

**LARGE POLARON MOBILITY IN A MAGNETIC  
FIELD OF ARBITRARY STRENGTH**

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Thesis  
entitled

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**LARGE POLARON MOBILITY IN A MAGNETIC FIELD OF ARBITRARY STRENGTH.**

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**ABSTRACT**

This research was done in the three stages. In the first stage, the propagator was obtained for a charged particle subjected to an electromagnetic field and being under the influence of a non-local oscillator. The method of derivation was based on a direct solution of the corresponding classical equation of motion.

In the second stage, an analytic expression of the ground state energy of the polaron in a magnetic field was derived by J.D. Devreese and F. Brosens but no numerical data was presented. So, the objective of this stage was to present some numerical results.

Finally, the steady-state condition of an electron interacting with the phonons of a crystal in finite electric and constant magnetic fields was determined via two methods utilizing Feynman path integrals. The first method was called "Double Path". The second method was called "Single Path". The loss rate of momentum when applying fields was expressed in a form in which the lattice coordinates had been eliminated exactly by path integrals methods. The quadratic influence functional used to simulate the electron-lattice interaction was shown to be derived from a self-consistent relation for the impedance tensor. The Feynman one-oscillator model is discussed in terms of the self-consistency relation. The applied magnetic and electric fields problem is discussed. Lastly, we have derived the explicit form of the effective mass and the mobility of the polaron in a magnetic field.

KEY WORDS : FRÖHLICH POLARON/ PATH INTEGRAL/ STEADY-STATE/  
EFFECTIVE MASS/ MOBILITY

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ความคล่องตัวของโพลารอนขนาดใหญ่ภายใต้สนามแม่เหล็กที่มีความเข้มใดๆ (LARGE POLARON MOBILITY IN A MAGNETIC FIELD OF ARBITRARY STRENGTH).

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### บทคัดย่อ

งานวิจัยชิ้นนี้ศึกษาสมบัติความคล่องตัวของโพลารอนโดยแบ่งการ แก้ปัญหาออกเป็น 3 ส่วน ส่วนแรก เราได้ทำการหา พรอพเพเกเตอร์ ของระบบที่ประกอบด้วยอนุภาคที่มีประจุเคลื่อนที่อยู่ในสนามแม่เหล็กไฟฟ้าและ ภายใต้อิทธิพลของศักย์แบบนอนโลคัลฮาร์โมนิคออสซิลเลเตอร์ วิธีที่ใช้ในการพิสูจน์พรอพเพเกเตอร์นั้นได้อาศัยคำตอบที่ได้จากการแก้สมการ การเคลื่อนที่แบบคลาสสิกคอลลของอนุภาคที่สอดคล้องกับระบบที่เราสนใจ

สำหรับส่วนที่สอง ผลลัพธ์ที่ได้จากการคำนวณด้วยวิธีแบบแอนนาไลติกของสมการสถานะพื้นของโพลารอนในสนามแม่เหล็กได้ถูกเสนอโดย J.D.Devreese และ F.Brosens แต่ไม่ได้แสดงผลการคำนวณเชิงตัวเลข ดังนั้น ในส่วนนี้เราจะทำการเสนอผลการคำนวณเชิงตัวเลขของสมการสถานะพื้น

ส่วนสุดท้าย เราได้แก้สมการการเคลื่อนที่สำหรับสภาวะคงตัวของอิเล็กตรอนซึ่งมีอันตรกิริยากับโฟนอนของผลึกเมื่ออยู่ในสนามไฟฟ้าที่มีค่าจำกัดและสนามแม่เหล็กที่มีค่าคงตัว ในกรณีนี้เราได้ใช้เทคนิค 2 วิธี กล่าวคือ วิธีแรกเรียกว่า “วิธีคู่” วิธีที่สองเรียกว่า “วิธีเดี่ยว” โดยอาศัยวิธีดังกล่าวเราได้ทำการคำนวณอัตราการสูญเสียโมเมนตัมของโพลารอนเมื่ออยู่ภายใต้สนามภายนอกซึ่งแสดงในรูปแบบที่มีการลดรูปพิกัดของโครงร่างผลึก เราเลือกฟังก์ชันศักย์กำลังสองซึ่งมีอิทธิพลต่อการเคลื่อนที่ของอิเล็กตรอนในการเลียนแบบการเกิดอัตรกิริยาระหว่างอิเล็กตรอนและโครงร่างผลึก ซึ่งสามารถคำนวณได้จากความสัมพันธ์แบบสอดคล้องในตัวเองของเทนเซอร์ความต้านทานเชิงซ้อน และกล่าวถึงรูปแบบจำลองโหมดของออสซิลเลเตอร์หนึ่งตัวมีการอธิบายปัญหาของโพลารอนเมื่ออยู่ในสนามไฟฟ้าและสนามแม่เหล็กในลำดับต่อมา สุดท้ายเราได้แก้ปัญหารูปแบบที่ถูกต้องของมวลยังผล และค่าความคล่องตัวของโพลารอนในสนามแม่เหล็กด้วย

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## CHAPTER 1

### REVIEW AND INTRODUCTION TO THE POLARON

#### 1.1 The polaron

The Feynman path-integral formulation of quantum mechanics has become a major tool in many areas of physics and chemistry, as illustrated by the various topics covered in the Handbook of Feynman path integrals [1]

The subject of the polaron has continued to attract the attention of physicists. Briefly, a polaron is an electron moving in a polar crystal together with the self-induced polarization of the lattice. In particular, the polaron is characterized by its binding energy, effective mass and by its response to external electric and magnetic fields (i.e. mobility and impedance).

In general, there are two distinct types of polarons formed depending on which electron-lattice interaction is of primary importance. A large polaron forms when the electron-lattice interaction due to long-range Coulombic interactions between an electronic carrier and a solid's ions is of paramount importance. Competing effects then determine the radius of a large polaron. By contrast, a small polaron can form when a short range electron-lattice interaction, is dominant. A small polaron is shrunk without limit until it is confined to a single site. This thesis is concerned with the large polaron, or Fröhlich polaron

The polaron concept is of interest, not only because it describes the particular physical properties of an electron in an polar crystal or ionic semiconductor but also because it is an interesting field theoretical model consisting of a fermion interacting with a scalar boson field.

The early work on polarons was devoted to the interaction between a charge carrier and the long - wavelength optical phonons. The field - theoretical Hamiltonian

describing this interaction was derived by Fröhlich [2]

$$H_{pol} = \frac{\mathbf{P}^2}{2m} + \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \left( C_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_\tau} + C_{\mathbf{k}}^* a_{\mathbf{k}}^\dagger e^{-i\mathbf{k}\cdot\mathbf{r}_\tau} \right) \quad (1.1)$$

where

$$C_{\mathbf{k}} = \frac{i\hbar\omega_{\mathbf{k}}}{\mathbf{k}} \sqrt{\frac{4\pi\alpha}{V}} \sqrt{\frac{\hbar}{2m\omega_{\mathbf{k}}}} \quad (1.2)$$

Here  $V$  is the volume of the crystal,  $\hbar$  is the Planck's constant,  $\omega_{\mathbf{k}}$  is the frequency of the longitudinal optical phonons and  $\alpha$  is the dimensionless Fröhlich coupling constant. The Hamiltonian  $H_{pol}$  is readily constructed by the standard conversion of the creation and annihilation operators  $a_{\mathbf{k}}^\dagger$  and  $a_{\mathbf{k}}$  of a harmonic oscillator to the corresponding position and momentum variables.  $\mathbf{r}$  is the position coordinate operator of the electron with mass  $m$  and  $\mathbf{P}$  is its canonically conjugate momentum operator.

In the past, most works on polarons were devoted to calculating the ground-state energy and the effective mass of the polaron at zero temperature. Analytical results are available for these properties only for the limits of small and large values of electron-phonon coupling strength [3–9]. The theory of Tyablikov [10] can prove results for both the weak coupling as well as strong-coupling limits, but the method can not resolve intermediate coupling behavior. Feynman's celebrated path integral [11,12] theory of the polaron [14] addresses this. The path integral method offers a unique advantage in discussing the electron-phonon system [15–17]. If the electron-lattice interaction is linear in the lattice variables (the phonon approximation), then these lattice variables can be eliminated exactly, and the problem can then be written in terms of the electronic coordinates alone. The simplification thus achieved is remarkable as demonstrated in previous papers discussing the polaron problem [14–17].

There is one difficulty, however. Written in terms of electron coordinates alone, the method cannot be completed without making some approximation. The most successful is due to Feynman [14] who attempted to simulate the exact influence functional by an approximate harmonic one which imitated the exact functional as well as possible while still permitting the calculation to be completed. After deriving

a variational principle which gave an upper bound to the ground state energy of an electron interacting with an arbitrary distribution of phonons, he used as an influence functional the now well-known one-oscillator trial distribution whose strength and frequency are variational parameters used to minimize the ground-state energy at zero temperature. This method was soon generalized to finite temperature [18].

Following this success for calculating self-energy, transport properties including mobility [19], impedance [15], and velocity-field characteristics [17] were investigated using harmonics in place of the exact influence functionals. More recently in the nonlinear problems of calculating the velocity-field dependence for arbitrary coupling, temperature, and field strength, Thornber-Feynman [17] were forced to fall back on the Feynman one-oscillator influence functional for lack of anything better. This was particularly unfortunate because in the region of maximum energy loss per unit distance the electron's relative motion is certainly appreciably faster than as given by the one-oscillator model at the lattice temperature. Also, one can apply a strong magnetic field to calculate Hall mobility and cyclotron mass, and again one expects the harmonic influence functional to depend on the applied field. Finally, while the one-oscillator model is physical for the polaron problem where an energy threshold exists for phonon emission, in order to deal with optical phonons where phonons of any energy can be emitted, it is clear one must have some procedure to determine a more physical model interaction. Moreover, little motivation for this can be sought from trying to minimize the free energy. For finite electric fields, the energy loss is so important that the real and imaginary parts of the self-energy are comparable. For the drifting electron problem, we must pass to imaginary velocity variables.

Thornber [20] has calculated both the linear and non-linear transport properties of electron-phonon systems with constant electric, a small time-dependent electric field and magnetic fields. The expectation value of the rate of change of momentum operator equation was calculated for a general harmonic influence functional. The electron will acquire some steady-state expectation drift velocity which can be related

to the strength of the electric and magnetic fields. Finally, he also comments on the Hall mobility, cyclotron mass, and magnetoresistance for the Fröhlich polaron in perpendicular electric and magnetic fields.

## 1.2 Objective of study

The purpose of this research is to study the following problem. Suppose we have an electron interacting with the phonon modes of a crystal. Let us assume that in the uniform lattice, the electron would move as a free particle. We are not interested in the problem of an electron weakly coupled to the phonons, in which the unperturbed electron states are better described by a band structure. We now take the crystal and apply a spatially uniform and time-dependent electric field  $\mathbf{E}$  and magnetic field  $\mathbf{B}$ . An electron is said to be in a steady-state if the expectation value of its acceleration is zero. We find the steady-state relation between  $\mathbf{E}$  and  $\mathbf{B}$  for arbitrary lattice temperature, electron-phonon coupling strengths and magnetic and small electric field. In various limits we can recover drift and Hall mobility, and other interesting transport properties. The specific objectives are stated as follows:

1. To study how to evaluate the ground state energy of a polaron in the magnetic field by using the Devreese assumption [21, 24] and minimize that energy to determine the four parameters  $(v_{\parallel}, w_{\parallel}, v_{\perp}, w_{\perp})$
2. To study the steady-state condition of a polaron in a small electric field and an arbitrary magnetic field. Of particular interest is the case where the electric field is modeled by

$$\mathbf{E}_{\tau} = \mathbf{E}_0 e^{-i\omega\tau} \quad (1.3)$$

where  $\mathbf{E}_0$  is a constant vector, and  $e^{-i\omega\tau}$  is the time dependence of the oscillation of frequency  $\omega$ .

## 1.3 Outline of thesis

Chapter 2 reviews some basics of Feynman's path integral and describes the elimination of the phonon coordinates. Chapter 3 evaluates the non-local action and the

propagator. Chapter 4 determines the ground-state energy of a polaron in a magnetic field by using the J.T.Devresse and F.Brosens [24](hereafter referred to as DB) technique and shows the numerical results. Chapter 5 evaluates the steady-state of the electron in the applied fields, and shows self-consistence of the solution. Lastly we express the effective mass and the mobility of the polaron in a magnetic field. Chapter 6 summaries conclusions.

## CHAPTER 2

### INTRODUCTION TO THE FEYNMAN PATH INTEGRAL

The conventional formulation of quantum mechanics in terms of operators in Hilbert space is a Hamiltonian approach. It was invented and developed by Bohr, Born, Dirac, Heisenberg, Jordan, Pauli, Schrödinger, and others in the years 1925-26. The basic quantity in quantum mechanics is a certain complex function  $\Psi$  called a probability amplitude or wave function associated with every quantum mechanical state. In the simplest case of a single particle the wave function  $\Psi(\mathbf{r}, t)$  is the total amplitude for the particle to arrive at a particular point  $(\mathbf{r}, t)$  in space and time from the past in some situation. The probability (density) of finding the particle at the point  $\mathbf{r}$  and at the time  $t$  is  $|\Psi(\mathbf{r}, t)|^2$ . In the usual approach to quantum mechanics the wave function is calculated by solving a differential equation, which for non-relativistic systems, is the Schrödinger Equation

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi \quad (2.1)$$

Here  $H$  is a differential operator called the Hamiltonian or Schrödinger operator, which is derived from the classical Hamiltonian  $H(\mathbf{p}, \mathbf{r})$  of the associated classical system. The Schrödinger Equation (2.1) is a kind of wave equation, and this explains why the probability amplitude  $|\Psi(\mathbf{r}, t)|^2$  is commonly called the (Schrödinger) wave function. Obviously, the Schrödinger Equation (2.1) is a deterministic equation, since knowledge of  $\Psi$  at  $t_a$  implies knowledge at all subsequent times  $t_b$ . However, the interpretation of the probability of an event is an indeterministic interpretation. Introduction of the Green function of the time-dependent Schrödinger Equation (2.1) allows the quantum mechanical time evolution of the wave function to be explicitly given by the integral relation

$$\Psi(\mathbf{r}_{t_b}, t_b) = \int d\mathbf{r}_{t_a} K(\mathbf{r}_{t_b}, t_b; \mathbf{r}_{t_a}, t_a) \Psi(\mathbf{r}_{t_a}, t_a) \quad (2.2)$$

which determines the probability amplitude at a final point  $\mathbf{r}_{t_b}$  at time  $t_b$  in terms of the probability amplitude  $\Psi(\mathbf{r}_{t_a}, t_a)$  at an initial point  $\mathbf{r}_{t_a}$  at time  $t_a$ . Eq(2.2) shown that the Green function  $K$  plays the role of an integral kernel. In fact,  $K$  is identical to the kernel of the quantum mechanical time-evolution operator ( $T = t_b - t_a > 0$ )

$$K(\mathbf{r}_{t_b}, t_b; \mathbf{r}_{t_a}, t_a) = \langle \mathbf{r}_{t_b} | e^{-\frac{i}{\hbar}TH} | \mathbf{r}_{t_a} \rangle \quad (2.3)$$

Since the integral relation Eq(2.2) is completely equivalent to the Schrödinger Equation(2.1), it offers the possibility of considering Eq(2.2) as the basic time-evolution equation in quantum mechanics and thus as an alternative to the operator Schrödinger equation. This is exactly Feynman's approach in his path integral formulation of quantum mechanics [12]. In this approach the integral kernel  $K$  is the primary object, and that is the reason why the time-dependent Green function  $K$  is in this context is commonly called the Feynman kernel. "A quantum mechanical system is described equally well by specifying the function  $K$ , or by specifying the Hamiltonian  $H$  from which it results. For some purpose the specification in terms of  $K$  is easier to use and visualize" [13]. It is clear from Eq(2.2) and Eq(2.3) that the Feynman kernel  $K(\mathbf{r}_{t_b}, t_b; \mathbf{r}_{t_a}, t_a)$  has the meaning of a transition-probability amplitude to get from the point  $(\mathbf{r}_{t_a}, t_a)$  and  $(\mathbf{r}_{t_b}, t_b)$ , or in Feynman's words: "A probability amplitude is associated with an entire motion of a particle as a function of time, rather than simply with a position of the particle at a particular time". [11]

## 2.1 The propagator

Let us briefly sketch how Feynman arrived at his path integral. At time  $t_a$  a particle is prepared at  $\mathbf{r}_{t_a}$ . The probability amplitude (complex) that the particle will be found at  $\mathbf{r}_{t_b}$  at time  $t_b$  is the propagator  $K$ . The propagator can be split in two parts: from  $t_a$  to an intermediate time  $t_1$  and from there to the final time  $t_b$ . By means of Eq(2.2) one can show that the propagator obeys the property

$$K(\mathbf{r}_{t_b}, t_b; \mathbf{r}_{t_a}, t_a) = \int d\mathbf{r}_{t_1} K(\mathbf{r}_{t_b}, t_b; \mathbf{r}_{t_1}, t_1) K(\mathbf{r}_{t_1}, t_1; \mathbf{r}_{t_a}, t_a) \quad (2.4)$$

We can also write

$$K(\mathbf{r}_{t_b}, t_b; \mathbf{r}_{t_a}, t_a) = \int d\mathbf{r}_{t_1} \int d\mathbf{r}_{t_2} K(\mathbf{r}_{t_b}, t_b; \mathbf{r}_{t_2}, t_2) K(\mathbf{r}_{t_2}, t_2; \mathbf{r}_{t_1}, t_1) K(\mathbf{r}_{t_1}, t_1; \mathbf{r}_{t_a}, t_a) \quad (2.5)$$

and so on. We slice time into  $N$  intervals, of width  $\varepsilon$ . By

$$\begin{aligned} t_N &= t_b > t_{N-1} > t_{N-2} > \dots > t_2 > t_1 > t_a = t_0 \\ t_0 &= t_a; t_N = t_b \\ t_n &= n\varepsilon + t_a; t_b - t_a = N\varepsilon, n = 1, 2, \dots, N-1 \end{aligned}$$

then

$$K(\mathbf{r}_{t_b}, t_b; \mathbf{r}_{t_a}, t_a) = \int d\mathbf{r}_{t_1} \dots \int d\mathbf{r}_{t_{N-1}} K(\mathbf{r}_{t_b}, t_b; \mathbf{r}_{t_{N-1}}, t_{N-1}) \times K(\mathbf{r}_{t_{N-1}}, t_{N-1}; \mathbf{r}_{t_{N-2}}, t_{N-2}) \dots K(\mathbf{r}_{t_1}, t_1; \mathbf{r}_{t_a}, t_a) \quad (2.6)$$

$$K(\mathbf{r}_{t_b}, t_b; \mathbf{r}_{t_a}, t_a) = \lim_{N \rightarrow \infty, \varepsilon \rightarrow 0} \left[ \prod_{n=1}^{N-1} \int d\mathbf{r}_n \right] K(\mathbf{r}_{t_b}, \mathbf{r}_{n-1}; \varepsilon) \dots K(\mathbf{r}_{t_1}, \mathbf{r}_{t_a}; \varepsilon) \quad (2.7)$$

To visualize this pictorially, we consider a space-time plane, as shown in Figure 2.1. The initial and final space-time points are fixed to be  $(\mathbf{r}_{t_a}, t_a)$  and  $(\mathbf{r}_{t_b}, t_b)$ , respectively. For each time segment, say between  $t_{n-1}$  and  $t_n$ , we consider the transition amplitude to go from  $(\mathbf{r}_{n-1}, t_{n-1})$  to  $(\mathbf{r}_n, t_n)$ ; we then integrate over  $\mathbf{r}_{t_1}, \mathbf{r}_{t_2}, \dots, \mathbf{r}_{t_{N-1}}$ . This means that we must sum over all possible paths in the space-time plane with the end points fixed.

