-spinor wave function since the Dirac Hamiltonian $\hat{H}_D$ is a 4×4 matrix of operators. The Dirac equation is first order in time *and* space, as desired.

Notice that $\hat{H}_D$ is Hermitian by virtue of the Hermiticity of the $\boldsymbol{\alpha}$ and β matrices. The square of each of these matrices is $\mathcal{I}$, and each pair of different matrices anticommute. These properties define the relevant matrices and are more important than the specific form shown in Eq. (6.27). Unlike the Klein-Gordon equation, the Dirac equation can take on a variety of forms in accordance with the choice of $\boldsymbol{\alpha}$ and β; we speak of different representations of the Dirac equation. The one in Eq. (6.29) is called the *spinor representation*.

To transform the Dirac equation before us to other representations, let us now multiply Eq. (6.29) on the left with a constant unitary 4×4 matrix U, and insert $U^{-1}U = \mathcal{I}$ in between $\hat{H}_D$ and ψ ($\mathcal{I}$ is the 4×4 unit matrix. With the notation $\phi' = U\phi$ and $\hat{H}'_D = U\hat{H}_D\,U^{-1}$ we find

$$\imath\hbar\,\partial_t\phi' = \hat{H}'_D\,\phi'\,, \tag{6.30}$$

which is again a Dirac equation but with a new Hamiltonian, $\hat{H}'_D$. This one is also Hermitian since a unitary transformation takes an Hermitian matrix into an Hermitian matrix.

Consider the particular unitary matrix

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} I & I \\ I & -I \end{pmatrix}. \tag{6.31}$$

Then $\hat{H}'_D = U\hat{H}_D\,U^{-1}$ is given by

$$\hat{H}'_D = c\boldsymbol{\alpha}'\cdot\frac{\hbar}{\imath}\boldsymbol{\nabla} + mc^2\beta' = c\begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}\cdot\frac{\hbar}{\imath}\boldsymbol{\nabla} + mc^2\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}. \tag{6.32}$$

To this corresponds the 4-spinor wave function ϕ' (which we call here ψ)

$$\psi = \frac{1}{\sqrt{2}}\begin{pmatrix} \phi_R + \phi_L \\ \phi_R - \phi_L \end{pmatrix}. \tag{6.33}$$

The corresponding form of the Dirac equation is the one Dirac used originally, and is still the most popular whenever manifest relativistic covariance is not important. We shall call the scheme (6.32)-(6.33) the *standard representation*. Henceforth we do not mark the $\hat{H}_D$ with a $'$ but simply indicate which representation is in use.

Exercises:

1. Show that both ϕ_L and ϕ_R individually satisfy the free Klein-Gordon equation.

2. Show that the relations

$$\begin{aligned} &\alpha_i\alpha_j + \alpha_j\alpha_i = 2I\delta_{ij}\,, \qquad \alpha_i\beta + \beta\alpha_i = 0\,, \qquad \beta^2 = I \\ &{\alpha_i}^\dagger = \alpha_i\,, \qquad \beta^\dagger = \beta\,. \end{aligned} \tag{6.34}$$

   hold in any representation. Thus Eq. (6.34) can be said to define the Dirac matrices.

3. Using Exercise 2, show that iteration of the free Dirac equation gives the Klein-Gordon equation. Thus any solution of the free Dirac equation is a solution of the Klein-Gordon equation. The reverse is not true.

4. Write down the Dirac equation in the presence of an electromagnetic field. Is it gauge invariant?

5. If $m = 0$ in the Dirac equation, is it possible to obtain a representation where the equations for the upper and lower parts of the 4-spinor decouple? Explain.

6.2.3 Conservation of probability

Dirac's strategy of devising a relativistic equation of first-order in time and space succeeded in giving a positive definite probability density. In Schrödinger theory we represent probability density by $\psi^*\psi$. Since here the spinor wave function ψ has four components, ψ_j, we should represent probability density by the positive definite expression

$$\rho = \psi^\dagger\psi = |\psi_1|^2 + |\psi_2|^2 + |\psi_3|^2 + |\psi_4|^2\,. \tag{6.35}$$

We have

$$\imath\hbar\,\partial_t\,\rho = (\imath\hbar\,\partial_t\,\psi^\dagger)\,\psi + \psi^\dagger\,\imath\hbar\,\partial_t\,\psi \tag{6.36}$$

$$= -(\hat{H}_D\psi)^\dagger\,\psi + \psi^\dagger\,\hat{H}_D\,\psi \tag{6.37}$$

$$= \frac{c\hbar}{\imath}\boldsymbol{\nabla}\psi^\dagger\cdot\boldsymbol{\alpha}\psi - mc^2\psi^\dagger\beta\psi + \frac{c\hbar}{\imath}\psi^\dagger\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}\psi + mc^2\psi^\dagger\beta\psi \tag{6.38}$$

$$= \frac{c\hbar}{\imath}\boldsymbol{\nabla}\cdot(\psi^\dagger\boldsymbol{\alpha}\psi) \tag{6.39}$$

Thus if we define the probability flux (or current) by

$$\boldsymbol{j} = c\,\psi^\dagger \boldsymbol{\alpha} \psi \tag{6.40}$$

we have the continuity equation $\partial_t \rho + \boldsymbol{\nabla} \cdot \boldsymbol{j} = 0$.

Observe that the values of ρ and of $\boldsymbol{j}$ are unchanged by a unitary transformation from one representation to another. Note also that since $\psi^\dagger\psi$ is a probability density, we can think of $c\boldsymbol{\alpha}$ as the velocity observable in Dirac theory [see Eq. (6.40)]. This will be confirmed in Sec. 6.2.6.

Thus, in contrast to the Klein-Gordon, the Dirac equation is equipped with the notion of a positive definite conserved probability. Whereas it is unprofitable to think of Klein-Gordon's ψ as a particle's wave function, and one must early in the game opt for a field-theoretic interpretation, Dirac's ψ can be thought of as a true wave function in many contexts, and the need for a field-theoretic framework for it is thus postponed.

6.2.4 The Dirac equation also has negative energies

Are we rid of the negative energies of the Klein-Gordon equation? As we know, the spectrum of an operator is unaffected by a unitary transformation of it: we can calculate the energy eigenvalues of $\hat{H}_D$ in any representation. We choose to do so in the standard representation, Eq. (6.32). We shall assume a plane wave solution

$$\phi = \begin{pmatrix} w_A \\ w_B \end{pmatrix} e^{\imath(\boldsymbol{p}\cdot\boldsymbol{r} - Et)/\hbar}\,, \tag{6.41}$$

where the spinors w_A and w_B are constant.

Substituting this in Eq. (6.29) and collecting terms we get

$$\begin{pmatrix} mc^2 I - EI & c\,\boldsymbol{\sigma}\cdot\boldsymbol{p} \\ c\,\boldsymbol{\sigma}\cdot\boldsymbol{p} & -mc^1 I - EI \end{pmatrix} \begin{pmatrix} w_A \\ w_B \end{pmatrix} = 0\,. \tag{6.42}$$

From linear algebra we know that this coupled set of linear equations can have a nontrivial solution for w_A and w_B only if the determinant of the 4×4 matrix vanishes. This gives us the condition

$$E^2 - m^2c^4 = (c\,\boldsymbol{\sigma}\cdot\boldsymbol{p})^2 = c^2\boldsymbol{p}^2\,. \tag{6.43}$$

which (not surprisingly) is just Eq. (6.3). We see that for given $\boldsymbol{p}$ both positive and negative energies E are allowed. Thus the problem of the negative energies resurfaces in the Dirac equation. The free Dirac equation energy eigenvalues are also distributed, as in Fig. 6.2, into two bands.

