Quantum Mechanics

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decoherence: -breakdown of quantum principles in the macroscopic universe\
- forcing an outcome, larger than the atom, ultra small

-thermodynamics and electrochemistry have shown us how energy moves between matter, however, total energy content of the universe is constant. Where does EMF come from?
-All atoms have U, and is in translational, rotational, vibrational, and electrical. Electrochemistry demonstrates that chemical processes access and alter primarily the electronic portion of U
-It's fair to assume that as the total internal energy of an atom decreases, U_{before} - EMF = U_{after}, the stability of the atom increases (noble gases and whatnot...)
-It's the before and after condition with respect to the electrical energy pocket that is understood by the science of Quantum Mech. Fundamental principles must first be covered.

-The 1st tenant of QM is particle-wave duality. It can be demonstrated that light travels as a wave (with all corresponding properties of frequency (v), wavelength (λ), and amplitude (a) where
$c=v\lambda$) and also as a particle (with momentum mv).

$C = V \times \lambda$, $C = 2.9979248 \times 10^8$ m/s

-3 properties of waves

1. Reflected
2. Refracted (bent)
3. Diffracted (taken apart)

-The speed of light changes when in a different medium
-When light moves, it has momentum (and mass); when it stops, it has nothing.
-Radiated heat is infrared light
-Not all light can be seen with human eyes, in fact, only a small portion of the electromagnetic spectrum is visible to us. Radiated heat (Q) travels as waves of infrared light while radio waves transmit information. All of these are types of radiated energy.
-Waves of light can be reflected and refracted (bent) just as all waves can. However, they also act as particles in that they can be blocked and they have momentum. This shows that light is both a particle and a wave at the same time.

Planck's Conjecture (93-94)

-According to the Maxwell-Boltzman interpretation of atomic behavior, as a body is heated, it should begin to glow, and heat would be radiated across the electromagnetic spectrum with a normal distribution. However, with the discovery of x-rays, this caused the problem known as the "Ultraviolet Catastrophe."
-Bodies that should radiate across all wavelengths (called universal black bodies) did not exist and they should! Also, very warm bodies should give off a lethal amount of x-rays.

Black Body	Emission
- temp should = color (but it doesn't!!!) - ultraviolet catastrophe(bad!!!) -Jeans predicted left side, Raleigh the right -black bodies radiate all visible colors -Planck = no atoms, found out curve was grainy - all solids, many liquids and gases	- cold spectra - not a complete spectrum -high pressure gases -hydrogen spectrum (5 lines) -positive and negative spectra -emission spectra are unique to the particular element/compound being energized -absorbs radiation completely and then releases it

-Lyman Series = UV
-Balmer Series = visible
-Paschen Series = near infrared
Bracket Series = far infrared
Pfund Series = Microwaves

Electromagnetic Spectrum

> > > > > >

wavelength

Gamma X UV Visible Infrared Microwave Radiowave Long waves

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frequency

-quanta = minimum quantity of energy that can be lost or gained by an atom

E = h x v H = 6.626×10^{-34}

λ = d sin(Θ)

E = (hc)/(d λ)

The First Quantum Number (94-97)

-Planck's Quantum Theory explained the Ultraviolet Catastrophe
-Rutherford's discovery of atomic structure and Planck's Quantum theory, Bohr discovered the first Quantum model
-Rutherford told Bohr that if he could explain the emission spectra of hydrogen and helium, we'd believe the rest. This is the first major flaw of Bohr!!!
-Light remains the same from hydrogen without any type of variance. Bohr realized that the process that caused light was linked to electrons.
-Electrons have specific energy levels, the electrons transition "upward" when light is absorbed. The greater the difference in the separation of the levels, the greater the amount of energy absorbed or emitted, and the increase in frequency of light absorbed or emitted.
-Energy levels are whole number integer multiples of Planck's constant, $2\pi/h$.