Now, we consider

$$K(\mathbf{r}_n, \mathbf{r}_{n-1}; \varepsilon) = \langle \mathbf{r}_n | e^{-\frac{i}{\hbar} \hat{H} \varepsilon} | \mathbf{r}_{n-1} \rangle \quad (2.8)$$

where  $\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{r}})$ , and

$$\begin{aligned} K(\mathbf{r}_n, \mathbf{r}_{n-1}; \varepsilon) &= \left\langle \mathbf{r}_n \left| e^{-\frac{i\varepsilon}{\hbar} \left( \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{r}}) \right)} \right| \mathbf{r}_{n-1} \right\rangle \\ &= \left\langle \mathbf{r}_n \left| e^{-\frac{i\varepsilon}{\hbar} \left( \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r}_{n-1}) \right)} \right| \mathbf{r}_{n-1} \right\rangle \end{aligned} \quad (2.9)$$

We know  $\int d\mathbf{p} |\mathbf{p}\rangle \langle \mathbf{p}| = 1$ , where  $\mathbf{p}$  is momentum, and Eq(2.9) becomes

$$\begin{aligned} K(\mathbf{r}_n, \mathbf{r}_{n-1}; \varepsilon) &= \int d\mathbf{p} \langle \mathbf{r}_n | e^{-\frac{i\varepsilon}{\hbar} \left( \frac{\mathbf{p}^2}{2m} \right)} | \mathbf{p} \rangle \langle \mathbf{p} | \mathbf{r}_{n-1} \rangle e^{-\frac{i\varepsilon}{\hbar} V(\mathbf{r}_{n-1})} \\ &= \int d\mathbf{p} e^{-\frac{i\varepsilon}{\hbar} \left( \frac{\mathbf{p}^2}{2m} \right)} \langle \mathbf{r}_n | \mathbf{p} \rangle \langle \mathbf{p} | \mathbf{r}_{n-1} \rangle e^{-\frac{i\varepsilon}{\hbar} V(\mathbf{r}_{n-1})} \end{aligned} \quad (2.10)$$

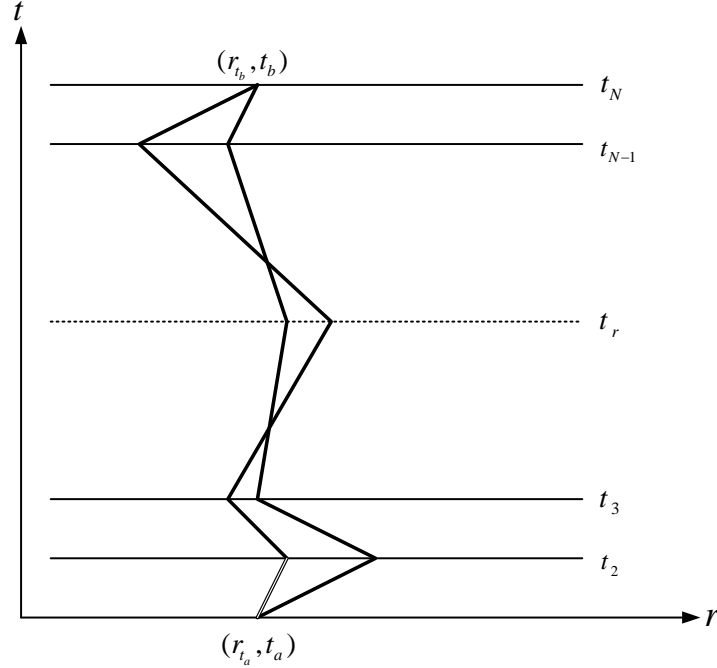


Figure 2.1: Paths in  $r$ - $t$  plane

We also know that  $\langle \mathbf{r} | \mathbf{p} \rangle = \left( \frac{1}{2\pi\hbar} \right)^{\frac{3}{2}} e^{\frac{i\mathbf{p}\mathbf{r}}{\hbar}}$ , so that

$$K(\mathbf{r}_n, \mathbf{r}_{n-1}; \varepsilon) = \left( \frac{1}{2\pi\hbar} \right)^{\frac{3}{2}} e^{-\frac{i\varepsilon}{\hbar} V(\mathbf{r}_{n-1})} \int d\mathbf{p} e^{\frac{-i\varepsilon}{\hbar} \left( \frac{\mathbf{p}^2}{2m} \right) + \frac{i\mathbf{p}(\mathbf{r}_n - \mathbf{r}_{n-1})}{\hbar}} \quad (2.11)$$

Consider

$$\begin{aligned} \int d\mathbf{p} e^{\frac{-i\varepsilon}{\hbar} \frac{\mathbf{p}^2}{2m} + \frac{i\mathbf{p}(\mathbf{r}_n - \mathbf{r}_{n-1})}{\hbar}} &= \int d\mathbf{p} e^{\frac{-i\varepsilon}{2m\hbar} \left( \mathbf{p}^2 + \frac{2m\mathbf{p}(\mathbf{r}_n - \mathbf{r}_{n-1})}{\varepsilon} \right)} \\ &= \int d\mathbf{p} e^{\frac{-i\varepsilon}{2m\hbar} \left[ \left( \mathbf{p} - \frac{m}{\varepsilon} (\mathbf{r}_n - \mathbf{r}_{n-1}) \right)^2 - \frac{m^2 (\mathbf{r}_n - \mathbf{r}_{n-1})^2}{\varepsilon^2} \right]} \end{aligned} \quad (2.12)$$

Let  $\mathbf{y} = \mathbf{p} - \frac{m}{\varepsilon} (\mathbf{r}_n - \mathbf{r}_{n-1})$ . Now Eq(2.11) becomes

$$\begin{aligned} K(\mathbf{r}_n, \mathbf{r}_{n-1}; \varepsilon) &= \left( \frac{1}{2\pi\hbar} \right)^{\frac{3}{2}} e^{-\frac{i\varepsilon}{\hbar} V(\mathbf{r}_{n-1})} e^{\frac{im(\mathbf{r}_n - \mathbf{r}_{n-1})^2}{2\hbar\varepsilon}} \int d\mathbf{y} e^{-\frac{i\varepsilon}{2m\hbar} \mathbf{y}^2} \\ &= \left( \frac{2\pi m\hbar}{i\varepsilon} \frac{1}{2\pi\hbar} \right)^{\frac{3}{2}} e^{\left( \frac{im}{2\varepsilon\hbar} (\mathbf{r}_n - \mathbf{r}_{n-1})^2 - \frac{i\varepsilon}{\hbar} V(\mathbf{r}_{n-1}) \right)} \\ &= \left( \frac{m}{2\pi\hbar i\varepsilon} \right)^{\frac{3}{2}} e^{\frac{i\varepsilon}{\hbar} \left( \frac{m}{2} \frac{(\mathbf{r}_n - \mathbf{r}_{n-1})^2}{\varepsilon^2} - V(\mathbf{r}_{n-1}) \right)} \end{aligned} \quad (2.13)$$

Finally we get the propagator of the particle from  $a \longrightarrow b$

$$\begin{aligned} K(\mathbf{r}_{t_b}, \mathbf{r}_{t_a}) &= \lim_{N \rightarrow \infty, \varepsilon \rightarrow 0} \left[ \prod_{n=1}^{N-1} \int d\mathbf{r}_n \right] \left( \frac{m}{2\pi i \varepsilon \hbar} \right)^{\frac{3N}{2}} e^{\left\{ \frac{i\varepsilon}{\hbar} \sum_{n=1}^N \left( \frac{m}{2} \left( \frac{\mathbf{r}_n - \mathbf{r}_{n-1}}{\varepsilon} \right)^2 - V(\mathbf{r}_{n-1}) \right) \right\}} \\ &= A \int D[\mathbf{r}_\tau] \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt \left( \frac{m}{2} \dot{\mathbf{r}}_\tau^2 - V(\mathbf{r}) \right) \right\} \end{aligned} \quad (2.14)$$

where  $S_{classical} = \int_{t_a}^{t_b} dt \left( \frac{m}{2} \dot{\mathbf{r}}_\tau^2 - V(\mathbf{r}) \right)$ , and

$$K(\mathbf{r}_{t_b}, \mathbf{r}_{t_a}) = A \int_{\mathbf{r}_{t_a}}^{\mathbf{r}_{t_b}} D[\mathbf{r}_\tau] e^{\frac{i}{\hbar} S_{classical}} \quad (2.15)$$

where  $A$  is a constant independent of the dynamics of the system and symbol the  $D[\mathbf{r}_\tau]$  is the “path differential measure” signifying summation or integration over all paths. In this integration, the end points are held fixed and only the intermediate points are integrated over the entire space. Any spatial configuration of the intermediate points, of course, gives rise to a trajectory between the initial and the final points. Thus, integrating over all such configurations is equivalent to summing over all the paths connecting the initial and the final points.

## 2.2 Elimination of the phonon coordinates

In this section we want to eliminate the phonon coordinates by using Feynman’s path integral. The Hamiltonian for this system may be written as

$$H_{pol} = H_e + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \sum_{\mathbf{k}} \left( C_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}_\tau} + C_{\mathbf{k}}^* a_{\mathbf{k}}^\dagger e^{-i\mathbf{k} \cdot \mathbf{r}_\tau} \right) \quad (2.16)$$

where  $H_e$  is the Hamiltonian of the electron and  $\mathbf{r}_\tau$  is the vector position of the electron. Since  $H_{pol}$  is written in terms of the creation and annihilation operators, we must first rewrite it using coordinates and momenta. If we quantize the motion of the crystal, we must choose the creation and annihilation operators, so that

$$q_{\mathbf{k}} = \sqrt{\frac{\hbar}{2\omega_{\mathbf{k}}}} (a_{\mathbf{k}} + a_{-\mathbf{k}}^\dagger) \quad (2.17)$$

$$p_{\mathbf{k}} = i \sqrt{\frac{\hbar \omega_{\mathbf{k}}}{2}} (a_{-\mathbf{k}}^\dagger - a_{\mathbf{k}}) \quad (2.18)$$

then

$$a_{\mathbf{k}} = \frac{1}{2} \left( \sqrt{\frac{2\omega_{\mathbf{k}}}{\hbar}} q_{\mathbf{k}} + i \sqrt{\frac{2}{\hbar\omega_{\mathbf{k}}}} p_{\mathbf{k}} \right) \quad (2.19)$$

$$a_{\mathbf{k}}^{\dagger} = \frac{1}{2} \left( \sqrt{\frac{2\omega_{\mathbf{k}}}{\hbar}} q_{\mathbf{k}}^{\dagger} - i \sqrt{\frac{2}{\hbar\omega_{\mathbf{k}}}} p_{\mathbf{k}}^{\dagger} \right) \quad (2.20)$$

From the Eq(2.16), the kinetic energy of the collective mode of the phonons is

$$\begin{aligned} H_{phonon} &\equiv \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \\ &= \frac{1}{4} \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} \left( \sqrt{\frac{2\omega_{\mathbf{k}}}{\hbar}} q_{\mathbf{k}} + i \sqrt{\frac{2}{\hbar\omega_{\mathbf{k}}}} p_{\mathbf{k}} \right) \left( \sqrt{\frac{2\omega_{\mathbf{k}}}{\hbar}} q_{\mathbf{k}}^{\dagger} - i \sqrt{\frac{2}{\hbar\omega_{\mathbf{k}}}} p_{\mathbf{k}}^{\dagger} \right) \\ &= \frac{1}{4} \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} \left( \frac{2\omega_{\mathbf{k}}}{\hbar} q_{\mathbf{k}}^{\dagger} q_{\mathbf{k}} + \frac{2}{\hbar\omega_{\mathbf{k}}} p_{\mathbf{k}}^{\dagger} p_{\mathbf{k}} + \frac{2i}{\hbar} [q_{\mathbf{k}}^{\dagger} p_{\mathbf{k}} - p_{\mathbf{k}}^{\dagger} q_{\mathbf{k}}] \right) \end{aligned} \quad (2.21)$$

From Eq(2.17) and Eq(2.18), we find  $q_{\mathbf{k}}^{\dagger} = q_{-\mathbf{k}}$  and  $p_{\mathbf{k}}^{\dagger} = p_{-\mathbf{k}}$ . We can show that

$$\sum_{\mathbf{k}} q_{\mathbf{k}}^{\dagger} p_{\mathbf{k}} = \sum_{\mathbf{k}} q_{-\mathbf{k}} p_{\mathbf{k}} = \sum_{\mathbf{k}} q_{\mathbf{k}} p_{-\mathbf{k}} = \sum_{\mathbf{k}} q_{\mathbf{k}} p_{\mathbf{k}}^{\dagger} \quad (2.22)$$

Since

$$[a_{\mathbf{k}}, a_{\mathbf{k}'}^{\dagger}] = \delta_{\mathbf{k}, \mathbf{k}'} \quad (2.23)$$

thus

$$[q_{\mathbf{k}}, p_{\mathbf{k}'}] = i\hbar\delta_{\mathbf{k}, -\mathbf{k}'} \quad (2.24)$$

By using the properties Eq(2.22)-(2.24), Eq(2.21) becomes

$$\begin{aligned} H_{phonon} &= \sum_{\mathbf{k}} \left( \frac{1}{2} p_{\mathbf{k}}^{\dagger} p_{\mathbf{k}} + \frac{1}{2} \omega_{\mathbf{k}}^2 q_{\mathbf{k}}^{\dagger} q_{\mathbf{k}} \right) + \frac{1}{2\hbar} \sum_{\mathbf{k}} [q_{\mathbf{k}}, p_{-\mathbf{k}}] \hbar\omega_{\mathbf{k}} \\ &= \sum_{\mathbf{k}} \left( \frac{1}{2} p_{\mathbf{k}}^{\dagger} p_{\mathbf{k}} + \frac{1}{2} \omega_{\mathbf{k}}^2 q_{\mathbf{k}}^{\dagger} q_{\mathbf{k}} - \frac{1}{2} \hbar\omega_{\mathbf{k}} \right) \end{aligned} \quad (2.25)$$

The interaction term between the electron and the phonons in Eq(2.16) is of the form

$$H_{interaction} = \sum_{\mathbf{k}} \sqrt{\frac{2\omega_{\mathbf{k}}}{\hbar}} C_{\mathbf{k}} q_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_{\tau}} \quad (2.26)$$

Substituting Eq(2.25) and Eq(2.26) into Eq(2.16), we have

$$H_{pol} = H_e + \sum_{\mathbf{k}} \left( \frac{1}{2} p_{\mathbf{k}}^{\dagger} p_{\mathbf{k}} + \frac{1}{2} \omega_{\mathbf{k}}^2 q_{\mathbf{k}}^{\dagger} q_{\mathbf{k}} - \frac{1}{2} \hbar\omega_{\mathbf{k}} \right) + \sum_{\mathbf{k}} \sqrt{\frac{2\omega_{\mathbf{k}}}{\hbar}} C_{\mathbf{k}} q_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_{\tau}} \quad (2.27)$$

The  $q_{\mathbf{k}}$  and  $p_{\mathbf{k}}$  are not canonical and some analysis is required. Let  $\xi$  be the set containing half the points in d-dimensional space for  $\mathbf{k} > 0$ . We then conclude that  $-\mathbf{k} \in \xi'$ , and  $\mathbf{k} = 0$  is a spacial point not contained in either  $\xi$  or  $\xi'$ . We now define

$$\begin{aligned} &= \frac{1}{\sqrt{2}} (p_{\mathbf{k}} + p_{-\mathbf{k}}) \quad \text{for } \mathbf{k} \in \xi \\ P_{\mathbf{k}} &= p_0 \quad \text{for } \mathbf{k} = 0 \\ &= \frac{i}{\sqrt{2}} (p_{\mathbf{k}} - p_{-\mathbf{k}}) \quad \text{for } \mathbf{k} \in \xi' \end{aligned} \quad (2.28)$$

and

$$\begin{aligned} &= \frac{1}{\sqrt{2}} (q_{\mathbf{k}} + q_{-\mathbf{k}}) \quad \text{for } \mathbf{k} \in \xi \\ Q_{\mathbf{k}} &= q_0 \quad \text{for } \mathbf{k} = 0 \\ &= \frac{i}{\sqrt{2}} (q_{\mathbf{k}} - q_{-\mathbf{k}}) \quad \text{for } \mathbf{k} \in \xi' \end{aligned} \quad (2.29)$$

which have the required property that

$$[Q_{\mathbf{k}}, P_{\mathbf{k}'}] = i\hbar\delta_{\mathbf{k},\mathbf{k}'} \quad (2.30)$$

Using Eq(2.28),(2.29), we obtain

$$\sum_{\mathbf{k}} p_{\mathbf{k}}^\dagger p_{\mathbf{k}} = \sum_{\mathbf{k}} P_{\mathbf{k}}^2 \quad (2.31)$$

and

$$\sum_{\mathbf{k}} q_{\mathbf{k}}^\dagger q_{\mathbf{k}} = \sum_{\mathbf{k}} Q_{\mathbf{k}}^2 \quad (2.32)$$