6.2.5 Conserved quantities of the free Dirac particle

Here we work in Heisenberg picture. As usual, any operator which commutes with the Hamiltonian is a conserved quantity. For example, in any representation H_D commutes with $-\imath\hbar\boldsymbol{\nabla}$ so that momentum is a conserved quantity of the free Dirac equation. Angular momentum should also be conserved in the absence of forces, not so? Let us try with $\hat{\boldsymbol{l}}$:

$$\begin{aligned}&[\hat{l}_z, \hat{H}_D] = [\hat{x}\,\hat{p}_y - \hat{y}\,\hat{p}_x, c\,\alpha_1\,\hat{p}_x + c\,\alpha_2\,\hat{p}_y]\\ &= \imath\hbar c\alpha_1\,\hat{p}_y - \imath\hbar c\alpha_2\,\hat{p}_x = \imath\hbar c(\boldsymbol{\alpha}\times\hat{\boldsymbol{p}})_3\end{aligned} \tag{6.44}$$

By cyclic symmetry no component of $\hat{\boldsymbol{l}}$ commutes with $\hat{H}_D$: $\hat{\boldsymbol{l}}$ is not conserved.

This is surprising. The Dirac particle is not subject to forces, so its physics is invariant under rotations. The generator of rotations should commute with $\hat{H}_D$. If $\hat{\boldsymbol{l}}$ does not, that means there is another contribution to the generator of rotation (the angular momentum). From the fact that the Dirac wave function has several components (spinor) we suspect the extra angular momentum is spin. Thus far we are only familiar with spin half, which we wrote as $\frac{1}{2}\hbar\boldsymbol{\sigma}$. If we assume that we have spin half here, we need a 4×4 matrix as the spin observable since the spinors here are 4-spinors. So let us consider the natural 4×4 extension of $\frac{1}{2}\hbar\boldsymbol{\sigma}$, namely

$$\tfrac{1}{2}\hbar\boldsymbol{\Sigma} = \tfrac{1}{2}\hbar\begin{pmatrix}\boldsymbol{\sigma} & 0\\ 0 & \boldsymbol{\sigma}\end{pmatrix}. \tag{6.45}$$

We first look at $[\Sigma_3, \hat{H}_D]$ with $\hat{H}_D$ in the form (6.32). Obviously $[\Sigma_3, \alpha_3] = [\Sigma_3, \beta] = 0$. Then

$$[\Sigma_3, \alpha_1] = \left[\begin{pmatrix}\sigma_3 & 0\\ 0 & \sigma_3\end{pmatrix}, \begin{pmatrix}0 & \sigma_1\\ \sigma_1 & 0\end{pmatrix}\right] = \begin{pmatrix}0 & [\sigma_3,\sigma_1]\\ [\sigma_3,\sigma_1] & 0\end{pmatrix} = \begin{pmatrix}0 & 2\imath\sigma_2\\ 2\imath\sigma_2 & 0\end{pmatrix} = 2\imath\alpha_2 \tag{6.46}$$

The analogous $[\Sigma_3, \alpha_2] = -2\imath\alpha_1$ is most effectively obtained by cycling the indices. Altogether

$$[\Sigma_3, \hat{H}_D] = -2\imath c(\boldsymbol{\alpha} \times \hat{\boldsymbol{p}})_3 \tag{6.47}$$

Comparing with Eq. (6.44) we get that $[l_z + \frac{1}{2}\hbar\Sigma_3, \hat{H}_D] = 0$. By extension this shows that

$$\hat{\boldsymbol{J}} \equiv \hat{\boldsymbol{l}} + \tfrac{1}{2}\hbar\boldsymbol{\Sigma} = \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}} + \tfrac{1}{2}\hbar\boldsymbol{\Sigma} \tag{6.48}$$

is a conserved quantity—the total angular momentum.

Let us check that the observable (6.45) really carries spin half. Consider

$$\left(\tfrac{1}{2}\hbar\boldsymbol{\Sigma}\right)^2 = \frac{\hbar^2}{4}\left[\begin{pmatrix}\sigma_1 & 0\\ 0 & \sigma_1\end{pmatrix}^2 + \begin{pmatrix}\sigma_2 & 0\\ 0 & \sigma_2\end{pmatrix}^2 + \begin{pmatrix}\sigma_3 & 0\\ 0 & \sigma_3\end{pmatrix}^2\right] = \frac{3\hbar^2}{4}\mathcal{I} \tag{6.49}$$

Now the eigenvalues of angular momentum have the form $j(j+1)\hbar^2$. Since $3/4 = \frac{1}{2}(1+\frac{1}{2})$, we conclude that $\frac{1}{2}\hbar\boldsymbol{\Sigma}$ does indeed represent spin half. The Dirac equation is thus suitable for describing fermions such as the electron, muon, the quarks and composite particles such as most of the baryons.

For a free Dirac particle we may trivially build from the conserved vector observables $\hat{\boldsymbol{J}}$ and $\hat{\boldsymbol{p}}$ a scalar conserved quantity called *helicity*:

$$\hat{h} = \frac{\hat{\boldsymbol{J}} \cdot \hat{\boldsymbol{p}}}{\hbar|\hat{\boldsymbol{p}}|} = \frac{\hat{\boldsymbol{J}} \cdot \hat{\boldsymbol{p}}}{\hbar\sqrt{\hat{\boldsymbol{p}}^2}} = \tfrac{1}{2}\frac{\boldsymbol{\Sigma} \cdot \hat{\boldsymbol{p}}}{|\hat{\boldsymbol{p}}|} \tag{6.50}$$

What are the eigenvalues of helicity? We square it to get

$$\hat{h}^2 = \tfrac{1}{4}\frac{(\boldsymbol{\Sigma} \cdot \hat{\boldsymbol{p}})^2}{\hat{\boldsymbol{p}}^2} = \frac{1}{4\hat{\boldsymbol{p}}^2}\begin{pmatrix}\boldsymbol{\sigma} \cdot \hat{\boldsymbol{p}} & 0\\ 0 & \boldsymbol{\sigma} \cdot \hat{\boldsymbol{p}}\end{pmatrix}^2 = \frac{1}{4\hat{\boldsymbol{p}}^2}\begin{pmatrix}(\boldsymbol{\sigma} \cdot \hat{\boldsymbol{p}})^2 & 0\\ 0 & (\boldsymbol{\sigma} \cdot \hat{\boldsymbol{p}})^2\end{pmatrix} = \tfrac{1}{4}\mathcal{I} \tag{6.51}$$

Thus the only eigenvalue of $\hat{h}^2$ is $\frac{1}{4}$ so the eigenvalues of helicity are $\pm\frac{1}{2}$. States with helicity $\frac{1}{2}$ are traditionally called *right handed* and those with helicity $-\frac{1}{2}$ are called *left handed*

6.2.6 The *Zitterbewegung*

Classically a free particle moves rectilinearly with fixed velocity; a consequence is that it conserves its momentum and its orbital angular momentum. Since the free Dirac particle conserves the former but not the later, it

would seem it does not move rectilinearly. But for a quantum particle what does it mean to move along a definite line or curve? This can have meaning only regarding the "motion" of the observables. So let us work out $\hat{\boldsymbol{r}}(t)$ in Heisenberg picture. The Heisenberg equation (1.97) for $\hat{\boldsymbol{r}}(t)$ is

$$\frac{d\hat{\boldsymbol{r}}}{dt} = \frac{1}{\imath\hbar}[\hat{\boldsymbol{r}}, c\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}} + mc^2\beta] = c\boldsymbol{\alpha} \tag{6.52}$$

where we have used the canonical commutation relation $[\hat{r}_i, \hat{p}_j] = \imath\hbar\delta_{ij}$. This result confirms our hunch at the end of Sec 6.2.3 that $c\boldsymbol{\alpha}$ is the velocity observable.