The Field Grows (97-99)

-Bohr: by using the principle quantum number (n) as a determination of energy level, color transitions in the visible, UV, IR, etc...can be explained.
-All other elements remained unexplained because of electrons and the behavior of this pesky particle.
-Maltese Cross and Electron Diffraction experiment: These proved that electrons behave as waves and particles (respectively), just as light does.

n = energy of the electron

-Louie deBroglie began to reason that all particles of matter could act as waves. This equation (Planck, Einstein, and wave equation): $\boldsymbol{\lambda = h/(mv)}$
-Heisenberg: uncertainty principles, impossible to find the electron in a single location around an atom and that the electron must, in actuality, inhabit all areas of the space.

The act of observation affects the data

More Quantum Numbers (101-104)

-fine structure and hyperfine structure
-fine structure = l, separate one line of emission spectra (angular momentum)(shape)
-fine structure is characterized by the 2nd quantum number (angular momentum)
-Zeeman effect = hyperfine structure = m_l (magnetic quantum number)
-final quantum number is found by observing the "spin" of the electron
-all quantum numbers related through the principle quantum number

n=	1	2	3	4	5
	s	p	d	f	g

n	principle quantum number, level electron inhabits	n
l	angular momentum	
	l=0, s; l=1, p; l=2, d; l=3, f; etc...	0 -> (n–1)
m_l	magnetic quantum number	-l ->l
m_s	spin quantum number	±½

-s,p,d,f,g thing = l number, s=0, p=1, d=2, f=3, etc...
-m_s : use + before -
-then change l, which changes m_l
-Schrodinger postulated a quantum theory that accounted for all observations by treating

electrons as standing waves that surround the nucleus. This meant that only specific frequencies (and energies) were allowed.
-equation describes how the energy of an electron wave in 3 spaces change
-Solutions to Schrodinger's equation are electron wave functions. Ψ^2 is a probability density, when the value of Ψ^2 is greater than 95%, or .95, the electron is said to be in an orbital, a region of space that surrounds the nucleus where the electron is most likely found.
    -orbital is a region of space with a probability 95% or greater
    -sublevel is a different type of orbital (suborbital)
-1 major problem: solutions to the equation can only be found using the "orbital approximation." This states that no electron in any orbital affects any other electron in any other orbital.
-The resulting shapes of the wave function produce the shapes and internal structure of the electron orbitals. The shapes (and hybrids of them) give rise to the valence and bonding structure of elements and molecules.

Orbital Structure (101-104)

-The resulting orbitals have discrete 3d shapes and internal structure. These include both axial and radial nodes.
-A node is a region of space where the wave amplitude is always 0. (Wave crosses itself).
-S-orbital (l=0) has no axial nodes. All s orbitals share this same basic shape.
-P-orbital (l=1) has 1 axial node. The location of the axial node is always the nucleus. Three p orbitals(p_x, p_y, p_z) have corresponding values of m_l (-1, 0, 1)
-d is always 1 behind the s, so 4s is filled immediately before 3d (and before 4p)
-f is always 2 behind s, so s is filled before f; f is filled before d, so 6s, 4f, 5d, 6p

1s	**2s**	**2p**	**3s**	**3p**	**4s**	**3d**	**4p**	**5s**	**4d**	**5p**	**6s**	**4f**	**5d**	**6p**
1 0	2 0	2 1	3 0	3 1	4 0	3 2	4 1	5 0	4 2	5 1	6 0	4 3	5 2	6 1

-s and p are always valence, d is sometimes, f is never, **find valence by bolded oxidation #**
-stability from most stable to least stable: full, empty, half full, partially full
- stability can use **resonance factor** to "steal" an electron from another orbital
-s holds 2 e
-p holds 6 e
-d holds 10 e
-f holds 14 e
-higher n=bluer line in emission spectra (by **E = h x v**)
-different l = different fine structure
-different m_l= different magnetic slitting
-different spin = opposite spin

Book Notes

-photoelectric effect: emission of electrons from a metal when light shines on the metal
-Aufblau principle: order of electron filling (1s, 2s, 2p, etc...)
-Pauli exclusion principle: no two electrons in the same atom can have the same set of quantum numbers
-Hund's rule: orbitals of equal energy are each occupied by one electron before any orbital is occupied by a second electron, and all electrons in singly occupied orbitals must have the same spin.