From Eq(2.29), we have

$$\begin{aligned} &= \frac{1}{\sqrt{2}} (Q_{\mathbf{k}} + iQ_{-\mathbf{k}}) \quad \text{for } \mathbf{k} \in \xi \\ q_{\mathbf{k}} &= Q_0 \quad \text{for } \mathbf{k} = 0 \\ &= \frac{i}{\sqrt{2}} (Q_{\mathbf{k}} - iQ_{-\mathbf{k}}) \quad \text{for } \mathbf{k} \in \xi' \end{aligned} \quad (2.33)$$

Substituting Eq(2.33) into Eq(2.26), we have

$$H_{interaction} = \sum_{\mathbf{k} \in \xi} \frac{1}{\sqrt{2}} \sqrt{\frac{2\omega_{\mathbf{k}}}{\hbar}} C_{\mathbf{k}} (Q_{\mathbf{k}} + iQ_{-\mathbf{k}}) e^{i\mathbf{k} \cdot \mathbf{r}_\tau} + \sqrt{\frac{2\omega_0}{\hbar}} C_0 Q_0$$

$$\begin{aligned}
 & + \sum_{\mathbf{k} \in \xi'} \frac{1}{\sqrt{2}} \sqrt{\frac{2\omega_{\mathbf{k}}}{\hbar}} C_{\mathbf{k}} (Q_{-\mathbf{k}} - iQ_{\mathbf{k}}) e^{i\mathbf{k} \cdot \mathbf{r}_{\tau}} \\
 = & \sqrt{\frac{2\omega_0}{\hbar}} C_0 Q_0 + \sum_{\mathbf{k} \in \xi} \sqrt{\frac{\omega_{\mathbf{k}}}{\hbar}} \left( e^{i\mathbf{k} \cdot \mathbf{r}_{\tau}} [Q_{\mathbf{k}} + iQ_{-\mathbf{k}}] \right. \\
 & \left. e^{-i\mathbf{k} \cdot \mathbf{r}_{\tau}} [Q_{\mathbf{k}} + iQ_{-\mathbf{k}}] \right) \\
 = & \sqrt{\frac{2\omega_0}{\hbar}} C_0 Q_0 + \sum_{\mathbf{k} \in \xi} 2\sqrt{\frac{\omega_{\mathbf{k}}}{\hbar}} C_{\mathbf{k}} Q_{\mathbf{k}} \cos \mathbf{k} \cdot \mathbf{r}_{\tau} + \sum_{\mathbf{k} \in \xi'} 2\sqrt{\frac{\omega_{\mathbf{k}}}{\hbar}} C_{\mathbf{k}} Q_{\mathbf{k}} \sin \mathbf{k} \cdot \mathbf{r}_{\tau} \\
 = & 2 \sum_{\mathbf{k}} \sqrt{\frac{\omega_{\mathbf{k}}}{\hbar}} C_{\mathbf{k}} Q_{\mathbf{k}} f_{\mathbf{k},\tau} \tag{2.34}
 \end{aligned}$$

where

$$\begin{aligned}
 & = \cos \mathbf{k} \cdot \mathbf{r}_{\tau} \quad \text{for } \mathbf{k} \in \xi \\
 f_{\mathbf{k},\tau} & = \frac{1}{\sqrt{2}} \quad \text{for } \mathbf{k} = 0 \\
 & = \sin \mathbf{k} \cdot \mathbf{r}_{\tau} \quad \text{for } \mathbf{k} \in \xi' \tag{2.35}
 \end{aligned}$$

We now substitute Eqs(2.31), (2.32) and (2.34) into Eq(2.27), and we have

$$H_{pol} = H_e + \sum_{\mathbf{k}} \left( \frac{P_{\mathbf{k}}^2}{2} + \frac{1}{2} \omega_{\mathbf{k}}^2 Q_{\mathbf{k}}^2 - \frac{1}{2} \hbar \omega_{\mathbf{k}} \right) + 2 \sum_{\mathbf{k}} \sqrt{\frac{\omega_{\mathbf{k}}}{\hbar}} C_{\mathbf{k}} Q_{\mathbf{k}} f_{\mathbf{k},\tau} \tag{2.36}$$

The propagator for the above system is given by

$$\begin{aligned}
 K \left( \mathbf{r}_{t_b}, Q_{\mathbf{k}}^b, t_b; \mathbf{r}_{t_a}, Q_{\mathbf{k}}^a, t_a \right) & \equiv \left\langle \mathbf{r}_{t_b}, Q_{\mathbf{k}}^b, t_b \middle| \mathbf{r}_{t_a}, Q_{\mathbf{k}}^a, t_a \right\rangle \\
 & = \int_{\mathbf{r}_{t_a}}^{\mathbf{r}_{t_b}} D[\mathbf{r}_{\tau}] \prod_{\mathbf{k}} \int_{Q_{\mathbf{k}}^a}^{Q_{\mathbf{k}}^b} D[Q_{\mathbf{k}}] e^{\frac{i}{\hbar} S} \tag{2.37}
 \end{aligned}$$

where

$$S = \int_{t_a}^{t_b} d\tau \left( L_e + \sum_{\mathbf{k}} \left( \frac{1}{2} \dot{Q}_{\mathbf{k}}^2 - \frac{1}{2} \omega_{\mathbf{k}}^2 Q_{\mathbf{k}}^2 - \frac{1}{2} \hbar \omega_{\mathbf{k}} \right) - 2 \sum_{\mathbf{k}} \sqrt{\frac{\omega_{\mathbf{k}}}{\hbar}} C_{\mathbf{k}} Q_{\mathbf{k}} f_{\mathbf{k},\tau} \right) \tag{2.38}$$

Now we write

$$K \left( \mathbf{r}_{t_b}, Q_{\mathbf{k}}^b, t_b; \mathbf{r}_{t_a}, Q_{\mathbf{k}}^a, t_a \right) = \int_{\mathbf{r}_{t_a}}^{\mathbf{r}_{t_b}} D[\mathbf{r}_{\tau}] e^{\frac{i}{\hbar} \int_{t_a}^{t_b} d\tau L_e} \prod_{\mathbf{k}} K_0 \left( Q_{\mathbf{k}}^b, t_b; Q_{\mathbf{k}}^a, t_a \right) \tag{2.39}$$

where

$$K_0 \left( Q_{\mathbf{k}}^b, t_b; Q_{\mathbf{k}}^a, t_a \right) = \int_{Q_{\mathbf{k}}^a}^{Q_{\mathbf{k}}^b} D[Q_{\mathbf{k}}] e^{\frac{i}{\hbar} \int_{t_a}^{t_b} d\tau L_{\mathbf{k}}} \tag{2.40}$$

with

$$L_{\mathbf{k}} = \frac{1}{2}\dot{Q}_{\mathbf{k}}^2 - \frac{1}{2}\omega_{\mathbf{k}}^2 Q_{\mathbf{k}}^2 + \frac{1}{2}\hbar\omega_{\mathbf{k}} + F_{\mathbf{k},\tau}Q_{\mathbf{k}} \quad (2.41)$$

is the transformation function for a force harmonic oscillator with the forcing function

$$F_{\mathbf{k},\tau} = -2\sqrt{\frac{\omega_{\mathbf{k}}}{\hbar}}C_{\mathbf{k}}f_{\mathbf{k},\tau} \quad (2.42)$$

The path integral over the phonon coordinates can be performed exactly because the potential energy is a quadratic function. Let us consider the following. The action integral is given as

$$S_{\mathbf{k}} = \int_{t_a}^{t_b} d\tau \left( \frac{1}{2}\dot{Q}_{\mathbf{k}}^2 - \frac{1}{2}\omega_{\mathbf{k}}^2 Q_{\mathbf{k}}^2 + F_{\mathbf{k},\tau}Q_{\mathbf{k}} \right) \quad (2.43)$$

We obtain the corresponding classical equation of motion as

$$\ddot{Q}_{\mathbf{k}} + \omega_{\mathbf{k}}^2 Q_{\mathbf{k}} = F_{\mathbf{k}} \quad (2.44)$$

which has solution

$$\begin{aligned} Q_{\mathbf{k},\tau} = & \frac{1}{\sin \omega_{\mathbf{k}}T} \left( Q_{\mathbf{k}}^b \sin \omega_{\mathbf{k}} (\tau - t_a) + Q_{\mathbf{k}}^a \sin \omega_{\mathbf{k}} (t_b - \tau) \right. \\ & - \frac{1}{\omega_{\mathbf{k}}} \int_{t_a}^{t_b} d\tau F_{\mathbf{k},\tau} \sin \omega_{\mathbf{k}} (\tau - t_a) \sin \omega_{\mathbf{k}} (t_b - \sigma) \\ & \left. - \frac{1}{\omega_{\mathbf{k}}} \int_{t_a}^{t_b} d\tau F_{\mathbf{k},\tau} \sin \omega_{\mathbf{k}} (\sigma - t_a) \sin \omega_{\mathbf{k}} (t_b - \tau) \right) \end{aligned} \quad (2.45)$$

Using Eq(2.44) and Eq(2.45), Eq(2.43) becomes; ( $T = t_b - t_a$ )

$$\begin{aligned} S_{\mathbf{k}} = & \frac{\omega_{\mathbf{k}}}{2 \sin \omega_{\mathbf{k}}T} \left\{ \left( (Q_{\mathbf{k}}^b)^2 + (Q_{\mathbf{k}}^a)^2 \right) \cos \omega_{\mathbf{k}}T - 2Q_{\mathbf{k}}^b Q_{\mathbf{k}}^a \right. \\ & + \frac{1}{\sin \omega_{\mathbf{k}}T} \int_{t_a}^{t_b} d\tau \left( Q_{\mathbf{k}}^a \sin \omega_{\mathbf{k}} (t_b - \tau) + Q_{\mathbf{k}}^b \sin \omega_{\mathbf{k}} (\tau - t_a) \right) F_{\mathbf{k},\tau} \\ & \left. - \frac{1}{\omega_{\mathbf{k}} \sin \omega_{\mathbf{k}}T} \int_{t_a}^{t_b} d\tau \int_{t_a}^{t_b} d\sigma \sin \omega_{\mathbf{k}} (t_b - \tau) \sin \omega_{\mathbf{k}} (\sigma - t_a) F_{\mathbf{k},\tau} F_{\mathbf{k},\sigma} \right\} \end{aligned} \quad (2.46)$$

We now introduce the following Fourier transforms

$$A(\omega_{\mathbf{k}}) = \frac{1}{2\omega_{\mathbf{k}}} \int_{t_a}^{t_b} d\tau e^{-i\omega_{\mathbf{k}}(\tau-t_a)} F_{\mathbf{k},\tau} \quad (2.47)$$

$$B(\omega_{\mathbf{k}}) = \frac{1}{2\omega_{\mathbf{k}}} \int_{t_a}^{t_b} d\tau e^{-i\omega_{\mathbf{k}}(t_b-\tau)} F_{\mathbf{k},\tau} = -A(-\omega_{\mathbf{k}}) e^{-i\omega_{\mathbf{k}}T} \quad (2.48)$$

Then the propagator  $K_0$  becomes

$$\begin{aligned}
 K_0(Q_{\mathbf{k}}^b, t_b; Q_{\mathbf{k}}^a, t_a) &= \left( \frac{e^{i\omega_{\mathbf{k}}T}}{2\pi i\hbar \sin \omega_{\mathbf{k}}T} \right)^{\frac{3}{2}} \exp \left\{ \sum_{\mathbf{k}} \left[ \frac{i\omega_{\mathbf{k}}}{2\hbar \sin \omega_{\mathbf{k}}T} \left( [(Q_{\mathbf{k}}^b)^2 + (Q_{\mathbf{k}}^a)^2] \cos \omega_{\mathbf{k}}T \right. \right. \right. \\
 &\quad \left. \left. - 2Q_{\mathbf{k}}^b \left( A(\omega_{\mathbf{k}}) e^{i\omega_{\mathbf{k}}T} - B(\omega_{\mathbf{k}}) \right) + 2Q_{\mathbf{k}}^a \left( B(\omega_{\mathbf{k}}) e^{i\omega_{\mathbf{k}}T} - A(\omega_{\mathbf{k}}) \right) \right) \right. \\
 &\quad \left. - \frac{i\omega_{\mathbf{k}}}{2\hbar \sin \omega_{\mathbf{k}}T} \left( e^{i\omega_{\mathbf{k}}T} \left( A^2(\omega_{\mathbf{k}}) + B^2(\omega_{\mathbf{k}}) \right) - 2A(\omega_{\mathbf{k}}) B(\omega_{\mathbf{k}}) \right) \right. \\
 &\quad \left. \left. - 2Q_{\mathbf{k}}^b Q_{\mathbf{k}}^a + \frac{i}{4\hbar\omega_{\mathbf{k}}} \int_{t_a}^{t_b} d\tau \int_{t_a}^{t_b} d\sigma e^{-i\omega_{\mathbf{k}}|\tau-\sigma|} F_{\mathbf{k},\tau} F_{\mathbf{k},\sigma} \right] \right\} \quad (2.49)
 \end{aligned}$$

We now take the trace over the field coordinates in Eq(2.49) according to the following steps. i) set  $Q_{\mathbf{k}}^a = Q_{\mathbf{k}}^b = Q_{\mathbf{k}}$ . ii) integrate over  $Q_{\mathbf{k}}$  by using  $\int e^{-ax^2+bx} dx = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}}$ .

Thus, the propagator in Eq(2.39) becomes

$$\begin{aligned}
 K(\mathbf{r}_{t_b}, t_b; \mathbf{r}_{t_a}, t_a) &= \prod_{\mathbf{k}} \left( \frac{e^{i\omega_{\mathbf{k}}T}}{2\pi i\hbar \sin \omega_{\mathbf{k}}T} \right)^3 \int_{\mathbf{r}_{t_a}^{t_b}} D[\mathbf{r}_{\tau}] e^{\frac{i}{\hbar} \int_{t_a}^{t_b} d\tau L_e} \\
 &\quad \times \exp \left\{ \sum_{\mathbf{k}} \left[ \frac{i}{4\hbar\omega_{\mathbf{k}}} \int_{t_a}^{t_b} d\tau \int_{t_a}^{t_b} d\sigma e^{-i\omega_{\mathbf{k}}|\tau-\sigma|} F_{\mathbf{k},\tau} F_{\mathbf{k},\sigma} \right. \right. \\
 &\quad \left. \left. + \frac{i\omega_{\mathbf{k}}}{2 \sin \omega_{\mathbf{k}}T/2} e^{i\omega_{\mathbf{k}}T} A(\omega_{\mathbf{k}}) B(\omega_{\mathbf{k}}) \right] \right\} \quad (2.50)
 \end{aligned}$$

We can rearrange the above equation by using Eq(2.47) and Eq(2.48) to read

$$\begin{aligned}
 K(\mathbf{r}_{t_b}, t_b; \mathbf{r}_{t_a}, t_a) &= \prod_{\mathbf{k}} \left( \frac{e^{i\omega_{\mathbf{k}}T}}{2\pi i\hbar \sin \omega_{\mathbf{k}}T} \right)^3 \int_{\mathbf{r}_{t_a}^{t_b}} D[\mathbf{r}_{\tau}] \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} d\tau L_e \right. \\
 &\quad \left. + \sum_{\mathbf{k}} \frac{i}{4\hbar\omega_{\mathbf{k}}} \int_{t_a}^{t_b} d\tau \int_{t_a}^{t_b} d\sigma \frac{\cos \omega_{\mathbf{k}} (|\tau - \sigma| - T/2)}{\sin \omega_{\mathbf{k}}T/2} F_{\mathbf{k},\tau}^* F_{\mathbf{k},\sigma} \right\} \quad (2.51)
 \end{aligned}$$

where

$$F_{\mathbf{k},\tau}^* F_{\mathbf{k},\sigma} = 4 \frac{\omega_{\mathbf{k}}}{\hbar} |C_{\mathbf{k}}|^2 e^{i\mathbf{k} \cdot (\mathbf{r}_{\tau} - \mathbf{r}_{\sigma})} \quad (2.52)$$

Substituting Eq(2.52) into Eq(2.51), we obtain

$$K(\mathbf{r}_{t_b}, t_b; \mathbf{r}_{t_a}, t_a) = \prod_{\mathbf{k}} \left( \frac{e^{i\omega_{\mathbf{k}}T}}{2\pi i\hbar \sin \omega_{\mathbf{k}}T} \right)^3 \int_{\mathbf{r}_{t_a}^{t_b}} D[\mathbf{r}_{\tau}] e^{\frac{i}{\hbar} S_{pol}(\dot{\mathbf{r}}, \mathbf{r}, \tau)} \quad (2.53)$$

with

$$S_{pol} = \int_{t_a}^{t_b} d\tau L_e + \frac{1}{2\hbar} \sum_{\mathbf{k}} |C_{\mathbf{k}}|^2 \int_{t_a}^{t_b} d\tau \int_{t_a}^{t_b} d\sigma \frac{\cos \omega_{\mathbf{k}} (|\tau - \sigma| - T/2)}{\sin \omega_{\mathbf{k}}T/2} e^{i\mathbf{k} \cdot (\mathbf{r}_{\tau} - \mathbf{r}_{\sigma})} \quad (2.54)$$

We now replace  $|C_{\mathbf{k}}|^2 = \frac{2\sqrt{2}\pi\alpha}{k^2} \sqrt{\frac{\hbar}{m\omega_{\mathbf{k}}}} \hbar^2 \omega_{\mathbf{k}}^2$ ,  $\sum_{\mathbf{k}} = \int \frac{d^3k}{(2\pi)^3}$  and performing integration over the wave number  $\mathbf{k}$ , we find

$$S_{pol} = \int_{t_a}^{t_b} d\tau L_e + \frac{\alpha}{2\sqrt{2}} \sqrt{\frac{\hbar}{m\omega_{\mathbf{k}}}} \hbar^2 \omega_{\mathbf{k}}^2 \int_{t_a}^{t_b} d\tau \int_{t_a}^{t_b} d\sigma \frac{\cos \omega_{\mathbf{k}} (|\tau - \sigma| - T/2)}{\sin \omega_{\mathbf{k}} T/2} \frac{1}{|\mathbf{r}_{\tau} - \mathbf{r}_{\sigma}|} \quad (2.55)$$

Eq(2.55) describes the coupling of an electron at a certain time with its position at an earlier time by a ‘‘Coulomb interaction’’.