It is strange that a physical vector is represented by a vector of matrices. Let us check on the eigenvalues of the velocity observable. According to Exercise 2 of Sec 6.2.2 the *square* of each α_i is $\mathcal{I}$. Thus the eigenvalues of each component of velocity are $\pm c$. This does not mean that velocities larger than c can be measured because the three components of $\boldsymbol{\alpha}$ do not commute, and cannot be measured simultaneously. But it is strange that c can be attained by a particle which has mass! We leave the clarification of this issue for later.

What is the acceleration? Using the anticommutation relations in Exercise 2 of Sec 6.2.2 we get

$$\frac{d\alpha_1}{dt} = \frac{[\alpha_1, \hat{H}_D]}{\imath\hbar} = \frac{\{\alpha_1, \hat{H}_D\} - 2\hat{H}_D\,\alpha_1}{\imath\hbar} = \frac{2c\hat{p}_x - 2\hat{H}_D\,\alpha_1}{\imath\hbar} \tag{6.53}$$

Since $\hat{p}_x$ and $\hat{H}_D$ are time independent, the solution of this equation is

$$c\alpha_1(t) = c^2\hat{p}_x\,{\hat{H}_D}^{-1} + e^{2\imath\hat{H}_D t/\hbar}\left(c\alpha_1(0) - c^2\hat{p}_x\,{\hat{H}_D}^{-1}\right). \tag{6.54}$$

This can be verified by differentiation. According to special relativity $c^2\hat{p}_x/E$ is the x component of velocity of a particle with momentum p_x and energy E, so the first term in the r.h.s. of Eq. (6.54) corresponds to the classical conserved velocity. However, our result says that superimposed on this is an oscillation of amplitude $\mathcal{O}(c)$ and frequency $2E/\hbar$ (assuming the particle in an eigenstate of $\hat{H}_D$). Thus, as we suspected, nonconservation of orbital angular momentum is reflected in a departure from rectilinear motion.

Integrating Eq. (6.52) in light of Eq. (6.54) gives the following expression

for the evolution of the particle's coordinate:

$$\hat{x}(t) = \hat{x}(0) + c^2\hat{p}_x\hat{H}_D{}^{-1}\,t - \frac{1}{2}\imath\hbar\,\hat{H}_D{}^{-1}e^{2\imath\hat{H}_D t/\hbar}\left(c\alpha_1(0) - c^2\hat{p}_x\,\hat{H}_D{}^{-1}\right)$$
$$= \hat{x}(0) + c^2\hat{p}_x\hat{H}_D{}^{-1}\,t - \frac{1}{2}\imath\hbar\,\hat{H}_D{}^{-1}\left(c\alpha_1(t) - c^2\hat{p}_x\,\hat{H}_D{}^{-1}\right). \qquad (6.55)$$

Although it is not obvious, this expression is Hermitian. To show this one must commute the order of $\alpha_1(t)$ and $\hat{H}_D{}^{-1}$ with help of Eq. (6.53). The first line of Eq. (6.55) shows that superimposed on the classical rectilinear motion represented by the first two terms on the r.h.s. is an oscillation of amplitude $\mathcal{O}(\hbar c/E)$ and frequency $2E/\hbar$. If the particle is an electron with energy $E = \gamma mc^2$ the parameters of the oscillation are

$$\delta x \sim c\hbar/E \approx 10^{-10}\,\gamma^{-1}\,\mathrm{cm}; \qquad \omega = 2E/\hbar \approx 10^{21}\,\gamma\,\mathrm{s}^{-1}. \qquad (6.56)$$

The "rest frame" amplitude of the oscillation is $\hbar/(mc)$, the Compton wavelength of the particle. In other frames this amplitude suffers a Lorentz-FitzGerald[5] contraction (division by γ). The oscillation phenomenon was first recognized by Schrödinger who named it *Zitterbewegung* (German for "trembling motion").

6.2.7 The gyromagnetic ratio of the Dirac particle

The Dirac particle automatically has a gyromagnetic ratio twice the classical, in accordance with experiment. We shall demonstrate this in two of the several possible ways. On the basis of Eq. (6.40) we may write the electric current of the Dirac particle with charge e as

$$\boldsymbol{J} = ec\,\psi^\dagger\boldsymbol{\alpha}\psi = \frac{1}{2}ec\left(\psi^\dagger\boldsymbol{\alpha}\psi + \psi^\dagger\boldsymbol{\alpha}\psi\right) \equiv \frac{1}{2}ec\,(\boldsymbol{I}/mc^2). \qquad (6.57)$$

Focus on I_x and employ the Dirac equation, (6.30) with (6.32), and its Hermitian conjugate, followed by repeated use of the anticommutation relations

[5]George Francis FitzGerald (1851-1901) was an Irish experimental physicist who explored consequences of the then new Maxwellian electromagnetic theory. He suggested (independently of Lorentz) that contraction of a moving body is the reason for the null result of the Michaelson-Morley experiment.

in Exercise 2 of Sec. 6.2.2; with the notation $\dot{\psi} = \partial_t \psi$ etc. we get

$$\begin{aligned} I_x &= mc^2(\psi^\dagger \alpha_1 \psi + \psi^\dagger \alpha_1 \psi) = mc^2\big(\psi^\dagger \alpha_1 \beta(\beta\psi) + (\psi^\dagger\beta)\beta\alpha_1\psi\big) \\ &= c\imath\hbar\big(\psi^\dagger\alpha_1\beta\,\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}\psi - \boldsymbol{\nabla}\psi^\dagger\cdot\boldsymbol{\alpha}\,\beta\alpha_1\psi\big) + \imath\hbar\big(\psi^\dagger\alpha_1\beta\dot{\psi} - \dot{\psi}^\dagger\beta\alpha_1\psi\big) \\ &= c\imath\hbar\Big(\psi^\dagger\alpha_1\beta\,\alpha_2\,\partial_y\psi + \psi^\dagger\alpha_1\beta\,\alpha_3\,\partial_z\psi - (\partial_y\psi^\dagger)\alpha_2\beta\alpha_1\psi - (\partial_z\psi^\dagger)\alpha_3\beta\alpha_1\psi\Big) \\ &-c\imath\hbar\Big(\psi^\dagger\beta\,\partial_x\psi - (\partial_x\psi^\dagger)\beta\psi\Big) + \imath\hbar\partial_t(\psi^\dagger\alpha_1\beta\psi)\,. \end{aligned} \tag{6.58}$$

We have separated the Dirac electric current into three parts; such procedure is known as Gordon's decomposition of the current.