### 2.3 Equilibrium density matrix (imaginary time path integral)

We write the equilibrium density operator

$$\rho = \frac{1}{Z} e^{-\beta H} \quad (2.56)$$

with the partition function

$$Z = Tr \left( e^{-\beta H} \right) \quad (2.57)$$

in position representation

$$\rho(\mathbf{r}_{\beta}, \mathbf{r}_0) = \frac{1}{Z} \langle \mathbf{r}_{\beta} | e^{-\beta H} | \mathbf{r}_0 \rangle \quad (2.58)$$

Comparing  $\langle \mathbf{r}_t | e^{-iHt/\hbar} | \mathbf{r}_0 \rangle$  and  $\langle \mathbf{r}_{\beta} | e^{-\beta H} | \mathbf{r}_0 \rangle$  one concludes that the equilibrium density matrix apart from the partition function is equivalent to a propagator in imaginary time  $t \rightarrow -i\hbar\beta$ .

How does the action look like in imaginary time?

$$\begin{aligned} \int_0^t d\tau \left[ \frac{m}{2} \dot{\mathbf{r}}_{\tau}^2 - V(\mathbf{r}) \right] &= \int_0^{-i\hbar\beta} d\tau \left[ \frac{m}{2} \left( \frac{d\mathbf{r}}{d\tau} \right)^2 - V(\mathbf{r}) \right] \\ &= -i \int_0^{\hbar\beta} d\sigma \left[ -\frac{m}{2} \left( \frac{d\mathbf{r}}{d\sigma} \right)^2 - V(\mathbf{r}) \right]; \sigma = i\tau \\ &= i \int_0^{\hbar\beta} d\sigma \left[ \frac{m}{2} \left( \frac{d\mathbf{r}}{d\sigma} \right)^2 + V(\mathbf{r}) \right] \\ &= iS^{\beta} \end{aligned} \quad (2.59)$$

where the last line define the so-called Euclidean action. We now have a path integral expression for the equilibrium density matrix.

$$\langle \mathbf{r}_{\beta} | e^{-\beta H} | \mathbf{r}_0 \rangle = \int_{\mathbf{r}_0}^{\mathbf{r}_{\beta}} D[\mathbf{r}_{\tau}] e^{-\frac{1}{\hbar} S^{\beta}} \quad (2.60)$$

For the polaron system considered in section 2.2, rewriting the expression for the propagator into imaginary time  $t \rightarrow -i\hbar\beta$  one obtains

$$\rho(\mathbf{r}_\beta, \mathbf{r}_0) = \prod_{\mathbf{k}} \frac{1}{Z} \left( \frac{e^{\hbar\omega_{\mathbf{k}}\beta/2}}{2\pi\hbar \sinh \omega_{\mathbf{k}}\hbar\beta} \right)^3 \int_{\mathbf{r}_0}^{\mathbf{r}_\beta} D[\mathbf{r}_\tau] e^{-\frac{1}{\hbar} S_{pol}^\beta} \quad (2.61)$$

where

$$S_{pol}^\beta = \int_0^{\hbar\beta} d\tau L_e - \frac{\alpha}{2\sqrt{2}} \sqrt{\frac{\hbar}{m\omega_{\mathbf{k}}}} \hbar^2 \omega_{\mathbf{k}}^2 \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma \frac{\cosh \omega_{\mathbf{k}} (|\tau - \sigma| - \hbar\beta/2)}{\sinh \omega_{\mathbf{k}}\hbar\beta/2} \frac{1}{|\mathbf{r}_\tau - \mathbf{r}_\sigma|} \quad (2.62)$$

## 2.4 Non-equilibrium statistical operator of the polaron system

In section 2.2 we had eliminated the phonon coordinates to obtain an effective action for the electron coordinates only by using Feynman's path integral or a "single path integral". In this section, we now want to perform the elimination of the phonon coordinates within the "double path integral" approach [12].

We first illustrate the idea by considering the time evolution of the density matrix

$$\begin{aligned} W(\mathbf{r}_t, Q_{\mathbf{k}}^t, t; \mathbf{r}_0, Q_{\mathbf{k}}^0, 0) &= \int d\mathbf{r}_t d\mathbf{r}'_0 dQ_{\mathbf{k}}^t dQ_{\mathbf{k}}^0 K(\mathbf{r}_t, Q_{\mathbf{k}}^t, t; \mathbf{r}_0, Q_{\mathbf{k}}^0, 0) W_0(\mathbf{r}_0, Q_{\mathbf{k}}^0; \mathbf{r}'_0, Q_{\mathbf{k}}^0) \\ &\times K^*(\mathbf{r}'_t, Q_{\mathbf{k}}^t, t; \mathbf{r}'_0, Q_{\mathbf{k}}^0, 0) \end{aligned} \quad (2.63)$$

where  $\mathbf{r}_{t_b} = \mathbf{r}_t, \mathbf{r}_{t_a} = \mathbf{r}_0, Q_{\mathbf{k}}^b = Q_{\mathbf{k}}^t, Q_{\mathbf{k}}^a = Q_{\mathbf{k}}^0$ . Eq(2.63) is just the coordinate representation of the familiar operator equation  $W(t) = e^{-iHt/\hbar} W_0 e^{iHt/\hbar}$ . The phonon is assumed to be in thermal equilibrium while the system may be in a non-equilibrium state. If we neglect initial correlations between electron and phonons, that is if we switch on the coupling after the initial state, the initial density matrix may be written in factorized form

$$W_0(\mathbf{r}_0, Q_{\mathbf{k}}^0; \mathbf{r}'_0, Q_{\mathbf{k}}^0) = \rho(\mathbf{r}_0; \mathbf{r}'_0) W_\beta(Q_{\mathbf{k}}^0; Q_{\mathbf{k}}^0) \quad (2.64)$$

If we are only interested in the dynamics of the electron, we may trace out the phonon coordinates. Then the time evolution may be expressed as

$$J(\mathbf{r}_t, \mathbf{r}'_t, t) = \int d\mathbf{r}_0 d\mathbf{r}'_0 \rho(\mathbf{r}_t, \mathbf{r}'_t, t; \mathbf{r}_0, \mathbf{r}'_0, 0) \rho(\mathbf{r}_0; \mathbf{r}'_0) \quad (2.65)$$

with the propagator function

$$\begin{aligned} \rho(\mathbf{r}_t, \mathbf{r}'_t, t; \mathbf{r}_0, \mathbf{r}'_0, 0) &= \int dQ_{\mathbf{k}}^t dQ_{\mathbf{k}}^0 dQ_{\mathbf{k}}^{\prime 0} K(\mathbf{r}_t, Q_{\mathbf{k}}^t, t; \mathbf{r}_0, Q_{\mathbf{k}}^0, 0) W_{\beta}(Q_{\mathbf{k}}^0; Q_{\mathbf{k}}^{\prime 0}) \\ &\times K^*(\mathbf{r}'_t, Q_{\mathbf{k}}^{\prime t}, t; \mathbf{r}'_0, Q_{\mathbf{k}}^{\prime 0}, 0) \end{aligned} \quad (2.66)$$

The propagators  $K$  and  $K^*$  may be written as real time path integrals while the equilibrium density matrix of the bath is given by a path integral in imaginary time.

The functional integration Eq(2.66) is over the set of paths  $\mathbf{r}_{\tau}, \mathbf{r}'_{\tau}$  of the polaron described above. We now write

$$\begin{aligned} \rho(\mathbf{r}_t, \mathbf{r}'_t, t; \mathbf{r}_0, \mathbf{r}'_0, 0) &= \int dQ_{\mathbf{k}}^t dQ_{\mathbf{k}}^0 dQ_{\mathbf{k}}^{\prime 0} \int_{\mathbf{r}_0}^{\mathbf{r}_t} D[\mathbf{r}_{\tau}] \int_{\mathbf{r}'_0}^{\mathbf{r}'_t} D[\mathbf{r}'_{\tau}] \int_{Q_{\mathbf{k}}^0}^{Q_{\mathbf{k}}^t} D[Q_{\mathbf{k}}^{\tau}] \int_{Q_{\mathbf{k}}^{\prime 0}}^{Q_{\mathbf{k}}^{\prime t}} D[Q_{\mathbf{k}}^{\prime \tau}] \\ &\int_{Q_{\mathbf{k}}^0}^{Q_{\mathbf{k}}^{\prime 0}} D[Q_{\mathbf{k}}^{\beta}] e^{\frac{i}{\hbar} \left\{ S_e[\mathbf{r}_{\tau}] - S_e[\mathbf{r}'_{\tau}] + S_{\mathbf{k}}[\mathbf{r}_{\tau}, Q_{\mathbf{k}}^{\tau}] - S_{\mathbf{k}}[\mathbf{r}'_{\tau}, Q_{\mathbf{k}}^{\prime \tau}] \right\} - \frac{1}{\hbar} S_{phonon}^{\beta}[Q_{\mathbf{k}}^{\beta}]} \end{aligned} \quad (2.67)$$

where

$$S_e[\mathbf{r}_{\tau}] = \int_0^t d\tau L_e \quad (2.68)$$

$$S_{\mathbf{k}}[\mathbf{r}_{\tau}, Q_{\mathbf{k}}] = \int_0^t d\tau \left( \frac{1}{2} \dot{Q}_{\mathbf{k}}^2 - \frac{1}{2} \omega_{\mathbf{k}}^2 Q_{\mathbf{k}}^2 + F_{\mathbf{k},\tau} Q_{\mathbf{k}} \right) \quad (2.69)$$

$$S_{phonon}^{\beta}[Q_{\mathbf{k}}^{\beta}] = \int_0^{\hbar\beta} d\tau \left( \frac{1}{2} \dot{Q}_{\mathbf{k}}^2 + \frac{1}{2} \omega_{\mathbf{k}}^2 Q_{\mathbf{k}}^2 \right) \quad (2.70)$$

and  $F_{\mathbf{k},\tau}$  is defined in Eq(2.42). Eq(2.69) is a Gaussian functional integral over all paths  $Q_{\mathbf{k}}^{\tau}$  which can be evaluated exactly[see Eq(2.46)]. One finds

$$\begin{aligned} S_{\mathbf{k}}[\mathbf{r}_{\tau}, Q_{\mathbf{k}}] &= \frac{\omega_{\mathbf{k}}}{2 \sin \omega_{\mathbf{k}} t} \left\{ \left( (Q_{\mathbf{k}}^t)^2 + (Q_{\mathbf{k}}^0)^2 \right) \cos \omega_{\mathbf{k}} t - 2Q_{\mathbf{k}}^t Q_{\mathbf{k}}^0 \right. \\ &+ \frac{1}{\sin \omega_{\mathbf{k}} t} \int_0^t d\tau \left( Q_{\mathbf{k}}^0 \sin \omega_{\mathbf{k}} (t - \tau) + Q_{\mathbf{k}}^t \sin \omega_{\mathbf{k}} (\tau) \right) F_{\mathbf{k},\tau} \\ &\left. - \frac{1}{\omega_{\mathbf{k}} \sin \omega_{\mathbf{k}} t} \int_0^t d\tau \int_0^t d\sigma \sin \omega_{\mathbf{k}} (t - \tau) \sin \omega_{\mathbf{k}} (\sigma) F_{\mathbf{k},\tau} F_{\mathbf{k},\sigma} \right\} \end{aligned} \quad (2.71)$$

The functional Eq(2.70) may also be decomposed according to

$$S_{phonon}^{\beta}[Q_{\mathbf{k}}^0, Q_{\mathbf{k}}^{\prime 0}] = \frac{\omega_{\mathbf{k}}}{2 \sinh \omega_{\mathbf{k}} \hbar \beta} \left\{ \left[ (Q_{\mathbf{k}}^0)^2 + (Q_{\mathbf{k}}^{\prime 0})^2 \right] \cosh \omega_{\mathbf{k}} \hbar \beta - 2Q_{\mathbf{k}}^0 Q_{\mathbf{k}}^{\prime 0} \right\} \quad (2.72)$$

Here, the trace has been performed by setting  $Q_{\mathbf{k}}^t = Q_{\mathbf{k}}^{\prime t}$  and integrating over these coordinates. The remaining evolution of the Gaussian integrals over the intermediate coordinates  $Q_{\mathbf{k}}^0, Q_{\mathbf{k}}^{\prime 0}$  is straightforward but tedious. After some algebra one obtains.

$$\rho(\mathbf{r}_t, \mathbf{r}'_t, t; \mathbf{r}_0, \mathbf{r}'_0, 0) = \int D[\mathbf{r}_\tau] \int D[\mathbf{r}'_\tau] e^{\frac{i}{\hbar} \{S_e[\mathbf{r}_\tau] - S_e[\mathbf{r}'_\tau]\} - \frac{1}{\hbar} \Phi[\mathbf{r}_\tau, \mathbf{r}'_\tau]} \quad (2.73)$$

where

$$\Phi[\mathbf{r}_\tau, \mathbf{r}'_\tau] = \int_0^t d\tau \int_0^\tau d\sigma \{F_{\mathbf{k},\tau}^* - F_{\mathbf{k},\tau}^{\prime*}\} \{T_{\omega_{\mathbf{k}}}(\tau - \sigma) F_{\mathbf{k},\tau} - T_{\omega_{\mathbf{k}}}^*(\tau - \sigma) F_{\mathbf{k},\tau}'\} \quad (2.74)$$

Substituting  $F_{\mathbf{k},\tau}$  into Eq(2.74) we have

$$\Phi[\mathbf{r}_\tau, \mathbf{r}'_\tau] = \sum_{\mathbf{k}} \frac{|C_{\mathbf{k}}|^2}{\hbar^2} \int_0^t d\tau \int_0^\tau d\sigma \{e^{i\mathbf{k}\cdot\mathbf{r}_\tau} - e^{i\mathbf{k}\cdot\mathbf{r}'_\tau}\} \{T_{\omega_{\mathbf{k}}}(\tau - \sigma) e^{-i\mathbf{k}\cdot\mathbf{r}_\sigma} - T_{\omega_{\mathbf{k}}}^*(\tau - \sigma) e^{-i\mathbf{k}\cdot\mathbf{r}'_\sigma}\} \quad (2.75)$$

Here we have introduced the kernel

$$T_{\omega_{\mathbf{k}}}(\tau - \sigma) = \frac{\cos[i\omega_{\mathbf{k}}(\tau - \sigma - i\hbar\beta/2)]}{\sinh \omega_{\mathbf{k}} \hbar\beta/2} \quad (2.76)$$

We can now completely express the non-equilibrium density matrix in terms of the electron coordinates only.

In Feynman [14], Feynman-Hellwarth-Iddings-Platzman [15] and Thornber-Feynman [17] a path integral similar to Eq(2.61) and Eq(2.73), had to be evaluated. They worked there in some rough approximation which we will show in details in chapters 3 and 5.

## CHAPTER 3

# THE NON-LOCAL ACTION AND THE PROPAGATOR

### 3.1 Introduction to the trial action

In the context of a path integral theory, a non-local action or two-time action arises in many physical systems. Historically, Feynman was the first to introduce a non-local action in his path integral theory of the polaron problem [14] to calculate the ground state energy. Subsequently many others have employed this type of action to treat several aspects of the polaron problem [15–17] and it has also been exploited in the calculation of the density of electronic states in disordered [25] systems.

It is convenient to describe the dynamics of the polaron system by a path integral over the electron and phonon coordinates. For Feynman’s approximation we use a “trial action” in which the electron is coupled to the lattice(a fictitious particle). The coupling is by some spring between the electron and the lattice particle. Such a system, in which the electron interacts with a single particle is described by the Lagrangian

$$L_{trial} = L_e + \frac{M}{2} \dot{\mathbf{y}}_\tau^2 - \frac{\kappa}{2} (\mathbf{r}_\tau - \mathbf{y}_\tau)^2 \quad (3.1)$$

where  $L_e$  is the Lagrangian for the electron system.  $M$  and  $\mathbf{y}$  refer to the mass and coordinate of the fictitious particle, and  $\kappa$  is a force constant. The propagator of the two-particle system can be written in the path integral form as

$$\begin{aligned} K(\mathbf{r}_{t_b}, \mathbf{y}_{t_b}, t_b; \mathbf{r}_{t_a}, \mathbf{y}_{t_a}, t_a) &= \int_{\mathbf{r}_{t_a}}^{\mathbf{r}_{t_b}} D[\mathbf{r}_\tau] \int_{\mathbf{y}_{t_a}}^{\mathbf{y}_{t_b}} D[\mathbf{y}_\tau] e^{\frac{i}{\hbar} \int_{t_a}^{t_b} d\tau (L_e - \kappa \mathbf{r}_\tau^2)} e^{\frac{i}{\hbar} \int_{t_a}^{t_b} d\tau (\frac{M}{2} \dot{\mathbf{y}}_\tau^2 - \frac{\kappa}{2} \mathbf{y}_\tau^2 + \kappa \mathbf{r}_\tau \cdot \mathbf{y}_\tau)} \\ &= \left( \frac{M\Omega}{2\pi i \sin \Omega T} \right)^3 \int_{\mathbf{r}_{t_a}}^{\mathbf{r}_{t_b}} D[\mathbf{r}_\tau] e^{\frac{i}{\hbar} \int_{t_a}^{t_b} d\tau (L_e - \kappa \mathbf{r}_\tau^2)} e^{\frac{i}{\hbar} S_0} \end{aligned} \quad (3.2)$$

where

$$\begin{aligned}
 S_0 = & \frac{M\Omega}{2\sin\Omega T} \left\{ (\mathbf{y}_{t_b}^2 - \mathbf{y}_{t_a}^2) \cos\Omega T - 2\mathbf{y}_{t_b}\mathbf{y}_{t_a} + 2\frac{\mathbf{y}_{t_b}\kappa}{M\Omega} \int_{t_a}^{t_b} d\tau \mathbf{r}_\tau \sin\Omega(\tau - t_a) \right. \\
 & \left. + 2\frac{\mathbf{y}_{t_a}\kappa}{M\Omega} \int_{t_a}^{t_b} d\tau \mathbf{r}_\tau \sin\Omega(t_b - \tau) - \frac{2\kappa^2}{M^2\Omega^2} \int_{t_a}^{t_b} d\tau \int_{t_a}^{t_b} d\sigma \mathbf{r}_\tau \sin\Omega(t_b - \tau) \sin\Omega(\sigma - t_a) \mathbf{r}_\sigma \right\}
 \end{aligned} \quad (3.3)$$

with  $\Omega = \sqrt{\frac{\kappa}{M}}$ . The fictitious particle coordinate can now be eliminated by first setting  $\mathbf{y}_{t_b} = \mathbf{y}_{t_a} = \mathbf{y}$  and then integrating with respect to  $\mathbf{y}$ , to obtain

$$K(\mathbf{r}_{t_b}, t_b; \mathbf{r}_{t_a}, t_a) = \left( \frac{M\Omega}{2\pi i \sin\Omega T} \right)^3 \int_{\mathbf{r}_{t_a}}^{\mathbf{r}_{t_b}} D[\mathbf{r}_\tau] e^{\frac{i}{\hbar} \int_{t_a}^{t_b} d\tau (L_e - \kappa \mathbf{r}_\tau^2)} e^{\frac{i}{\hbar} \frac{\kappa^2}{M\Omega} \int_{t_a}^{t_b} d\tau \int_{t_a}^{t_b} d\sigma \mathbf{r}_\tau \frac{\cos\Omega(|\tau - \sigma| - T/2)}{\sin\Omega T/2} \mathbf{r}_\sigma}$$
(3.4)

Using;  $T = t_b - t_a$

$$\int_{t_a}^{t_b} d\tau \mathbf{r}_\tau^2 = \frac{\Omega}{2\sin\Omega T/2} \int_{t_a}^{t_b} d\tau \int_{t_a}^{t_b} d\sigma \cos\Omega(|\tau - \sigma| - T/2) (\mathbf{r}_\tau^2 + \mathbf{r}_\sigma^2) \quad (3.5)$$

and rearranging terms in the exponent of Eq(3.4) with the help of Eq(3.5), we have  
 $(t_a = 0, t_b = t)$

$$K(\mathbf{r}_t, t; \mathbf{r}_0, 0) = \left( \frac{M\Omega}{2\pi i \sin\Omega T} \right)^3 \int_{\mathbf{r}_0}^{\mathbf{r}_t} D[\mathbf{r}_\tau] e^{\frac{i}{\hbar} S_{trial}(\dot{\mathbf{r}}, \mathbf{r}, \tau)} \quad (3.6)$$

where  $S_{trial}$  is the trial action for the system after the coordinates of the fictitious particle have been eliminated

$$S_{trial} = \int_0^t d\tau L_e - \frac{\kappa\Omega}{8} \int_0^t d\tau \int_0^t d\sigma \frac{\cos\Omega(|\tau - \sigma| - t/2)}{\sin\Omega t/2} (\mathbf{r}_\tau - \mathbf{r}_\sigma)^2 \quad (3.7)$$

We now interested in solving for the propagator which  $L_e$  consists of

$$L_e = \frac{m}{2} (\dot{\mathbf{r}}_\tau^2 - \omega_0^2 \mathbf{r}_\tau^2 + \omega_c [\dot{x}_\tau y_\tau - x_\tau \dot{y}_\tau]) + \mathbf{f}_\tau \cdot \mathbf{r}_\tau \quad (3.8)$$

where  $\omega_c$  is the cyclotron frequency. Then for 3-dimensions, the form of such a trial action considered in this section is

$$\begin{aligned}
 S_{trial} = & \frac{m}{2} \int_0^t d\tau (\dot{\mathbf{r}}_\tau^2 - \omega_0^2 \mathbf{r}_\tau^2 + \omega_c \dot{\mathbf{r}}_\tau \mathbf{J} \mathbf{r}_\tau) + \int_0^t d\tau \mathbf{f}_\tau \cdot \mathbf{r}_\tau \\
 & - \frac{1}{2} \int_0^t d\tau \int_0^t d\sigma (\mathbf{r}_\tau - \mathbf{r}_\sigma) \cdot \mathbf{G}_{|\tau - \sigma|} \cdot (\mathbf{r}_\tau - \mathbf{r}_\sigma)
 \end{aligned} \quad (3.9)$$

where

$$\mathbf{J} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (3.10)$$

with the diagonal tensor

$$G_{|\tau-\sigma|}^{ij} = \delta_{ij} \frac{\kappa_{ij}\Omega_{ij}}{4} \frac{\cos \Omega_{ij} (|\tau - \sigma| - t/2)}{\sin \Omega_{ij} t/2} \quad (3.11)$$

$\omega_0$ ,  $\omega_c$ ,  $\Omega_{ij}$  and  $\kappa_{ij}$  are distinct positive parameters where  $\Omega_{11} = \Omega_{22} = \Omega_{\perp}$ ,  $\kappa_{11} = \kappa_{22} = \kappa_{\perp}$ ,  $\Omega_{33} = \Omega_{\parallel}$  and  $\kappa_{33} = \kappa_{\parallel}$ . The final expression for the propagator will depend on the time parameter  $t$  and the end point parameters  $\mathbf{r}_t$  and  $\mathbf{r}_0$ . We emphasize that these parameters are kept absolutely general throughout the derivation. The meanings of the terms in the action Eq(3.9) are as follows. The first term is the kinetic energy of the particle of mass  $m$ . The second term is the local harmonic oscillator. The third term is the interaction of the particle with a magnetic field. The fourth is due to an arbitrary driving force  $\mathbf{f}_{\tau}$ . The last term consists of a non-local oscillator. We now propose a new equivalent form for the trial action as

$$S_{trial} = \frac{m}{2} \int_0^t d\tau \dot{\mathbf{r}}_{\tau}^2 + \int_0^t d\tau \mathbf{f}_{\tau} \cdot \mathbf{r}_{\tau} + \frac{1}{2} \int_0^t d\tau \int_0^t d\sigma \mathbf{r}_{\tau} \cdot \bar{\mathbf{G}}_{|\tau-\sigma|} \cdot \mathbf{r}_{\sigma} \quad (3.12)$$

where

$$\bar{G}_{|\tau-\sigma|}^{ij} = m \left( \frac{\kappa_{ij}}{m} - \omega_0^2 \right) \delta(\tau - \sigma) + m\omega_c J_{ij} \dot{\delta}(\tau - \sigma) - \frac{\kappa_{ij}\Omega_{ij}\delta_{ij}}{2} \frac{\cos \Omega_{ij} (|\tau - \sigma| - t/2)}{\sin \Omega_{ij} t/2} \quad (3.13)$$

After integrating by parts of Eq(3.12), we obtain for the classical action

$$\bar{S}_{trial} = \frac{m}{2} (\mathbf{r}_t \cdot \dot{\mathbf{r}}_t - \mathbf{r}_0 \cdot \dot{\mathbf{r}}_0) + \int_0^t d\tau \mathbf{f}_{\tau} \cdot \mathbf{r}_{\tau} \quad (3.14)$$

Since the action  $S_{trial}$  is a quadratic function of the coordinates, it can be shown [12] that

$$K(\mathbf{r}_t, t; \mathbf{r}_0, 0) = F(t, 0) e^{\frac{i}{\hbar} \bar{S}_{trial}(\mathbf{r}_t, t; \mathbf{r}_0, 0)} \quad (3.15)$$

The prefactor  $F$  is given by [26]

$$F(t, 0) = \int_0^0 D[\mathbf{r}_{\tau}] e^{\frac{i}{\hbar} S_{trial, f=0}} \quad (3.16)$$

and is independent of the coordinates  $\mathbf{r}_0$  and  $\mathbf{r}_t$ . An explicit expression for this prefactor may be derived from the classical solution.

### 3.2 The classical solution

To solve the stationary parts, we start from the equation of motion

$$m\ddot{\mathbf{r}}_\tau - \int_0^t d\sigma \bar{\mathbf{G}}_{\tau-\sigma} \cdot \mathbf{r}_\sigma = \mathbf{f}_\tau \quad (3.17)$$

We now introduce a transformation matrix

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i & 0 \\ i & -1 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix} \quad \text{with} \quad U^\dagger = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i & 0 \\ i & -1 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix} \quad (3.18)$$

So we write

$$m\ddot{\mathbf{R}}_\tau - \int_0^t d\sigma \mathbf{g}_{\tau-\sigma} \cdot \mathbf{R}_\sigma = \mathbf{F}_\tau \quad (3.19)$$

where

$$\mathbf{R}_\tau = U^\dagger \mathbf{r}_\tau \quad (3.20)$$

$$\mathbf{F}_\tau = U^\dagger \mathbf{f}_\tau \quad (3.21)$$

$$\mathbf{g}_{\tau-\sigma} = U^\dagger \bar{\mathbf{G}}_{\tau-\sigma} U = g_{\tau-\sigma}^{ij} \delta_{ij} \quad (3.22)$$

We now solve for  $R_\tau^1$  using

$$m\ddot{R}_\tau^1 - \int_0^t d\sigma g_{\tau-\sigma}^{11} R_\sigma^1 = F_\tau^1 \quad (3.23)$$

and  $R_\tau^1$  may be written as

$$R_\tau^1 = \mu_\tau^1 + \int_0^t d\sigma C_{\tau-\sigma}^1 F_\sigma^1 \quad (3.24)$$

where  $\mu_\tau^1$  is the solution of Eq(3.23) for the homogeneous case. It satisfies

$$m\ddot{\mu}_\tau^1 - \int_0^t d\sigma g_{\tau-\sigma}^{11} \mu_\sigma^1 = 0 \quad (3.25)$$

$C_{\tau-\sigma}^1$  is the Green's function from

$$m \frac{\partial^2}{\partial \tau^2} C_{\tau-\sigma}^1 - \int_0^t d\sigma' g_{\tau-\sigma'}^{11} C_{\sigma'-\sigma}^1 = \delta(\tau - \sigma) \quad (3.26)$$

with “boundary conditions” as  $C^1(t, \sigma) = C^1(0, \sigma) = 0$  and  $R_t^1 = \mu_t^1$ ,  $R_0^1 = \mu_0^1$ . We now let  $g_{\tau-\sigma}^{11} = \sum_n g_n^{11} e^{i\nu_n(\tau-\sigma)}$ ;  $g_n^{11} = g_{-n}^{11}$ ,  $\nu_n = \frac{2\pi n}{t}$ , and Eq(3.23) becomes

$$m\ddot{R}_\tau^1 - \sum_n g_n^{11} \int_0^t d\sigma e^{i\nu_n(\tau-\sigma)} R_\sigma^1 = F_\tau^1 \quad (3.27)$$

or

$$\begin{aligned} \frac{m}{t} \int_0^t d\tau \ddot{R}_\tau^1 e^{-i\nu_n\tau} &= g_n^{11} \int_0^t d\tau R_\tau^1 e^{-i\nu_n\tau} + \frac{1}{t} \int_0^t d\tau F_\tau^1 e^{-i\nu_n\tau} \\ &= B_n^1 \end{aligned} \quad (3.28)$$

Then

$$B_n^1 = B_0^1 + i\nu_n \frac{m}{t} (R_t^1 - R_0^1) - \nu_n^2 \frac{m}{t} \int_0^t d\tau R_\tau^1 e^{-i\nu_n\tau} \quad (3.29)$$

and

$$\begin{aligned} \sum_{n \neq 0} \frac{B_n^1}{\nu_n^2} (e^{i\nu_n\tau} - 1) &= B_0^1 \sum_{n \neq 0} \frac{(e^{i\nu_n\tau} - 1)}{\nu_n^2} + \frac{m}{t} (R_t^1 - R_0^1) \sum_{n \neq 0} \frac{i(e^{i\nu_n\tau} - 1)}{\nu_n} \\ &\quad - \frac{m}{t} \int_0^t d\sigma R_\sigma^1 \sum_{n \neq 0} e^{-i\nu_n\sigma} (e^{i\nu_n\tau} - 1) \end{aligned} \quad (3.30)$$

where

$$\sum_{n \neq 0} \frac{(e^{i\nu_n\tau} - 1)}{\nu_n^2} = 2 \sum_{n=1} \frac{(\cos \nu_n\tau - 1)}{\nu_n^2} \quad (3.31)$$

$$i \sum_{n \neq 0} \frac{(e^{i\nu_n\tau} - 1)}{\nu_n} = -2 \sum_{n=1} \frac{\sin \nu_n\tau}{\nu_n} \quad (3.32)$$

and

$$\sum_{n \neq 0} e^{-i\nu_n\sigma} (e^{i\nu_n\tau} - 1) = \sum_{n=1} e^{-i\nu_n\sigma} (e^{i\nu_n\tau} - 1) = t \sum_{n=1} (\delta(\sigma - \tau - nt) - \delta(\sigma - nt)) \quad (3.33)$$

So Eq(3.30) becomes

$$\begin{aligned} \sum_{n \neq 0} \frac{B_n^1}{\nu_n^2} (e^{i\nu_n\tau} - 1) &= B_0^1 \frac{\tau}{2} (\tau - t) + m (R_t^1 - R_0^1) \left( \frac{\tau}{t} - \frac{1}{2} \right) \\ &\quad - m R_\tau^1 + \frac{m}{2} (R_t^1 + R_0^1) \end{aligned} \quad (3.34)$$

We can obtain  $R_\tau^1$  as

$$R_\tau^1 = R_0^1 + (R_t^1 - R_0^1) \frac{\tau}{t} + \frac{B_0^1}{m} \frac{\tau}{2} (\tau - t) - \frac{1}{m} \sum_{n \neq 0} \frac{B_n^1}{\nu_n^2} (e^{i\nu_n\tau} - 1) \quad (3.35)$$

Now defining

$$F_n^1 = \frac{1}{t} \int_0^t d\tau F_\tau^1 e^{-i\nu_n \tau} \quad (3.36)$$

Eq(3.28) becomes

$$B_n^1 = F_n^1 + g_n^{11} \int_0^t d\tau R_\tau^1 e^{-i\nu_n \tau} \quad (3.37)$$

From Eq(3.35), we have ( $n \neq 0$ )

$$\begin{aligned} \int_0^t d\tau R_\tau^1 e^{-i\nu_n \tau} &= \int_0^t d\tau \left( R_0^1 + [R_t^1 - R_0^1] \frac{\tau}{t} \right) e^{-i\nu_n \tau} + \frac{B_0^1}{2m} \int_0^t d\tau e^{-i\nu_n \tau} \tau (\tau - t) \\ &\quad - \frac{1}{m} \sum_{n' \neq 0} \frac{B_{n'}^1}{\nu_{n'}^2} \int_0^t d\tau \left( e^{-i\nu_{n'} \tau} - 1 \right) e^{-i\nu_n \tau} \\ &= \frac{i}{\nu_n} \left( R_t^1 - R_0^1 \right) + \frac{B_0^1 t}{m\nu_n^2} - \frac{B_n^1 t}{m\nu_n^2} \end{aligned} \quad (3.38)$$

and

$$\left( 1 + \frac{tg_n^{11}}{m\nu_n^2} \right) B_n^1 = F_n^1 + \frac{ig_n^{11}}{\nu_n} \left( R_t^1 - R_0^1 \right) + \frac{g_n^{11} B_0^1 t}{m\nu_n^2} \quad (3.39)$$

For  $n = 0$ , Eq(3.38) becomes

$$\int_0^t d\tau R_\tau^1 = \frac{t}{2} \left( R_t^1 + R_0^1 \right) - \frac{B_0^1 t^3}{12m} + \sum_{n \neq 0} \frac{B_n^1 t}{m\nu_n^2} \quad (3.40)$$

From Eq(3.39), we have

$$\begin{aligned} \frac{B_n^1}{m\nu_n^2} &= \frac{F_n^1}{m\nu_n^2 + tg_n^{11}} + \frac{ig_n^{11}}{\nu_n (m\nu_n^2 + tg_n^{11})} \left( R_t^1 - R_0^1 \right) + \frac{g_n^{11} B_0^1 t}{m\nu_n^2 (m\nu_n^2 + tg_n^{11})} \quad (3.41) \\ \sum_{n \neq 0} \frac{B_n^1}{m\nu_n^2} &= \sum_{n \neq 0} \frac{F_n^1}{m\nu_n^2 + tg_n^{11}} + \sum_{n \neq 0} \frac{ig_n^{11}}{\nu_n (m\nu_n^2 + tg_n^{11})} \left( R_t^1 - R_0^1 \right) + \sum_{n \neq 0} \frac{g_n^{11} B_0^1 t}{m\nu_n^2 (m\nu_n^2 + tg_n^{11})} \\ &= \sum_{n \neq 0} \frac{F_n^1}{m\nu_n^2 + tg_n^{11}} + \sum_{n \neq 0} \frac{ig_n^{11}}{\nu_n (m\nu_n^2 + tg_n^{11})} \left( R_t^1 - R_0^1 \right) \\ &\quad + i \sum_{n \neq 0} \left( \frac{1}{m\nu_n^2} - \frac{1}{m\nu_n^2 + tg_n^{11}} \right) B_0^1 \\ t \sum_{n \neq 0} \frac{B_n^1}{m\nu_n^2} &= t \sum_{n \neq 0} \frac{F_n^1}{m\nu_n^2 + tg_n^{11}} + t \sum_{n \neq 0} \frac{ig_n^{11}}{\nu_n (m\nu_n^2 + tg_n^{11})} \left( R_t^1 - R_0^1 \right) \\ &\quad + \frac{B_0^1 t^3}{12m} - \sum_{n \neq 0} \frac{B_0^1 t}{m\nu_n^2 + tg_n^{11}} \end{aligned} \quad (3.42)$$

Substituting Eq(3.42) into Eq(3.40), we obtain

$$\begin{aligned} \int_0^t d\tau R_\tau^1 &= \frac{t}{2} \left( R_t^1 + R_0^1 \right) + t \sum_{n \neq 0} \frac{ig_n^{11}}{\nu_n (m\nu_n^2 + tg_n^{11})} \left( R_t^1 - R_0^1 \right) \\ &\quad + t \sum_{n \neq 0} \frac{F_n^1}{m\nu_n^2 + tg_n^{11}} - \sum_{n \neq 0} \frac{B_0^1 t}{m\nu_n^2 + tg_n^{11}} \end{aligned} \quad (3.43)$$