We shall work in the standard representation. Assume we are dealing with a stationary state ($\psi \sim e^{-\imath Et/\hbar}$) so that the last term in the last equation drops out. We further recognize that the next to last term, which gives rise to the contribution

$$J_x^{(1)} = \frac{e\hbar}{2m\imath}\Big(\psi^\dagger\beta\,\partial_x\psi - (\partial_x\psi^\dagger)\beta\psi\Big) \tag{6.59}$$

to J_x, has, except for the β matrix intercalation, the form of the x component of the Klein-Gordon current (6.8). Since every solution of the Dirac equation solves the Klein-Gordon equation, this is not surprising but it does underline that the part $\boldsymbol{J}_x^{(1)}$ of $\boldsymbol{J}$ is not related to the spin. Given the form of β in the standard representation, it is evident that the lower 2-spinor of ψ contributes current in the opposite sense from the upper one. This already hints at the connection of the lower 2-spinor with antiparticles.

As for the part of the current arising from the penultimate line in Eq. (6.58), since $\alpha_1\beta\alpha_2 = -\alpha_2\beta\alpha_1 = -\imath\beta\Sigma_3$ and $\alpha_1\beta\alpha_3 = -\alpha_3\beta\alpha_1 = \imath\beta\Sigma_2$, it simplifies to

$$J_x^{(2)} = \frac{e}{m}\Big[\boldsymbol{\nabla}\times(\psi^\dagger\beta\,\tfrac{1}{2}\hbar\boldsymbol{\Sigma}\,\psi)\Big]_x\,. \tag{6.60}$$

By cycling indexes we conclude that

$$\boldsymbol{J}^{(2)} = \frac{e}{m}\boldsymbol{\nabla}\times(\psi^\dagger\beta\,\tfrac{1}{2}\hbar\boldsymbol{\Sigma}\,\psi)\,. \tag{6.61}$$

Now recall that in electrodynamics magnetization of the material contributes to the microscopic electric current: if $\mathcal{M}$ is the magnetization density, then the current is $c\boldsymbol{\nabla}\times\mathcal{M}$. If we interpret $\boldsymbol{J}^{(2)}$ as this type of current, then it is obvious that the magnetic moment operator is

$$\hat{\boldsymbol{\mu}} = \frac{e}{mc}\beta\,\tfrac{1}{2}\hbar\boldsymbol{\Sigma}\,. \tag{6.62}$$

Here as in our previous discussion, β causes the magnetic moment and current from the lower 2-spinor in ψ to be opposite in sign to those from the upper 2-spinor (all of $\boldsymbol{J}$ has this character). Since $\frac{1}{2}\hbar\boldsymbol{\Sigma}$ is the spin, we see that the gyromagnetic ratio of the Dirac particle is (e/mc), in harmony with experiment. The argument here is unambiguous, unlike Feynman's derivation of the Pauli equation in Sec. 4.2.2 (to be sure Feynman gave this pedagogical argument well after the Dirac equation's prediction of the correct gyromagnetic ratio was discovered).

But one might be uneasy about the former derivation. It works only for stationary states, and it appeals to the form of the Klein-Gordon current. We thus present a different argument leading to the gyromagnetic ratio which has neither of the above weak points.

First we couple the Dirac equation to the electromagnetic field in the same way we coupled the Schrödinger equation. This *minimal coupling* guarantees that the equation will be gauge covariant:

$$\imath\hbar\,\partial_t\psi - e\Phi = c\boldsymbol{\alpha}\cdot\big(\frac{\hbar}{\imath}\boldsymbol{\nabla} - \frac{e}{c}\boldsymbol{A}\big)\psi + mc^2\beta\psi \tag{6.63}$$

We now define two 2-spinor wave functions, ξ and η, by

$$\psi(\boldsymbol{r},t) = \begin{pmatrix}\xi(\boldsymbol{r},t)\\ \eta(\boldsymbol{r},t)\end{pmatrix} e^{-\imath mc^2 t/\hbar}\,. \tag{6.64}$$

One is *not* assuming here that the state is stationary: there is no claim that ξ and η vary sinusoidally in time. We are simply factoring out the time dependence coming from the rest mass of the Dirac particle, part of the time dependence, but not all of it. Crudely $\imath\hbar\,\partial_t\xi \sim \epsilon\,\xi$ and $\imath\hbar\,\partial_t\eta \sim \epsilon\eta$ where ϵ is a measure of the energy above the rest energy. Substituting Eq. (6.64) into Eq. (6.63) gives (in the standard representation)

$$\imath\hbar\,\partial_t\xi - e\Phi\,\xi = c\boldsymbol{\sigma}\cdot\big(\frac{\hbar}{\imath}\boldsymbol{\nabla} - \frac{e}{c}\boldsymbol{A}\big)\,\eta\,, \tag{6.65}$$

$$\imath\hbar\,\partial_t\eta - e\Phi\,\eta + 2mc^2\eta = c\boldsymbol{\sigma}\cdot\big(\frac{\hbar}{\imath}\boldsymbol{\nabla} - \frac{e}{c}\boldsymbol{A}\big)\,\xi\,. \tag{6.66}$$

No approximation has yet been made; the equations are equivalent to Dirac's.

We now assume that the system is nonrelativistic, namely that $|\epsilon| \ll mc^2$. Since $\imath\hbar\,\partial_t\eta \sim \epsilon\eta$ and we expect ϵ to be of the order of $e\Phi$, the first two

terms in Eq. (6.66) are negligible compared to the third, so we can write that equation as

$$\eta \approx \frac{1}{2mc}\,\boldsymbol{\sigma}\cdot\big(\frac{\hbar}{\imath}\boldsymbol{\nabla}-\frac{e}{c}\boldsymbol{A}\big)\,\xi\,. \tag{6.67}$$

If we now substitute this in Eq. (6.65) we obtain the equation

$$\imath\hbar\,\partial_t\,\xi = \frac{1}{2m}\left(\boldsymbol{\sigma}\cdot\big(\frac{\hbar}{\imath}\boldsymbol{\nabla}-\frac{e}{c}\boldsymbol{A}\big)\right)^2\xi + e\Phi\,\xi\,. \tag{6.68}$$

But the Hamiltonian here is precisely that in Eq. (4.43) which leads from Feynman's ansatz to the Pauli Hamiltonian (4.45). Thus proceeding as in Sec. 4.2.2 we reduce the previous equation to

$$\imath\hbar\,\partial_t\,\xi = -\frac{\hbar^2}{2m}\left(\boldsymbol{\nabla}-\frac{\imath e}{\hbar c}\boldsymbol{A}\right)^2\xi - \frac{e\hbar}{2mc}\boldsymbol{B}\cdot\boldsymbol{\sigma}\,\xi + e\Phi\,\xi\,. \tag{6.69}$$

Of course this Pauli type equation refers only to half of the Dirac 4-spinor. However, note that Eq. (6.67) tells us that η is of order of ξ times the kinematical momentum (mv) divided by mc. In the nonrelativistic limit the ratio is very small and Dirac's spinor is basically all ξ. Thus Eq. (6.69) is the only relevant wave equation. It shows, again, that the gyromagnetic ratio of the Dirac particle of charge e is (e/mc), as measured.