Using Eq(3.43), we obtain for  $B_0^1$

$$\begin{aligned} B_0^1 &= F_0^1 + \frac{tg_0^{11}}{2} (R_t^1 + R_0^1) + tg_0^{11} \sum_{n \neq 0} \frac{F_n^1}{m\nu_n^2 + tg_n^{11}} - g_0^{11} \sum_{n \neq 0} \frac{B_0^1 t}{m\nu_n^2 + tg_n^{11}} \\ &\quad + itg_0^{11} \sum_{n \neq 0} \frac{ig_n^{11}}{\nu_n (m\nu_n^2 + tg_n^{11})} (R_t^1 - R_0^1) \end{aligned} \quad (3.44)$$

and

$$\begin{aligned} \left( 1 + tg_0^{11} \sum_{n \neq 0} \frac{1}{m\nu_n^2 + tg_n^{11}} \right) B_0^1 &= F_0^1 + \frac{tg_0^{11}}{2} (R_t^1 + R_0^1) + tg_0^{11} \sum_{n \neq 0} \frac{F_n^1}{m\nu_n^2 + tg_n^{11}} \\ &\quad + itg_0^{11} \sum_{n \neq 0} \frac{ig_n^{11}}{\nu_n (m\nu_n^2 + tg_n^{11})} (R_t^1 - R_0^1) \end{aligned} \quad (3.45)$$

For  $F_n^1 = 0$ , Eq(3.35) becomes

$$\mu_\tau^1 = R_0^1 + \frac{\tau}{t} (R_t^1 - R_0^1) + \frac{B_0^1 \tau}{2m} (\tau - t) - \frac{1}{m} \sum_{n \neq 0} \frac{B_n^1}{\nu_n^2} (e^{i\nu_n \tau} - 1) \quad (3.46)$$

From Eq(3.41), we can write

$$\begin{aligned} \frac{1}{m} \sum_{n \neq 0} \frac{B_n^1}{m\nu_n^2} (e^{i\nu_n \tau} - 1) &= i (R_t^1 - R_0^1) \sum_{n \neq 0} \frac{g_n^{11} (e^{i\nu_n \tau} - 1)}{\nu_n (m\nu_n^2 + tg_n^{11})} \\ &\quad + B_0^1 t \sum_{n \neq 0} \frac{g_n^{11} (e^{i\nu_n \tau} - 1)}{m\nu_n^2 (m\nu_n^2 + tg_n^{11})} \\ &= \frac{im}{t} (R_t^1 - R_0^1) \sum_{n \neq 0} \left( \frac{\nu_n}{m\nu_n^2} - \frac{\nu_n}{m\nu_n^2 + tg_n^{11}} \right) (e^{i\nu_n \tau} - 1) \\ &\quad + \sum_{n \neq 0} \left( \frac{1}{m\nu_n^2} - \frac{1}{m\nu_n^2 + tg_n^{11}} \right) (e^{i\nu_n \tau} - 1) B_0^1 \\ &= \frac{m}{t} (R_t^1 - R_0^1) \sum_{n \neq 0} \frac{\partial}{\partial \tau} \left( \frac{1}{m\nu_n^2} - \frac{1}{m\nu_n^2 + tg_n^{11}} \right) (e^{i\nu_n \tau} - 1) \\ &\quad + \sum_{n \neq 0} \left( \frac{1}{m\nu_n^2} - \frac{1}{m\nu_n^2 + tg_n^{11}} \right) (e^{i\nu_n \tau} - 1) B_0^1 \end{aligned} \quad (3.47)$$

Defining

$$D_\tau^1 \equiv \frac{1}{t} \sum_{n \neq 0} \frac{e^{i\nu_n \tau}}{m\nu_n^2 + tg_n^{11}} \quad (3.48)$$

We have

$$\begin{aligned} \sum_{n \neq 0} \frac{B_n^1}{m\nu_n^2} (e^{i\nu_n \tau} - 1) &= (R_t^1 - R_0^1) \frac{m}{t} \left( \frac{1}{m} \left( \tau - \frac{t}{2} \right) - tD_\tau^1 \right) - \left( \frac{1}{2} + D_0^1 \right) (R_t^1 - R_0^1) \\ &\quad + \left( \frac{\tau}{2m} (\tau - t) - tD_\tau^1 + tD_0^1 \right) B_0^1 \end{aligned} \quad (3.49)$$

Inserting Eq(3.49) into Eq(3.46), we have

$$\mu_\tau^1 = \frac{1}{2} (R_t^1 + R_0^1) + m\dot{D}_\tau^1 (R_t^1 - R_0^1) + (D_\tau^1 - D_0^1) B_0^1 t - \left(\frac{1}{2} + \dot{D}_0^1\right) (R_t^1 - R_0^1) \quad (3.50)$$

From Eq(3.45), for  $F_0^1 = 0$

$$B_0^1 t = \frac{tg_0^{11}}{2(1 + tg_0^{11}D_0^1)} (R_t^1 + R_0^1) - \frac{tg_0^{11}}{(1 + tg_0^{11}D_0^1)} \left(\frac{1}{2} + \dot{D}_0^1\right) (R_t^1 - R_0^1) \quad (3.51)$$

Then Eq(3.50) becomes

$$\begin{aligned} \mu_\tau^1 &= \frac{1}{2} \left(\frac{1 + tg_0^{11}D_\tau^1}{1 + tg_0^{11}D_0^1}\right) (R_t^1 + R_0^1) + m\dot{D}_\tau^1 (R_t^1 - R_0^1) \\ &\quad - \left(\frac{1 + tg_0^{11}D_\tau^1}{1 + tg_0^{11}D_0^1}\right) \left(\frac{1}{2} + \dot{D}_0^1\right) (R_t^1 - R_0^1) \end{aligned} \quad (3.52)$$

If  $g_0^{11} \neq 0$ , we define

$$\bar{D}_\tau^1 = \frac{1}{t} \sum_{n=0} \frac{e^{i\nu_n \tau}}{m\nu_n^2 + tg_n^{11}} \quad (3.53)$$

Then we have  $\bar{D}_\tau^1 = D_\tau^1 + \frac{1}{t^2 g_0^{11}}$ ,  $\dot{\bar{D}}_\tau^1 = \dot{D}_\tau^1$ , and we can rewrite Eq(3.52) as

$$\mu_\tau^1 = \frac{1}{2} \left(\frac{\bar{D}_\tau^1}{\bar{D}_0^1}\right) (R_t^1 + R_0^1) + m\dot{\bar{D}}_\tau^1 (R_t^1 - R_0^1) - \frac{\bar{D}_\tau^1}{\bar{D}_0^1} \left(\frac{1}{2} + \dot{\bar{D}}_0^1\right) (R_t^1 - R_0^1) \quad (3.54)$$

Next we evaluate  $C_{\tau-\sigma}^1$ . Consider

$$C_{\tau-\sigma}^1 = \frac{\delta R_\tau^1}{\delta F_\tau^1} = \frac{\delta B_0^1}{\delta F_\tau^1} \frac{\tau}{2m} (\tau - t) - \frac{1}{m} \sum_{n \neq 0} \frac{1}{\nu_n^2} \frac{\delta B_0^1}{\delta F_\tau^1} (e^{i\nu_n \tau} - 1) \quad (3.55)$$

For  $n \neq 0$

$$\begin{aligned} \frac{\delta B_0^1}{\delta F_\tau^1} \left(1 + \frac{tg_n^{11}}{m\nu_n^2}\right) &= \frac{\delta F_n^1}{\delta F_\sigma^1} + \frac{tg_n^{11}}{m\nu_n^2} \frac{\delta B_0^1}{\delta F_\sigma^1} \\ &= \frac{e^{-i\nu_n \sigma}}{t} + \frac{tg_n^{11}}{m\nu_n^2} \frac{\delta B_0^1}{\delta F_\sigma^1} \end{aligned} \quad (3.56)$$

and

$$\begin{aligned} \frac{\delta B_0^1}{\delta F_\tau^1} (1 + tg_n^{11}D_0^1) &= \frac{\delta F_n^1}{\delta F_\sigma^1} + tg_n^{11} \sum_{n \neq 0} \frac{\delta F_0^1}{\delta F_\sigma^1} \frac{1}{m\nu_n^2 + tg_n^{11}} \\ &= \frac{1}{t} + g_0^{11} \sum_{n \neq 0} \frac{e^{-i\nu_n \sigma}}{m\nu_n^2 + tg_n^{11}} \\ &= \frac{1}{t} (1 + t^2 g_0^{11} D_\sigma^1) \\ \frac{\delta B_0^1}{\delta F_\sigma^1} &= \frac{1}{t} \left(\frac{1 + t^2 g_0^{11} D_\sigma^1}{1 + t^2 g_0^{11} D_0^1}\right) \end{aligned} \quad (3.57)$$

and

$$\begin{aligned}
\frac{1}{m} \sum_{n \neq 0} \frac{1}{\nu_n^2} \frac{\delta B_0^1}{\delta F_\sigma^1} \left( e^{i\nu_n \tau} - 1 \right) &= \frac{1}{t} \sum_{n \neq 0} \frac{e^{-i\nu_n \sigma} (e^{i\nu_n \tau} - 1)}{m\nu_n^2 + tg_n^{11}} \\
&+ \frac{\delta B_0^1}{\delta F_\sigma^1} \sum_{n \neq 0} \left( \frac{1}{m\nu_n^2} - \frac{1}{m\nu_n^2 + tg_n^{11}} \right) (e^{i\nu_n \tau} - 1) \\
&= D_{\tau-\sigma}^1 - D_\sigma^1 + \frac{\delta B_0^1}{\delta F_\sigma^1} \left( \frac{\tau}{2m} (\tau - t) - tD_\tau^1 + tD_0^1 \right)
\end{aligned} \tag{3.58}$$

then for  $0 \leq \tau \leq t$

$$\begin{aligned}
C_{\tau-\sigma}^1 &= -D_{\tau-\sigma}^1 + D_\sigma^1 + t \frac{\delta B_0^1}{\delta F_\sigma^1} (D_\tau^1 - D_0^1) \\
&= D_\tau^1 + D_\sigma^1 - D_{\tau-\sigma}^1 + D_0^1 + t \frac{t^2 g_0^{11}}{1 + t^2 g_0^{11} D_0^1} (D_\tau^1 - D_0^1) (D_\sigma^1 - D_0^1)
\end{aligned} \tag{3.59}$$

For  $g_0^{11} \neq 0$ ,  $C_{\tau-\sigma}^1$  becomes

$$C_{\tau-\sigma}^1 = \frac{\bar{D}_\tau^1 \bar{D}_\sigma^1}{\bar{D}_0^1} - \bar{D}_{\tau-\sigma}^1 \tag{3.60}$$

We now write

$$\begin{aligned}
R_\tau^1 &= \frac{1}{2} \frac{\bar{D}_\tau^1}{\bar{D}_0^1} (R_t^1 + R_0^1) + \left( m\dot{\bar{D}}_\tau^1 - \frac{\bar{D}_\tau^1}{\bar{D}_0^1} \left( \frac{1}{2} + \dot{\bar{D}}_0^1 \right) \right) (R_t^1 - R_0^1) \\
&+ \int_0^t d\sigma \left( \frac{\bar{D}_\tau^1 \bar{D}_\sigma^1}{\bar{D}_0^1} - \bar{D}_{\tau-\sigma}^1 \right) F_\sigma^1
\end{aligned} \tag{3.61}$$

In the same manner as the calculation of  $R_\tau^1$ , we can write  $R_\tau^2$  and  $R_\tau^3$  as

$$\begin{aligned}
R_\tau^2 &= \frac{1}{2} \frac{\bar{D}_\tau^2}{\bar{D}_0^2} (R_t^2 + R_0^2) + \left( m\dot{\bar{D}}_\tau^2 - \frac{\bar{D}_\tau^2}{\bar{D}_0^2} \left( \frac{1}{2} + \dot{\bar{D}}_0^2 \right) \right) (R_t^2 - R_0^2) \\
&+ \int_0^t d\sigma \left( \frac{\bar{D}_\tau^2 \bar{D}_\sigma^2}{\bar{D}_0^2} - \bar{D}_{\tau-\sigma}^2 \right) F_\sigma^2
\end{aligned} \tag{3.62}$$

and

$$\begin{aligned}
R_\tau^3 &= \frac{1}{2} \frac{\bar{D}_\tau^3}{\bar{D}_0^3} (R_t^3 + R_0^3) + \left( m\dot{\bar{D}}_\tau^3 - \frac{\bar{D}_\tau^3}{\bar{D}_0^3} \left( \frac{1}{2} + \dot{\bar{D}}_0^3 \right) \right) (R_t^3 - R_0^3) \\
&+ \int_0^t d\sigma \left( \frac{\bar{D}_\tau^3 \bar{D}_\sigma^3}{\bar{D}_0^3} - \bar{D}_{\tau-\sigma}^3 \right) F_\sigma^3
\end{aligned} \tag{3.63}$$

So we now have the relation

$$\begin{aligned}
 \begin{pmatrix} R_\tau^1 \\ R_\tau^2 \\ R_\tau^3 \end{pmatrix} &= \frac{1}{2} \begin{pmatrix} \frac{\bar{D}_\tau^1}{\bar{D}_0^1} & 0 & 0 \\ 0 & \frac{\bar{D}_\tau^2}{\bar{D}_0^2} & 0 \\ 0 & 0 & \frac{\bar{D}_\tau^3}{\bar{D}_0^3} \end{pmatrix} \begin{pmatrix} R_t^1 + R_0^1 \\ R_t^2 + R_0^2 \\ R_t^3 + R_0^3 \end{pmatrix} + m \begin{pmatrix} \dot{\bar{D}}_\tau^1 & 0 & 0 \\ 0 & \dot{\bar{D}}_\tau^2 & 0 \\ 0 & 0 & \dot{\bar{D}}_\tau^3 \end{pmatrix} \begin{pmatrix} R_t^1 - R_0^1 \\ R_t^2 - R_0^2 \\ R_t^3 - R_0^3 \end{pmatrix} \\
 &- \begin{pmatrix} \frac{\bar{D}_\tau^1}{\bar{D}_0^1} \left( \frac{1}{2} + \dot{\bar{D}}_0^1 \right) & 0 & 0 \\ 0 & \frac{\bar{D}_\tau^2}{\bar{D}_0^2} \left( \frac{1}{2} + \dot{\bar{D}}_0^2 \right) & 0 \\ 0 & 0 & \frac{\bar{D}_\tau^3}{\bar{D}_0^3} \left( \frac{1}{2} + \dot{\bar{D}}_0^3 \right) \end{pmatrix} \begin{pmatrix} R_t^1 - R_0^1 \\ R_t^2 - R_0^2 \\ R_t^3 - R_0^3 \end{pmatrix} \\
 &+ \int_0^t d\sigma \begin{pmatrix} \frac{\bar{D}_\tau^1 \bar{D}_\sigma^1}{\bar{D}_0^1} - \bar{D}_{\tau-\sigma}^1 & 0 & 0 \\ 0 & \frac{\bar{D}_\tau^2 \bar{D}_\sigma^2}{\bar{D}_0^2} - \bar{D}_{\tau-\sigma}^2 & 0 \\ 0 & 0 & \frac{\bar{D}_\tau^3 \bar{D}_\sigma^3}{\bar{D}_0^3} - \bar{D}_{\tau-\sigma}^3 \end{pmatrix} \begin{pmatrix} F_\sigma^1 \\ F_\sigma^2 \\ F_\sigma^3 \end{pmatrix} \quad (3.64)
 \end{aligned}$$

Using  $\mathbf{r}_\tau = U\mathbf{R}_\tau$ , we obtain for  $\mathbf{r}_\tau$

$$\begin{aligned}
 \mathbf{r}_\tau &= \frac{1}{8} \mathbf{D}_0^{-1} \cdot \mathbf{D}_\tau \cdot (\mathbf{r}_t + \mathbf{r}_0) + \frac{1}{4} \left( m \dot{\mathbf{D}}_\tau - \left( \frac{1}{2} + \dot{\mathbf{D}}_0 \right) \cdot \mathbf{D}_0^{-1} \cdot \mathbf{D}_\tau \right) \cdot (\mathbf{r}_t - \mathbf{r}_0) \\
 &+ \frac{1}{4} \int_0^t d\sigma \left( \mathbf{D}_0^{-1} \cdot \mathbf{D}_\tau \cdot \mathbf{D}_\sigma - \mathbf{D}_{\tau-\sigma} \right) \cdot \mathbf{f}_\sigma \quad (3.65)
 \end{aligned}$$

where

$$\mathbf{D}_\tau = \begin{pmatrix} \bar{D}_\tau^1 + \bar{D}_\tau^2 & -i(\bar{D}_\tau^1 - \bar{D}_\tau^2) & 0 \\ i(\bar{D}_\tau^1 - \bar{D}_\tau^2) & \bar{D}_\tau^1 + \bar{D}_\tau^2 & 0 \\ 0 & 0 & \bar{D}_\tau^3 \end{pmatrix} \quad (3.66)$$

Next we consider

$$g_{\tau-\sigma}^{11} = m \left( \frac{\kappa_\perp}{m} - \omega_0^2 \right) \delta(\tau - \sigma) - i\omega_c \dot{\delta}(\tau - \sigma) - \kappa_\perp \Omega_\perp \frac{\cos \Omega_\perp (|\tau - \sigma| - t/2)}{\sin \Omega_\perp t/2} \quad (3.67)$$

and the Fourier expansion of

$$\Omega_\perp \frac{\cos \Omega_\perp (|\tau - \sigma| - t/2)}{2 \sin \Omega_\perp t/2} = \frac{\Omega_\perp^2}{t} \sum_{n=-\infty}^{\infty} \frac{e^{-i\nu_n(\tau-\sigma)}}{\nu_n^2 - \Omega_\perp^2} \quad (3.68)$$

Then

$$\begin{aligned}
 tg_n^{11} &= -m\omega_0^2 - \frac{\kappa_\perp \nu_n^2}{\nu_n^2 - \Omega_\perp^2} - m\omega_c \nu_n \\
 \frac{m}{m\nu_n^2 + tg_n^{11}} &= \frac{\nu_n^2 - \Omega_\perp^2}{\nu_n^4 - \nu_n^2 (\Omega_\perp^2 + \frac{\kappa_\perp}{m}) + \nu_n^3 \omega_c - \nu_n \omega_c \Omega_\perp^2 + \omega_0^2 \Omega_\perp^2} \\
 &= \sum_{l=1}^4 \frac{(s_l^2 - \Omega_\perp^2)}{\prod_{l \neq k} (s_l - s_k)} \frac{1}{\nu_n - s_l} \quad (3.69)
 \end{aligned}$$

where  $s_l$  is a root of the polynomial of degree four in the denominator. Then

$$\frac{1}{t} \sum_n \frac{e^{i\nu_n \tau}}{m\nu_n^2 + tg_n^{11}} = \bar{D}_\tau^1 = \frac{1}{m} \sum_{l=1}^4 \frac{(s_l^2 - \Omega_\perp^2)}{\prod_{l \neq k} (s_l - s_k)} \frac{1}{t} \sum_{n=-\infty}^{\infty} \frac{e^{i\nu_n \tau}}{\nu_n - s_l} \quad (3.70)$$

We let

$$G_\tau(s_l) = \frac{1}{t} \sum_{n=-\infty}^{\infty} \frac{e^{i\nu_n \tau}}{\nu_n - s_l} \quad (3.71)$$

and to calculate the sum we use the Poisson summation formula [27]

$$\sum_{m=-\infty}^{\infty} f(m) = \int_{-\infty}^{\infty} d\varsigma \sum_n e^{2\pi i \varsigma n} f(\varsigma) \quad (3.72)$$

so that

$$\begin{aligned} G_\tau(s_l) &= \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \frac{e^{i\nu_n \tau}}{\nu_n - s_l} e^{i\nu t n} \\ &= \sum_{n=-\infty}^{\infty} e^{i\nu t n} \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \frac{e^{i\nu_n \tau}}{\nu_n - s_l + i\eta} \\ &= \sum_{n=-\infty}^{\infty} e^{is_l(\tau+tn)} \Theta(\tau + tn) \end{aligned} \quad (3.73)$$

where  $\Theta$  is the Heaviside function. Since this expression is periodic in  $t$  we can restrict our attention to the basic interval  $\tau \in [0, t)$ . Then the sum can be done right-away giving

$$\begin{aligned} G_\tau(s_l) &= \sum_{n=-\infty}^0 e^{is_l(\tau+tn)} \\ &= \frac{e^{is_l \tau}}{1 - e^{is_l t}} \end{aligned} \quad (3.74)$$

Inserting Eq(3.74) into Eq(3.70), we obtain

$$D_\tau^1 = -\frac{1}{m} \Delta_\tau^+ \quad (3.75)$$

where

$$\Delta_\tau^+ = \sum_{l=1}^4 \frac{(s_l^2 - \Omega_\perp^2)}{\prod_{l \neq k} (s_l - s_k)} \frac{e^{is_l \tau}}{(e^{is_l t} - 1)} \quad (3.76)$$

In the same way, we can write

$$D_\tau^2 = \frac{1}{m} \Delta_\tau^- \quad (3.77)$$

with

$$\Delta_{\tau}^{-} = - \sum_{l=1}^4 \frac{(s_l^2 - \Omega_{\perp}^2)}{\prod_{l \neq k} (s_l - s_k)} \frac{e^{-is_l \tau}}{(e^{-is_l t} - 1)} \quad (3.78)$$

Next, we consider

$$g_{\tau-\sigma}^{33} = m \left( \frac{\kappa_{\parallel}}{m} - \omega_0^2 \right) \delta(\tau - \sigma) - \kappa_{\parallel} \Omega_{\parallel} \frac{\cos \Omega_{\parallel} (|\tau - \sigma| - t/2)}{2 \sin \Omega_{\parallel} t/2} \quad (3.79)$$

and

$$\begin{aligned} t g_n^{33} &= - \frac{\kappa_{\parallel} \nu_n^2}{\nu_n^2 - \Omega_{\parallel}^2} \\ \frac{m}{m \nu_n^2 + t g_n^{33}} &= \frac{\nu_n^2 - \Omega_{\parallel}^2}{\nu_n^4 - \nu_n^2 \left( \Omega_{\parallel}^2 + \frac{\kappa_{\parallel}}{m} \right)} \\ &= \frac{1}{z_1^2 - z_2^2} \left( \frac{z_1^2 - \Omega_{\parallel}^2}{\nu_n^2 - z_1^2} - \frac{z_2^2 - \Omega_{\parallel}^2}{\nu_n^2 - z_2^2} \right) \end{aligned} \quad (3.80)$$

where  $2z_{1,2}^2 = \left( \Omega_{\parallel}^2 + \frac{\kappa_{\parallel}}{m} \right)^2 \pm \sqrt{\left( \Omega_{\parallel}^2 + \frac{\kappa_{\parallel}}{m} \right)^4 - 4\omega_0^2 \Omega_{\parallel}^2}$ . Then

$$\begin{aligned} \bar{D}_{\tau}^3 &= \frac{1}{t} \sum_n \frac{e^{i\nu_n \tau}}{m \nu_n^2 + t g_n^{33}} \\ &= \frac{1}{m(z_1^2 - z_2^2)} \left( \frac{z_1^2 - \Omega_{\parallel}^2}{z_1^2} \frac{z_1^2}{t} \sum_n \frac{e^{i\nu_n \tau}}{\nu_n^2 - z_1^2} - \frac{z_2^2 - \Omega_{\parallel}^2}{z_2^2} \frac{z_2^2}{t} \sum_n \frac{e^{i\nu_n \tau}}{\nu_n^2 - z_2^2} \right) \end{aligned} \quad (3.81)$$

Using Eq(3.72), we obtain

$$\bar{D}_{\tau}^3 = - \frac{1}{m} \Delta_{\tau}^3 \quad (3.82)$$

with

$$\Delta_{\tau}^3 = \frac{1}{2} \frac{z_1^2 - \Omega_{\parallel}^2}{z_1^2 - z_2^2} \frac{\cos z_1 (\tau - t/2)}{z_1 \sin z_1 t/2} - \frac{1}{2} \frac{z_2^2 - \Omega_{\parallel}^2}{z_1^2 - z_2^2} \frac{\cos z_2 (\tau - t/2)}{z_2 \sin z_2 t/2} \quad (3.83)$$

The solution of the classical equation of motion is now given. From equation Eq(3.65), Eq(3.75), Eq(3.77) and Eq(3.82), we see that

$$\begin{aligned} \mathbf{r}_{\tau} &= \frac{1}{2} \mathbf{\Delta}_0^{-1} \cdot \mathbf{\Delta}_{\tau} \cdot (\mathbf{r}_t + \mathbf{r}_0) + \left( \dot{\mathbf{\Delta}}_{\tau} - \left( \frac{1}{2} + \dot{\mathbf{\Delta}}_0 \right) \cdot \mathbf{\Delta}_0^{-1} \cdot \mathbf{\Delta}_{\tau} \right) \cdot (\mathbf{r}_t - \mathbf{r}_0) \\ &\quad + \frac{1}{m} \int_0^t d\sigma \left( \mathbf{\Delta}_0^{-1} \cdot \mathbf{\Delta}_{\tau} \cdot \mathbf{\Delta}_{t-\sigma} - \mathbf{\Delta}_{\tau-\sigma} \right) \cdot \mathbf{f}_{\sigma} \end{aligned} \quad (3.84)$$

where

$$\mathbf{\Delta}_{\tau} = \frac{1}{2} \begin{pmatrix} \Delta_{\tau}^{+} + \Delta_{\tau}^{-} & -i(\Delta_{\tau}^{+} - \Delta_{\tau}^{-}) & 0 \\ i(\Delta_{\tau}^{+} - \Delta_{\tau}^{-}) & \Delta_{\tau}^{+} + \Delta_{\tau}^{-} & 0 \\ 0 & 0 & \Delta_{\tau}^3 \end{pmatrix} \quad (3.85)$$

With the classical action  $\bar{S}_{trial}$  given by Eq(3.14),  $\mathbf{r}_\tau$  given by Eq(3.84), the velocity  $\dot{\mathbf{r}}_\tau$  is given by differentiating Eq(3.84)

$$\begin{aligned}\dot{\mathbf{r}}_\tau &= \frac{1}{2}\mathbf{\Delta}_0^{-1} \cdot \dot{\mathbf{\Delta}}_\tau \cdot (\mathbf{r}_t + \mathbf{r}_0) + \left( \ddot{\mathbf{\Delta}}_\tau - \left( \frac{1}{2} + \dot{\mathbf{\Delta}}_0 \right) \cdot \mathbf{\Delta}_0^{-1} \cdot \dot{\mathbf{\Delta}}_\tau \right) \cdot (\mathbf{r}_t - \mathbf{r}_0) \\ &\quad + \frac{1}{m} \int_0^t d\sigma \mathbf{\Delta}_0^{-1} \cdot \dot{\mathbf{\Delta}}_\tau \cdot \mathbf{\Delta}_{t-\sigma} \cdot \mathbf{f}_\sigma - \frac{1}{m} \int_0^\tau d\sigma \dot{\mathbf{\Delta}}_{\tau-\sigma} \cdot \mathbf{f}_\sigma + \frac{1}{m} \int_\tau^t d\sigma \dot{\mathbf{\Delta}}_{\sigma-\tau} \cdot \mathbf{f}_\sigma\end{aligned}\quad (3.86)$$

so that

$$\begin{aligned}\dot{\mathbf{r}}_t &= \frac{1}{2}\mathbf{\Delta}_0^{-1} \cdot \dot{\mathbf{\Delta}}_t \cdot (\mathbf{r}_t + \mathbf{r}_0) + \left( \ddot{\mathbf{\Delta}}_t - \left( \frac{1}{2} + \dot{\mathbf{\Delta}}_0 \right) \cdot \mathbf{\Delta}_0^{-1} \cdot \dot{\mathbf{\Delta}}_t \right) \cdot (\mathbf{r}_t - \mathbf{r}_0) \\ &\quad + \frac{1}{m} \int_0^t d\sigma \mathbf{\Delta}_0^{-1} \cdot \dot{\mathbf{\Delta}}_t \cdot \mathbf{\Delta}_{t-\sigma} \cdot \mathbf{f}_\sigma - \frac{1}{m} \int_0^t d\sigma \dot{\mathbf{\Delta}}_{t-\sigma} \cdot \mathbf{f}_\sigma\end{aligned}\quad (3.87)$$

and

$$\begin{aligned}\dot{\mathbf{r}}_0 &= \frac{1}{2}\mathbf{\Delta}_0^{-1} \cdot \dot{\mathbf{\Delta}}_0 \cdot (\mathbf{r}_t + \mathbf{r}_0) + \left( \ddot{\mathbf{\Delta}}_0 - \left( \frac{1}{2} + \dot{\mathbf{\Delta}}_0 \right) \cdot \mathbf{\Delta}_0^{-1} \cdot \dot{\mathbf{\Delta}}_0 \right) \cdot (\mathbf{r}_t - \mathbf{r}_0) \\ &\quad + \frac{1}{m} \int_0^t d\sigma \mathbf{\Delta}_0^{-1} \cdot \dot{\mathbf{\Delta}}_0 \cdot \mathbf{\Delta}_{t-\sigma} \cdot \mathbf{f}_\sigma + \frac{1}{m} \int_0^t d\sigma \dot{\mathbf{\Delta}}_\sigma \cdot \mathbf{f}_\sigma\end{aligned}\quad (3.88)$$

A final expression for  $\bar{S}_{trial}$  is obtain by substitution in Eq(3.14). The manipulations are straightforward but somewhat lengthy. We find that  $(\mathbf{\Gamma} = \left( \frac{1}{2} + \dot{\mathbf{\Delta}}_0 \right) \mathbf{\Delta}_0^{-1})$

$$\begin{aligned}\bar{S}_{trial} &= \frac{m}{2} (\mathbf{r}_t - \mathbf{r}_0) \cdot \left( \ddot{\mathbf{\Delta}}_0 - \mathbf{\Gamma}^2 \mathbf{\Delta}_0 \right) \cdot (\mathbf{r}_t - \mathbf{r}_0) + \frac{m}{2} (\mathbf{r}_t + \mathbf{r}_0) \cdot \mathbf{\Delta}_0^{-1} \cdot (\mathbf{r}_t + \mathbf{r}_0) \\ &\quad + \frac{m}{4} (\mathbf{r}_t - \mathbf{r}_0) \cdot (\mathbf{\Gamma} - \mathbf{J}) \cdot (\mathbf{r}_t - \mathbf{r}_0) - \frac{m}{4} (\mathbf{r}_t - \mathbf{r}_0) \cdot \mathbf{\Gamma} \cdot (\mathbf{r}_t - \mathbf{r}_0) \\ &\quad - \frac{(\mathbf{r}_t - \mathbf{r}_0)}{2} \int_0^t d\tau \left( \mathbf{\Gamma} \mathbf{\Delta}_{t-\tau} - \dot{\mathbf{\Delta}}_{t-\tau} \right) \cdot \mathbf{f}_\tau + \frac{1}{2} \int_0^t d\tau \mathbf{f}_\tau \cdot \left( \mathbf{\Gamma} \mathbf{\Delta}_\tau - \dot{\mathbf{\Delta}}_\tau \right) \cdot (\mathbf{r}_t - \mathbf{r}_0) \\ &\quad - \frac{(\mathbf{r}_t + \mathbf{r}_0)}{4} \int_0^t d\tau \mathbf{\Delta}_0^{-1} \cdot \mathbf{\Delta}_{t-\tau} \cdot \mathbf{f}_\tau - \frac{1}{4} \int_0^t d\tau \mathbf{f}_\tau \cdot \mathbf{\Delta}_0^{-1} \cdot \mathbf{\Delta}_\tau \cdot (\mathbf{r}_t + \mathbf{r}_0) \\ &\quad + \frac{(\mathbf{r}_t - \mathbf{r}_0)}{2} \int_0^t d\tau \dot{\mathbf{\Delta}}_{t-\tau} \cdot \mathbf{f}_\tau - \frac{1}{2m} \int_0^t d\tau \int_0^t d\sigma \mathbf{f}_\tau \cdot \left( \mathbf{\Delta}_0^{-1} \cdot \mathbf{\Delta}_\tau \cdot \mathbf{\Delta}_{t-\sigma} - \mathbf{\Delta}_{|\tau-\sigma|} \right) \cdot \mathbf{f}_\sigma\end{aligned}\quad (3.89)$$

### 3.3 The prefactor

The prefactor  $F(t, 0)$  for the propagator is defined in Eq(3.16). An explicit expression for this function may be given from the classical solution by introducing a generating

functional. Firstly, we consider a generating functional

$$Z(\mathbf{f}_\tau) \equiv \left\langle e^{\frac{i}{\hbar} \int_0^t d\tau \mathbf{f}_\tau \cdot \mathbf{r}_\tau} \right\rangle \quad (3.90)$$

$$= e^{\frac{i}{\hbar} \int_0^t d\tau \mathbf{f}_\tau \cdot \mathbf{r}_\tau + \frac{1}{2} \int_0^t d\tau \int_0^t d\sigma \mathbf{f}_\tau \cdot \mathbf{C}(\tau-\sigma) \cdot \mathbf{f}_\sigma} \quad (3.91)$$

where

$$\mathbf{C}_{\tau-\sigma} = \begin{pmatrix} C_{\tau-\sigma}^{11} & C_{\tau-\sigma}^{12} & 0 \\ C_{\tau-\sigma}^{21} & C_{\tau-\sigma}^{22} & 0 \\ 0 & 0 & C_{\tau-\sigma}^{33} \end{pmatrix} \quad (3.92)$$

with

$$C_{\tau-\sigma}^{11} = \frac{1}{4} \left( \frac{\bar{D}_\tau^1 \bar{D}_\sigma^1}{\bar{D}_0^1} - \bar{D}_{\tau-\sigma}^1 + \frac{\bar{D}_\tau^2 \bar{D}_\sigma^2}{\bar{D}_0^2} - \bar{D}_{\tau-\sigma}^2 \right) = C_{\tau-\sigma}^{22} \quad (3.93)$$

$$C_{\tau-\sigma}^{21} = \frac{-i}{4} \left( \frac{\bar{D}_\tau^1 \bar{D}_\sigma^1}{\bar{D}_0^1} - \bar{D}_{\tau-\sigma}^1 - \frac{\bar{D}_\tau^2 \bar{D}_\sigma^2}{\bar{D}_0^2} + \bar{D}_{\tau-\sigma}^2 \right) = -C_{\tau-\sigma}^{12} \quad (3.94)$$

$$C_{\tau-\sigma}^{33} = \frac{1}{4} \left( \frac{\bar{D}_\tau^3 \bar{D}_\sigma^3}{\bar{D}_0^3} - \bar{D}_{\tau-\sigma}^3 \right) \quad (3.95)$$

Using Eq(3.92), Eq(3.91) becomes

$$Z(\mathbf{f}_\tau) = \exp \frac{i}{\hbar} \left( \int_0^t d\tau \left[ f_\tau^1 r_\tau^1 + f_\tau^2 r_\tau^2 + f_\tau^3 r_\tau^3 \right] + \frac{1}{2} \int_0^t d\tau \int_0^t d\sigma \left[ C_{\tau-\sigma}^{33} f_\tau^3 f_\sigma^3 \right. \right. \\ \left. \left. C_{\tau-\sigma}^{11} \left( f_\tau^1 f_\sigma^1 + f_\tau^2 f_\sigma^2 \right) + C_{\tau-\sigma}^{21} \left( f_\tau^1 f_\sigma^2 - f_\tau^2 f_\sigma^1 \right) \right] \right) \quad (3.96)$$

Now, we replace  $\bar{\mathbf{G}}$  by  $\lambda \bar{\mathbf{G}}$ . The propagator is

$$e^{M_\lambda(\mathbf{f}_\tau)} \equiv \int_{\mathbf{r}_0}^{\mathbf{r}_t} D[\mathbf{r}_\tau] e^{\frac{i}{\hbar} S_\lambda(\dot{\mathbf{r}}_\tau, \mathbf{r}_\tau, \tau)} \quad (3.97)$$

where

$$S_\lambda = \int_0^t d\tau \left( \frac{m}{2} \dot{\mathbf{r}}^2 + \mathbf{f}_\tau \cdot \mathbf{r}_\tau \right) + \frac{1}{2} \int_0^t d\tau \int_0^t d\sigma \mathbf{r}_\tau \cdot \lambda \bar{\mathbf{G}}_{\tau-\sigma} \cdot \mathbf{r}_\sigma \quad (3.98)$$