To be precise, the measured gyromagnetic ratio exceeds (e/mc) by one part in a thousand. The extra contribution comes from a *radiative effect*—the interaction of the particle with the quantum radiation field. Schwinger was the first to show how to calculate the corresponding *radiative correction*. Today the calculated gyromagnetic ratio agrees with experiment to 10 significant figures!

6.2.8 The Hamiltonian to $\mathcal{O}(v^2/c^2)$

Because in Eq. (6.67) η is expressed to accuracy $\mathcal{O}(v/c)$ with respect to ξ, that approximation (and the ensuing Pauli equation) is regarded as the approximation to the Dirac equation to $\mathcal{O}(v/c)$. Let us proceed to $\mathcal{O}(v^2/c^2)$. To simplify matters we assume there is no magnetic field anywhere $(\boldsymbol{A}=0)$ and that we deal with a stationary state. Thus $\imath\hbar\,\partial_t\xi = \epsilon\,\xi$ and $\imath\hbar\,\partial_t\eta = \epsilon\eta$

with ϵ the nonrelativistic part of the energy. Eqs. (6.65)-(6.66) become

$$(\epsilon - e\Phi)\,\xi = c\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}}\,\eta\,, \tag{6.70}$$

$$(\epsilon - e\Phi)\,\eta + 2mc^2\eta = c\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}}\,\xi\,. \tag{6.71}$$

Is it possible to formulate an energy eigenvalue problem for a 2-spinor which is equivalent to these equations to $\mathcal{O}(v/c)^2$? At first we may think that ξ serves as such spinor. But there is a problem. Conservation of probability means the norm of the exact wave function ψ, even when not in a stationary state, is conserved. The normalization integral

$$\int \psi^\dagger\psi\, d^3r = \int (\xi^\dagger\xi + \eta^\dagger\eta)\, d^3r = 1 \tag{6.72}$$

refers to both ξ and η. We cannot just drop η because this amounts to making an error of $\mathcal{O}(v/c)^2$ in the normalization. For according to Eq. (6.67), we may rewrite the normalization integral correct to $\mathcal{O}(v^2/c^2)$ as

$$\int \left(\xi^\dagger\xi + \frac{1}{4m^2c^2}\xi^\dagger(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})^2\,\xi\right) d^3r = 1\,. \tag{6.73}$$

According to Eq. (4.41), $(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})^2 = \hat{\boldsymbol{p}}^2$, so to $\mathcal{O}(v^2/c^2)$ it is the spinor

$$\chi = \left(1 + \frac{\hat{\boldsymbol{p}}^2}{8m^2c^2}\right)\xi \tag{6.74}$$

which is properly normalized. Thus to $\mathcal{O}(v^2/c^2)$, χ is the Dirac particle's wave function. We shall need the inverse relation to the same order:

$$\xi = \left(1 - \frac{\hat{\boldsymbol{p}}^2}{8m^2c^2}\right)\chi\,. \tag{6.75}$$

The next step is to obtain η to higher accuracy than in Eq. (6.67); from Eq. (6.71) we have to $\mathcal{O}(v^3/c^3)$

$$\eta = \frac{1}{2mc}\left(1 - \frac{\epsilon - e\Phi}{2mc^2}\right)\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}}\,\xi\,. \tag{6.76}$$

Then substituting the last two equations in Eq. (6.70) we have

$$\begin{aligned}(\epsilon - e\Phi)\left(1 - \frac{\hat{\boldsymbol{p}}^2}{8m^2c^2}\right)\chi &= \frac{(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})}{2m}\left(1 - \frac{\epsilon - e\Phi}{2mc^2}\right)\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}}\left(1 - \frac{\hat{\boldsymbol{p}}^2}{8m^2c^2}\right)\chi \\ &= \left(\frac{\hat{\boldsymbol{p}}^2}{2m} - \frac{1}{4m^2c^2}\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}}\,(\epsilon - e\Phi)\,\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}} - \frac{\hat{\boldsymbol{p}}^4}{16m^3c^2} + \mathcal{O}\Big(\frac{mv^6}{c^4}\Big)\right)\chi\,.\end{aligned} \tag{6.77}$$

Using Eq. (4.41) with $\hat{\boldsymbol{a}} = \hat{\boldsymbol{p}}$ and $\hat{\boldsymbol{b}} = (\epsilon - e\Phi)\,\hat{\boldsymbol{p}}$ allows us to write

$$\begin{aligned}
&\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}}\,(\epsilon - e\Phi)\,\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}} = \hat{\boldsymbol{p}}\cdot(\epsilon - e\Phi)\,\hat{\boldsymbol{p}} + \imath\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}}\times(\epsilon - e\Phi)\,\hat{\boldsymbol{p}} \\
&= \hat{\boldsymbol{p}}^2\,(\epsilon - e\Phi) - \imath e\hbar\,\hat{\boldsymbol{p}}\cdot\boldsymbol{\nabla}\Phi - e\hbar\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\Phi\times\hat{\boldsymbol{p}} \\
&= \hat{\boldsymbol{p}}^2\,(\epsilon - e\Phi) + e\hbar^2\boldsymbol{\nabla}\cdot\boldsymbol{E} + e\hbar\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\hat{\boldsymbol{p}})\,. \qquad (6.78)
\end{aligned}$$

with $\boldsymbol{E} \equiv -\boldsymbol{\nabla}\Phi$ the electric field. With this result we rewrite Eq. (6.77) as

$$\begin{aligned}
(\epsilon - e\Phi)\chi = &\left(\frac{\hat{\boldsymbol{p}}^2}{2m} - \frac{1}{8m^2c^2}\,\hat{\boldsymbol{p}}^2\,(\epsilon - e\Phi) - \frac{1}{8m^2c^2}\left[\hat{\boldsymbol{p}}^2\,(\epsilon - e\Phi) - (\epsilon - e\Phi)\,\hat{\boldsymbol{p}}^2\right]\right)\chi \\
&- \left(\frac{e\hbar^2}{4m^2c^2}\boldsymbol{\nabla}\cdot\boldsymbol{E} + \frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\hat{\boldsymbol{p}}) + \frac{\hat{\boldsymbol{p}}^4}{16m^3c^2}\right)\chi + \cdots\,. \qquad (6.79)
\end{aligned}$$

There are further simplifications possible. For example

$$\hat{\boldsymbol{p}}^2\,(\epsilon - e\Phi) - (\epsilon - e\Phi)\,\hat{\boldsymbol{p}}^2 = -e\hbar^2\boldsymbol{\nabla}\cdot\boldsymbol{E}\,. \qquad (6.80)$$

In addition, since to zeroth order $(\epsilon - e\Phi)\chi = (\hat{\boldsymbol{p}}^2/2m)\chi$ we may write

$$\hat{\boldsymbol{p}}^2\,(\epsilon - e\Phi)\,\chi = \frac{\hat{\boldsymbol{p}}^4}{2m}\chi \qquad (6.81)$$

With all these results we can write Eq. (6.79) as the following eigenvalue problem correct to $\mathcal{O}(v^2/c^2)$:

$$\begin{aligned}
&\hat{H}^{(2)}\chi = \epsilon^{(2)}\chi\,, \qquad (6.82)\\
&\hat{H}^{(2)} \equiv \frac{\hat{\boldsymbol{p}}^2}{2m} + e\Phi - \frac{\hat{\boldsymbol{p}}^4}{8m^3c^2} - \frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\hat{\boldsymbol{p}}) - \frac{e\hbar^2}{8m^2c^2}\boldsymbol{\nabla}\cdot\boldsymbol{E}\,.
\end{aligned}$$

How to understand the various terms of the Hamiltonian? The first two are obviously the ones in Schrödinger's equation. In regard to the third, let us expand the classical expression for energy as a function of momentum:

$$E = \sqrt{c^2\boldsymbol{p}^2 + m^2c^4} = mc^2 + \frac{\boldsymbol{p}^2}{2m} - \frac{\boldsymbol{p}^4}{8m^3c^2} + \cdots \qquad (6.83)$$

Since ϵ means $E - mc^2$ we understand the origin of the third term in the Hamiltonian.

It is easiest to understand the fourth term in the case of a spherically symmetric potential Φ. This will generate an electric field

$$\boldsymbol{E} = -\frac{\boldsymbol{r}}{r}\frac{d\Phi}{dr}\,. \tag{6.84}$$

From this follows that

$$-\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\hat{\boldsymbol{p}}) = \frac{e\hbar\, d\Phi/dr}{4m^2c^2r}\boldsymbol{\sigma}\cdot(\boldsymbol{r}\times\hat{\boldsymbol{p}}) = \frac{e}{2m^2c^2r}\frac{d\Phi}{dr}\boldsymbol{s}\cdot\hat{\boldsymbol{l}}\,. \tag{6.85}$$

This is exactly the contribution to the Hamiltonian of the spin-orbit interaction. In elementary accounts of this energy, it is customary to separate it into (a) the energy of the electron's magnetic moment in the magnetic field induced by the electron's motion through the nucleus' electric field, and (b) the energy from the kinematic Thomas' precession,[6] which is half as big and opposite in sign. The Dirac equation gives the full contribution to the Hamiltonian in one blow.

The fourth term in Eq. (6.82) is called the Darwin term.[7] As we know, in vacuum $\boldsymbol{\nabla}\cdot\boldsymbol{E} = 0$; however, in the presence of a "point source", for example a nucleus of charge $Z|e|$ situated at $\boldsymbol{r} = 0$, $\boldsymbol{\nabla}\cdot\boldsymbol{E} = 4\pi Z|e|\delta(\boldsymbol{r})$. Substituting this in Eq. (6.82) and collecting all our results we have

$$\hat{H}^{(2)} = \frac{\hat{\boldsymbol{p}}^2}{2m} + e\Phi - \frac{\hat{\boldsymbol{p}}^4}{16m^3c^2} + \frac{e}{2m^2c^2}\frac{d\Phi/dr}{r}\boldsymbol{s}\cdot\hat{\boldsymbol{l}} + \frac{Ze^2\hbar^2\pi\delta(\boldsymbol{r})}{2m^2c^2}\,. \tag{6.86}$$

The Darwin term has here the appearance of a contact interaction with the nucleus.

But what is the physics the Darwin term? Where does it come from?

[6] Llewellyn Hilleth Thomas (1903-1992) was a British American physicist and applied mathematician. Apart from discovering the eponymous precession, he invented the Thomas-Fermi model of the atom, discovered the Thomas-Reiche-Kuhn quantum sum rule, and invented the Thomas algorithm for solving sets of coupled linear equations of a certain type.

[7] Sir Charles Galton Darwin (1987-1962), a British physicist, was a grandson of the Charles Darwin of evolution fame. Sir Charles was the first, with Gordon, to work out the exact energy levels of Hydrogen according to the Dirac equation and thereby discovered the eponymous term in the levels. He worked out the Lagrangian and Hamiltonian for classical motion of several interacting charges correct to $\mathcal{O}(v^2/c^2)$. He also worked on statistical mechanics (Darwin-Fowler method). Later in life he took part in the Manhattan project.

6.2.9 Darwin term reflects the *Zitterbewegung*

The *Zitterbewegung* means the Dirac particle moves with rapid oscillations about a mean path obtained by averaging out the rapid oscillation *in time*. In Heisenberg picture

$$\hat{\boldsymbol{r}}(t) = \overline{\hat{\boldsymbol{r}}(t)} + \delta\hat{\boldsymbol{r}}(t)\,, \tag{6.87}$$

where $\overline{\delta\hat{\boldsymbol{r}}(t)} = 0$. The actual potential felt by the charged can be expanded about this mean path:

$$\begin{aligned} V(\hat{\boldsymbol{r}}(t)) = e\Phi(\hat{\boldsymbol{r}}(t)) = e\Phi(\overline{\hat{\boldsymbol{r}}(t)}) + e\boldsymbol{\nabla}\Phi(\boldsymbol{r})\big|_{\boldsymbol{r}=\overline{\hat{\boldsymbol{r}}(t)}} \cdot \delta\hat{\boldsymbol{r}}(t) \\ + \tfrac{1}{2}e\sum_{a,b=1}^{3} \frac{\partial^2\Phi(\boldsymbol{r})}{\partial r_a\,\partial r_b}\Big|_{\boldsymbol{r}=\overline{\hat{\boldsymbol{r}}(t)}} \hat{\delta}r_a(t)\,\hat{\delta}r_b(t) + \cdots\,. \end{aligned} \tag{6.88}$$

Clearly the difference $\overline{V(\hat{\boldsymbol{r}}(t))} - e\Phi(\overline{\hat{\boldsymbol{r}}(t)})$ is the perturbation to the potential on the mean path, $e\Phi(\overline{\hat{\boldsymbol{r}}(t)})$, due to the *Zitterbewegung*. Evidently the term linear in $\delta\hat{\boldsymbol{r}}(t)$ in Eq. (6.88) averages out to zero. Thus the contribution to the Hamiltonian due to the *Zitterbewegung* is

$$\Delta\hat{H}^{(Z)} = \overline{V(\hat{\boldsymbol{r}}(t))} - e\Phi(\overline{\hat{\boldsymbol{r}}(t)}) = \tfrac{1}{2}e\sum_{a,b=1}^{3} \frac{\partial^2\Phi(\boldsymbol{r})}{\partial r_a\,\partial r_b}\Big|_{\boldsymbol{r}=\overline{\hat{\boldsymbol{r}}(t)}} \overline{\delta\hat{r}_a(t)\,\delta\hat{r}_b(t)}\,. \tag{6.89}$$

We may assume that the *Zitterbewegung* is isotropic; then

$$\overline{\delta\hat{r}_a(t)\,\delta\hat{r}_b(t)} = \tfrac{1}{3}\overline{\delta\boldsymbol{r}^2}\,\delta_{ab}\,. \tag{6.90}$$

By the result (6.56) we may estimate $\overline{\delta\boldsymbol{r}^2} \approx (\hbar/mc)^2$. Thus

$$\Delta\hat{H}^{(Z)} \approx \frac{1}{6}\frac{e\hbar^2}{m^2c^2}\sum_{a,b=1}^{3}\delta_{ab}\,\frac{\partial^2\Phi(\boldsymbol{r})}{\partial r_a\,\partial r_b}\Big|_{\boldsymbol{r}=\overline{\hat{\boldsymbol{r}}(t)}} = \frac{1}{6}\frac{e\hbar^2}{m^2c^2}\Delta\Phi(\boldsymbol{r})\Big|_{\boldsymbol{r}=\overline{\hat{\boldsymbol{r}}(t)}} = -\frac{1}{6}\frac{e\hbar^2}{m^2c^2}\boldsymbol{\nabla}\cdot\boldsymbol{E}(\boldsymbol{r})\Big|_{\boldsymbol{r}=\overline{\hat{\boldsymbol{r}}(t)}} \tag{6.91}$$

Comparing our result with Eq. (6.82) we see we have reproduced the functional dependence, order of magnitude and sign of the Darwin term, but have an error of 30% in its amplitude. This last is hardly a worry in view of the approximate nature of the result (6.56). We are thus encouraged to see in the Darwin term (which has observable consequences in the spectrum of Hydrogen—see below) a manifestation of the *Zitterbewegung*.

6.2.10 The fine structure of the hydrogenic spectrum

The famous Bohr spectrum of an hydrogenic atom (atomic number Z) was recovered by Schrödinger by using just the zeroth order part of $\hat{H}^{(2)}$:

$$\hat{H}^{(0)} = \frac{\hat{\boldsymbol{p}}^2}{2m} - \frac{Ze^2}{r}\,. \tag{6.92}$$

The spectrum is

$$\epsilon_n^{(0)} = -\frac{Z^2e^4m}{2\hbar^2n^2}; \qquad n = 1, 2, \cdots \tag{6.93}$$

In Schrödinger's solution there is degeneracy; the levels do not depend on the quantum numbers $l = 0, 1, 2, \cdots n-1$ and $\mu_l = -l, -l+1, \cdots 0, 1, \cdots l$. In actuality, relativistic effects remove part of the above degeneracy giving rise to *fine structure*.

Darwin and Gordon obtained the exact eigenvalues of the Dirac equation coupled to the Coulomb potential. The method is complicated, the final formula[8] complex, and in a sense too exact. This is because interaction of the electron with the quantum vacuum radiation field generates radiative corrections to the energy levels of the Dirac equation which compete with rather low order terms in a suitable expansion of the Darwin-Gordon formula. (These radiative effects can be calculated with *quantum electrodynamics*, which we shall meet in the second part of this course.) It is thus simpler to go beyond Schrödinger's theory using perturbation theory.

In first order perturbation theory we need to average the purely $\mathcal{O}(v^2/c^2)$ part of the Hamiltonian,

$$\Delta\hat{H}^{(2)} = -\frac{\hat{\boldsymbol{p}}^4}{16m^3c^2} + \frac{e}{2m^2c^2}\frac{d\Phi/dr}{r}\boldsymbol{s}\cdot\hat{\boldsymbol{l}} + \frac{Ze^2\hbar^2\pi\delta(\boldsymbol{r})}{2m^2c^2}\,, \tag{6.94}$$

with respect to the appropriate zeroth order hydrogenic eigenfunction. We call this last $\Psi^{(0)}$ and denote a mean value with respect to it by just $\langle\cdots\rangle$.

Using Eq. (6.92) we have

$$\langle\hat{\boldsymbol{p}}^4\rangle = 4m^2\Big\langle(\hat{H}^{(0)} + Ze^2/r)^2\Big\rangle = 4m^2\Big[\epsilon_n^{(0)2} + 2Ze^2\epsilon_n^{(0)}\Big\langle\frac{1}{r}\Big\rangle + Z^2e^4\Big\langle\frac{1}{r^2}\Big\rangle\Big] \tag{6.95}$$

[8] $E_{nj} = mc^2\left[1 + \left(\frac{Z\alpha}{n-j-\frac{1}{2}+\sqrt{(j+\frac{1}{2})^2-Z^2\alpha^2}}\right)^2\right]^{-1/2}$ with $j = l \pm \frac{1}{2}$ and $0 \le l \le n-1$.

To evaluate the second term in $\Delta\hat{H}^{(2)}$ we need $(\hat{\boldsymbol{l}} + \boldsymbol{s} = \hat{\boldsymbol{j}})$

$$\boldsymbol{s}\cdot\hat{\boldsymbol{l}} = \tfrac{1}{2}\big(\hat{\boldsymbol{j}}^2 - \hat{\boldsymbol{l}}^2 - \boldsymbol{s}^2\big)\,. \tag{6.96}$$

When averaging this over $\Psi^{(0)}$ the $\boldsymbol{s}^2$ is replaced by $s(s+1)\hbar^2 = \frac{3}{4}\hbar^2$, $\hat{\boldsymbol{l}}^2$ by $l(l+1)\hbar^2$, and $\hat{\boldsymbol{j}}^2$ by $j(j+1)\hbar^2$ because $\hat{\boldsymbol{j}}^2, \hat{\boldsymbol{l}}^2$ and $\boldsymbol{s}^2$ commute among themselves, so $\Psi^{(0)}$ can be taken an eigenfunction of all of them. Thus

$$\Big\langle \frac{e}{2m^2c^2}\frac{d\Phi/dr}{r}\boldsymbol{s}\cdot\hat{\boldsymbol{l}}\Big\rangle = \frac{Ze^2}{4m^2c^2}\big[j(j+1) - l(l+1) - s(s+1)\big]\Big\langle\frac{1}{r^3}\Big\rangle \tag{6.97}$$

In regard to the last term in Eq. (6.94) we remark that $\langle\delta(\boldsymbol{r})\rangle = |\Psi^{(0)}(0)|^2$. Now all the hydrogenic eigenfunctions with $l \neq 0$ vanish at the origin. In regard to $l = 0$ we have

$$\Psi^{(0)}(0) = \left(\frac{Ze^2m}{n\hbar^2}\right)^{3/2} \qquad l = 0\,. \tag{6.98}$$

In addition we have from atomic physics

$$\Big\langle\frac{1}{r}\Big\rangle = \frac{Ze^2m}{n^2\hbar^2}\,, \tag{6.99}$$

$$\Big\langle\frac{1}{r^2}\Big\rangle = \frac{(Ze^2m)^2}{n^3\,(l+\frac{1}{2})\hbar^4}\,, \qquad l = 0, 1, \cdots n-1 \tag{6.100}$$

$$\Big\langle\frac{1}{r^3}\Big\rangle = \frac{(Ze^2m)^3}{n^3\,l(l+\frac{1}{2})(l+1)\hbar^6}\,, \qquad l \neq 0\,. \tag{6.101}$$

The value of the last for $l = 0$ is irrelevant: it is multiplied by zero in the term (6.97). Substituting from Eqs. (6.95) and (6.97)-(6.101) into $\langle\Delta\hat{H}^{(2)}\rangle$ from Eq. (6.94), and simplifying appropriately we can write the shift in energy eigenvalue due to $\mathcal{O}(v^2/c^2)$ perturbations for either $j = l + \frac{1}{2}$, $j = l - \frac{1}{2}$ or $j = \frac{1}{2}, l = 0$ as

$$\epsilon^{(2)}_{nj} = -\frac{Z^4e^8m}{2\hbar^4c^2n^3}\Big(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\Big)\,. \tag{6.102}$$

The above formula was first obtained by Sommerfeld[9] in 1916 from the

[9] Arnold Johannes Wilhelm Sommerfeld (1868-1951) was a German theoretical physicist. He devised a more sophisticated form of Bohr quantization, authored the Sommerfeld-Wilson quantization rule, and introduced the fine-structure constant. He was the first to compute the anomalous specific heat of a metal. Four of his doctoral students received Nobel prizes. Sommerfeld was famous as a teacher.

old quantum mechanics. It can also be obtained by expanding the Darwin-Gordon formula in powers of the fine structure constant α up to $\mathcal{O}(\alpha^4)$. Just like $\epsilon^{(2)}_{nj}$, the exact formula depends on the quantum numbers, n and j but not on l. Aside from $j = \frac{1}{2}$, all values of j correspond to two values of l and these two states are degenerate, e.g. the $ns^{1/2}$ and $np^{1/2}$ levels. Hence the Dirac energy spectrum of atomic Hydrogen, although less degenerate than the Bohr energy spectrum, retains a two-fold degeneracy with respect to l, and of course the degeneracy with respect to μ_l and μ_s.

As comparison of Eqs. (6.93) and (6.102) shows, in the perturbation series (or expansion in α of the Darwin-Gordon formula), each term is smaller than the preceding one by $\mathcal{O}(Z^2\alpha^2)$. Thus the spacing of the Bohr levels is on the order $10Z^2$ eV, the fine structure splitting is $\sim 10Z^4\alpha^2$ eV $\sim 10^{-3}Z^4$ eV, and the next correction would be of order $\sim 10Z^6\alpha^4$ eV $\sim 10^{-7}Z^6$ eV. Experiments, however, indicate a departure from the Darwin-Gordon formula, or from the perturbation series, at the level of 10^{-5} eV for Hydrogen. In particular, as shown in 1947 by Lamb[10] and Retherford, the $2s^{1/2}$ and $2p^{1/2}$ levels are split by this order. This paradox is resolved by quantum electrodynamics, as first shown by Bethe[11] in that year. Two effects, polarization of the vacuum and the actual Lamb effect, combine to split the $2s^{1/2}$ and $2p^{1/2}$ by an amount $\sim 10Z^4\alpha^3 \ln(1/\alpha)$ eV, which agrees to one part in 10^5 with the observed split. Thus there is no point to compute the corrections coming from the $\mathcal{O}(v^4/c^4)$ terms of the Dirac Hamiltonian.

According to the Dirac equation levels such as $1s^{1/2}$, $2p^{3/2}$ and $3d^{5/2}$ should be single levels, but again experiment indicates they are split at the level of 10^{-3} of the fine structure splittings discussed above. Pauli showed that this *hyperfine structure* results from the interaction between the magnetic moment of the nucleus and the magnetic field generated by the motion of the electron. Now, the magnetic moment of the proton is a fraction $\sim 10^{-3}$ of that of the electron [see Eq. (4.33) for the mass dependence of the gyromag-

[10] Willis Eugene Lamb (1913-2008) was an American physicist and Nobel Laureate who together with Robert Curtis Retherford measured the split in energy called today the Lamb shift. He later researched in quantum optics.

[11] Nobel laureate Hans Albrecht Bethe (1906-2005) was a German-American physicist of Jewish origin. Working in nuclear physics he identified one of the cycles of nuclear reactions by which the states shine, did early work in quantum electrodynamics, and was then director of the theory division of the Manhattan project. Later he worked on solid state physics and supernova theory.

netic ratio]. Therefore, hyperfine structure splittings are a fraction 10^{-3} of fine-structure splittings.

Exercises:

1. Use the quantum virial theorem to prove Eq. (6.99) without using the explicit wave functions.

6.3 The need for quantum field theories

We saw that one cannot associate with the Klein-Gordon wave equation a positive probability density. This immediately suggests that a good formulation of the theory of spin-0 particles must refer to particles which can be created or destroyed so that probability for a single particle is not a good concept. Such a theory calls for creation and annihilation operators, that is, it should be a quantum field theory.

A second problem with the Klein-Gordon equation is the negative energy solutions. As mentioned, these cannot be ignored; they are needed to explain the Klein paradox. However, the negative energies with no lower bound imply instability of the theory. Now, as we saw, there are negative energy solutions also in the Dirac equation. In fact Klein originally discovered his paradox in the Dirac equation, and the negative energy solutions are as central for understanding it in that context as they are in the Klein-Gordon case. Negative energies and the consequent propagation of waves in classically forbidden regions under sufficiently high potentials are features of all covariant wave equations.

Specifically with regard to his equation, Dirac proposed the following way to deal with the instability that surfaces because the negative energies. As we saw, that equation describes particles of spin $\frac{1}{2}$; these are necessarily fermions. Dirac suggested that in the real world all energy levels belonging to the lower band in the Dirac equation analog of Fig. 6.2 are already filled by the fermions of charge e (the parameter entering into Eq. (6.63) below). This is called the *Dirac sea*. Pauli's exclusion principle forbids any additional fermions from falling to lower energies. Thus there is no instability.

Dirac remarked that if a photon of sufficient energy is able to eject a fermion of the lower band of energies into the upper band, the hole so produced behaves as particle of charge $-e$ and positive energy. With this remark he predicted the existence of *antiparticles* for all types of fermions, and the possibility of particle-antiparticle production by radiation. Another obvious prediction is that an antiparticle can annihilate with a particle (a fermion in the upper band can fall into and plug a hole in the lower band), and this annihilation will liberate energy, possibly as radiation.

The positron (antiparticle of the electron) was discovered soon after Dirac's prediction, and positron-electron annihilation is a common occurrence in the laboratory and in astrophysical scenarios; it is even used in medicine—PET (positron emission tomography) to image tissues where malignant activity is suspected. The antiproton, antineutrinos and antineutron have also been seen in the lab (the former also in cosmic rays).

But despite the predictive power of Dirac's idea, it cannot be taken literally. Dirac's sea requires an infinite density of each kind of fermion all over space. There are absolutely no signs that such colossal density actually exists. We do not see strong electromagnetic or gravitational fields when external fields perturb the exact symmetry envisaged by Dirac. Further, Dirac's solution demands an asymmetry between matter and antimatter: there is infinite density of each type of fermions, but not of antifermions. Yet, as we shall see in the second part of this course, measurements assure us of complete symmetry in the properties of particle and antiparticle. How come the high density of the particles has not perturbed this symmetry? And whatever the merits of Dirac's sea, it is not relevant for spin 0 particles which are bosons. The negative energies instability associated with the Klein-Gordon equation remains unresolved.

The dilemma gave rise to quantum field theory, founded by Heisenberg, Born, Jordan and Dirac, whose development continues to this day. In this new approach there is no Dirac sea: bosons and fermions are treated along parallel lines. Particles and antiparticles enter on an equal footing, and a rigorous theorem guarantees the symmetry between their respective properties. There is no conservation of probability for a specific particle; particles and antiparticles can be created or destroyed. In fact particles are not the fundamental objects; fields are fundamental and particles (antiparticles) are mere excitations of the fields in the theory.