So

$$e^{M_\lambda(\mathbf{f}_\tau)} \frac{\partial}{\partial \lambda} M_\lambda(\mathbf{f}_\tau) = \frac{i}{2\hbar} \int_0^t d\tau \int_0^t d\sigma \int_{\mathbf{r}_0}^{\mathbf{r}_t} D[\mathbf{r}_\tau] (\mathbf{r}_\tau \cdot \bar{\mathbf{G}}_{\tau-\sigma} \cdot \mathbf{r}_\sigma) e^{\frac{i}{\hbar} S_\lambda(\dot{\mathbf{r}}_\tau, \mathbf{r}_\tau, \tau)} \\ = \frac{i}{2\hbar} \int_0^t d\tau \int_0^t d\sigma \int_{\mathbf{r}_0}^{\mathbf{r}_t} D[\mathbf{r}_\tau] \left\{ g_{\tau-\sigma}^{33} \left( r_\tau^1 r_\sigma^1 + r_\tau^2 r_\sigma^2 + r_\tau^3 r_\sigma^3 \right) \right. \\ \left. + m\omega_c \dot{\delta}(\tau-\sigma) \left( r_\tau^2 r_\sigma^1 - r_\tau^1 r_\sigma^2 \right) \right\} e^{\frac{i}{\hbar} S_\lambda(\dot{\mathbf{r}}_\tau, \mathbf{r}_\tau, \tau)} \quad (3.99)$$

Next we consider

$$\langle r_\tau^i \rangle = \left. \frac{\hbar}{i} \frac{\delta Z}{\delta f_\tau^i} \right|_{f=0} = \mu_\tau^i, \text{ then } \langle \mathbf{r}_\tau \rangle = \mu_\tau \quad (3.100)$$

$$\langle r_\sigma^i \rangle = \left. \frac{\hbar}{i} \frac{\delta Z}{\delta f_\sigma^i} \right|_{f=0} = \mu_\sigma^i, \text{ then } \langle \mathbf{r}_\sigma \rangle = \mu_\sigma \quad (3.101)$$

$$\langle r_\tau^i r_\sigma^i \rangle = \left. \left( \frac{\hbar}{i} \right)^2 \frac{\delta^2 Z}{\delta f_\tau^i \delta f_\sigma^i} \right|_{f=0} = \mu_\tau^i \mu_\sigma^i - \frac{i\hbar}{2} (C_{\tau-\sigma}^{ij} + C_{\sigma-\tau}^{ij}) \delta_{ij} \quad (3.102)$$

so that

$$\langle r_\tau^i r_\sigma^j \rangle = \mu_\tau^i \mu_\sigma^j - \frac{i\hbar}{2} (C_{\tau-\sigma}^{ij} + C_{\sigma-\tau}^{ij}) \quad (3.103)$$

$$\langle r_\tau^j r_\sigma^i \rangle = \mu_\tau^j \mu_\sigma^i + \frac{i\hbar}{2} (C_{\tau-\sigma}^{ij} + C_{\sigma-\tau}^{ij}) \quad (3.104)$$

Using Eq(3.100)-(3.104), Eq(3.99) gives

$$\begin{aligned} e^{M_\lambda(\mathbf{f}_\tau)} \frac{\partial}{\partial \lambda} M_\lambda(\mathbf{f}_\tau) &= \frac{i}{2\hbar} \int_0^t d\tau \int_0^t d\sigma \int_{\mathbf{r}_0}^{\mathbf{r}_t} D[\mathbf{r}_\tau] \left\{ g_{\tau-\sigma}^{33} \sum_{i=1}^3 \frac{\delta^2}{\delta f_\tau^i \delta f_\sigma^i} \right. \\ &\quad \left. + m\omega_c \dot{\delta}(\tau - \sigma) \left( \frac{\delta^2}{\delta f_\tau^2 \delta f_\sigma^1} - \frac{\delta^2}{\delta f_\tau^1 \delta f_\sigma^2} \right) \right\} e^{\frac{i}{\hbar} S_\lambda(\dot{\mathbf{r}}_\tau, \mathbf{r}_\tau, \tau)} \\ \frac{\partial}{\partial \lambda} M_\lambda(\mathbf{f}_\tau) &= \frac{i}{2\hbar} \int_0^t d\tau \int_0^t d\sigma \int_{\mathbf{r}_0}^{\mathbf{r}_t} D[\mathbf{r}_\tau] \left\{ g_{\tau-\sigma}^{33} e^{-M_\lambda(\mathbf{f}_\tau)} \sum_{i=1}^3 \frac{\delta^2}{\delta f_\tau^i \delta f_\sigma^i} e^{M_\lambda(\mathbf{f}_\tau)} \right. \\ &\quad \left. + m\omega_c \dot{\delta}(\tau - \sigma) e^{-M_\lambda(\mathbf{f}_\tau)} \left( \frac{\delta^2}{\delta f_\tau^2 \delta f_\sigma^1} - \frac{\delta^2}{\delta f_\tau^1 \delta f_\sigma^2} \right) e^{M_\lambda(\mathbf{f}_\tau)} \right\} \\ \frac{\partial}{\partial \lambda} M_\lambda(\mathbf{f}_\tau) &= \frac{1}{2} \int_0^t d\tau \int_0^t d\sigma \left\{ g_{\tau-\sigma}^{33} \sum_{i=1}^3 \left( \frac{\delta^2 S_\lambda}{\delta f_\tau^i \delta f_\sigma^i} + \frac{i}{\hbar} \frac{\delta S_\lambda}{\delta f_\tau^i} \frac{\delta S_\lambda}{\delta f_\sigma^i} \right) \right. \\ &\quad \left. + m\omega_c \dot{\delta}(\tau - \sigma) \left( \frac{\delta^2 S_\lambda}{\delta f_\tau^2 \delta f_\sigma^1} + \frac{i}{\hbar} \frac{\delta S_\lambda}{\delta f_\tau^2} \frac{\delta S_\lambda}{\delta f_\sigma^1} \right. \right. \\ &\quad \left. \left. - \frac{\delta^2 S_\lambda}{\delta f_\tau^1 \delta f_\sigma^2} - \frac{i}{\hbar} \frac{\delta S_\lambda}{\delta f_\tau^1} \frac{\delta S_\lambda}{\delta f_\sigma^2} \right) \right|_{f=0} \quad (3.105) \end{aligned}$$

Consider now the case  $\mathbf{r}_t = \mathbf{r}_0 = 0$  for which

$$\int_0^t d\tau \mathbf{f}_\tau \cdot \mathbf{r}_\tau = 0 \quad (3.106)$$

i.e.  $\mu_\tau = 0$ . Then

$$\frac{\partial}{\partial \lambda} M_\lambda(f_\tau) = \int_0^t d\tau \int_0^t d\sigma \left( g_{\tau-\sigma}^{33} C_{\tau-\sigma, \lambda}^{11} + \frac{1}{2} g_{\tau-\sigma}^{33} C_{\tau-\sigma, \lambda}^{33} + m\omega_c \dot{\delta}(\tau - \sigma) C_{\tau-\sigma, \lambda}^{21} \right) \quad (3.107)$$

From Eq(3.15), we have

$$K_\lambda(0, t; 0, 0) = F(t, 0) e^{\frac{i}{\hbar} \bar{S}_\lambda(0,0)} \quad (3.108)$$

Now consider the quantity

$$M_\lambda(f_\tau) = \ln K_\lambda(0, t; 0, 0) \quad (3.109)$$

According to Eq(3.108) we will only need  $M_1(0)$  in the final stage. Writing

$$M_1(0) = M_0(0) + \int_0^1 d\lambda \frac{\partial}{\partial \lambda} M_\lambda(0) \quad (3.110)$$

we have to specify the “initial” value  $M_0(0)$  and the derivative  $\frac{\partial}{\partial \lambda} M_\lambda(\mathbf{f}_\tau)$ . From the normalization factor of the transition probability density of the Wiener process or, equivalently, from the canonical density matrix of a free particle [12], it is well known that

$$M_0(0) = \ln \left[ \frac{m}{2\pi i \hbar t} \right]^{\frac{3}{2}} \quad (3.111)$$

so that

$$\begin{aligned} \ln F(t, 0) &= \ln \left[ \frac{m}{2\pi i \hbar t} \right]^{\frac{3}{2}} + \int_0^1 d\lambda \int_0^t d\tau \int_0^t d\sigma \left( g_{\tau-\sigma}^{33} C_{\tau-\sigma, \lambda}^{11} \right. \\ &\quad \left. + \frac{1}{2} g_{\tau-\sigma}^{33} C_{\tau-\sigma, \lambda}^{33} + m\omega_c \delta(\tau - \sigma) C_{\tau-\sigma, \lambda}^{21} \right) \end{aligned} \quad (3.112)$$

Next we consider

$$\begin{aligned} \frac{1}{2} \int_0^t d\tau \int_0^t d\sigma g_{\tau-\sigma}^{33} C_{\tau-\sigma, \lambda}^{33} &= \frac{1}{2} \int_0^t d\tau \int_0^t d\sigma g_{\tau-\sigma}^{33} \left\{ D_{\tau, \lambda}^3 + D_{\sigma, \lambda}^3 - D_{\tau-\sigma, \lambda}^3 - D_{0, \lambda}^3 \right. \\ &\quad \left. + \frac{t^2 \lambda g_0^{33}}{1 + t^2 \lambda g_0^{33} D_{0, \lambda}^3} \left( D_{\tau, \lambda}^3 - D_{0, \lambda}^3 \right) \left( D_{\sigma, \lambda}^3 - D_{0, \lambda}^3 \right) \right\} \end{aligned} \quad (3.113)$$

where

$$\begin{aligned} \int_0^t d\tau \int_0^t d\sigma g_{\tau-\sigma}^{33} D_{\tau-\sigma, \lambda}^3 &= \int_0^t d\tau \int_0^t d\sigma \sum_{n=0} g_n^{33} e^{i\nu_n(\tau-\sigma)} \frac{1}{t} \sum_{n'=0} \frac{e^{i\nu_{n'}(\tau-\sigma)}}{m\nu_{n'}^2 + t\lambda g_{n'}^{33}} \\ &= t \sum_{n \neq 0} \frac{g_n^{33}}{m\nu_n^2 + t\lambda g_n^{33}} \end{aligned} \quad (3.114)$$

$$\begin{aligned}
\int_0^t d\tau \int_0^t d\sigma g_{\tau-\sigma}^{33} D_{\tau,\lambda}^3 D_{\sigma,\lambda}^3 &= \sum_{n=0} g_n^{33} \left( \int_0^t d\tau e^{i\nu_n \tau} \frac{1}{t} \sum_{n' \neq 0} \frac{e^{i\nu_{n'} \tau}}{m\nu_{n'}^2 + t\lambda g_{n'}^{33}} \right)^2 \\
&= \sum_{n \neq 0} g_n^{33} \left( \frac{1}{m\nu_n^2 + t\lambda g_n^{33}} \right)^2 \\
&= -\frac{\partial}{\partial \lambda} D_{0,\lambda}^3
\end{aligned} \tag{3.115}$$

$$\int_0^t d\tau \int_0^t d\sigma g_{\tau-\sigma}^{33} D_{\tau,\lambda}^3 = t g_0^{33} \int_0^t d\tau D_{\tau,\lambda}^3 = 0 \tag{3.116}$$

and

$$\int_0^t d\tau \int_0^t d\sigma g_{\tau-\sigma}^{33} = t g_0^{33} \tag{3.117}$$

Inserting Eqs(3.114)-(3.117) into Eq(3.113) we find that

$$\begin{aligned}
\int_0^t d\tau \int_0^t d\sigma g_{\tau-\sigma}^{33} C_{\tau-\sigma,\lambda}^{33} &= -t \sum_{n \neq 0} \frac{g_n^{33}}{m\nu_n^2 + t\lambda g_n^{33}} - t^2 g_0^{33} D_{0,\lambda}^3 \\
&\quad + \frac{t^2 \lambda g_0^{33}}{1 + t^2 \lambda g_0^{33} D_{0,\lambda}^3} \left( t^2 g_0^{33} D_{0,\lambda}^3 D_{0,\lambda}^3 - \frac{\partial}{\partial \lambda} D_{0,\lambda}^3 \right) \\
&= -\frac{\partial}{\partial \lambda} \left\{ \sum_{n \neq 0} \ln(m\nu_n^2 + t\lambda g_n^{33}) + \ln(1 + t^2 \lambda g_0^{33} D_{0,\lambda}^3) \right\}
\end{aligned} \tag{3.118}$$

so that

$$\frac{1}{2} \int_0^1 d\lambda \int_0^t d\tau \int_0^t d\sigma g_{\tau-\sigma}^{33} C_{\tau-\sigma,\lambda}^{33} = \sum_{n \neq 0} \ln \left( 1 + \frac{t g_n^{33}}{m\nu_n^2} \right)^{-\frac{1}{2}} + \ln \left( 1 + t^2 g_0^{33} D_0^3 \right)^{-\frac{1}{2}} \tag{3.119}$$

Next we consider

$$\begin{aligned}
&\int_0^t d\tau \int_0^t d\sigma \left( g_{\tau-\sigma}^{33} C_{\tau-\sigma,\lambda}^{11} + m\omega_c \delta(\tau - \sigma) C_{\tau-\sigma,\lambda}^{21} \right) \\
&= \int_0^t d\tau \int_0^t d\sigma g_{\tau-\sigma}^{11} \left( \frac{\bar{D}_{\tau,\lambda}^1 \bar{D}_{\sigma,\lambda}^1}{\bar{D}_{0,\lambda}^1} - \bar{D}_{\tau-\sigma,\lambda}^1 \right) + \int_0^t d\tau \int_0^t d\sigma g_{\tau-\sigma}^{22} \left( \frac{\bar{D}_{\tau,\lambda}^2 \bar{D}_{\sigma,\lambda}^2}{\bar{D}_{0,\lambda}^2} - \bar{D}_{\tau-\sigma,\lambda}^2 \right) \\
&= \int_0^t d\tau \int_0^t d\sigma g_{\tau-\sigma}^{11} \left\{ D_{\tau,\lambda}^1 + D_{\sigma,\lambda}^1 - D_{\tau-\sigma,\lambda}^1 - D_{0,\lambda}^1 + \frac{t^2 \lambda g_0^{11}}{1 + t^2 \lambda g_0^{11} D_{0,\lambda}^1} (D_{\tau,\lambda}^1 - D_{0,\lambda}^1) \right. \\
&\quad \left. (D_{\sigma,\lambda}^1 - D_{0,\lambda}^1) \right\} + \int_0^t d\tau \int_0^t d\sigma g_{\tau-\sigma}^{22} \left\{ D_{\tau,\lambda}^2 + D_{\sigma,\lambda}^2 - D_{\tau-\sigma,\lambda}^2 - D_{0,\lambda}^2 \right. \\
&\quad \left. + \frac{t^2 \lambda g_0^{22}}{1 + t^2 \lambda g_0^{22} D_{0,\lambda}^2} (D_{\tau,\lambda}^2 - D_{0,\lambda}^2) (D_{\sigma,\lambda}^2 - D_{0,\lambda}^2) \right\}
\end{aligned} \tag{3.120}$$

and

$$\begin{aligned}
 & \int_0^1 d\lambda \int_0^t d\tau \int_0^t d\sigma \left( g_{\tau-\sigma}^{33} C_{\tau-\sigma,\lambda}^{11} + m\omega_c \delta(\tau - \sigma) C_{\tau-\sigma,\lambda}^{21} \right) \\
 &= \sum_{n \neq 0} \ln \left( 1 + \frac{tg_n^{11}}{m\nu_n^2} \right)^{-1} \left( 1 + \frac{tg_n^{22}}{m\nu_n^2} \right)^{-1} + \ln \left( 1 + t^2 g_0^{11} D_0^1 \right)^{-1} \left( 1 + t^2 g_0^{22} D_0^2 \right)^{-1}
 \end{aligned} \tag{3.121}$$

Inserting Eq(3.119) and (3.121) into Eq(3.112), we obtain the prefactor as

$$\begin{aligned}
 F(t, 0) &= \left[ \frac{m}{2\pi i \hbar t} \right]^{\frac{3}{2}} \prod_{n \neq 0} \left( 1 + \frac{tg_n^{11}}{m\nu_n^2} \right)^{-1} \prod_{n \neq 0} \left( 1 + \frac{tg_n^{22}}{m\nu_n^2} \right)^{-1} \prod_{n \neq 0} \left( 1 + \frac{tg_n^{33}}{m\nu_n^2} \right)^{-1} \\
 &\quad \times \left( 1 + t^2 g_0^{11} D_0^1 \right)^{-1} \left( 1 + t^2 g_0^{22} D_0^2 \right)^{-1} \left( 1 + t^2 g_0^{33} D_0^3 \right)^{-\frac{1}{2}}
 \end{aligned} \tag{3.122}$$

Using Eq(3.67) and Eq(3.79)

$$\begin{aligned}
 F(t, 0) &= \left[ \frac{m}{4\pi i \hbar t} \right]^{\frac{3}{2}} \frac{\sin \left( \Omega_{\parallel} \frac{t}{2} \right) \sin^2 \left( \Omega_{\perp} \frac{t}{2} \right)}{\sin \left( z_1 \frac{t}{2} \right) \sin \left( z_2 \frac{t}{2} \right) \prod_{l=1}^4 \sin \left( s_l \frac{t}{2} \right)} \\
 &\quad \times \left( \frac{z_1^2 - \Omega_{\parallel}^2 \cot \left( z_1 \frac{t}{2} \right)}{z_1^2 - z_2^2} \frac{1}{z_1} + \frac{z_2^2 - \Omega_{\parallel}^2 \cot \left( z_2 \frac{t}{2} \right)}{z_2^2 - z_1^2} \frac{1}{z_2} \right)^{-\frac{1}{2}} \\
 &\quad \times \left( \sum_{j=1}^4 \frac{\left( s_j^2 - \Omega_{\perp}^2 \right) \cot \left( s_j \frac{t}{2} \right)}{\prod_{j \neq k} (s_j - s_k)} \right)^{-1}
 \end{aligned} \tag{3.123}$$

We now have a complete expression for the propagator corresponding to the action of Eq(3.9) by using the Adamowski-Gerlach-Leschke [28] technique. It is given by Eqs(3.6), (3.89), (3.123) and agrees with reference [29] for  $\Lambda_x$  and  $\Lambda_y$  zero. For the case of zero magnetic field ( $\Omega_{\perp} \rightarrow \Omega_{\parallel}$ ) this expression agrees with reference [30].

## CHAPTER 4

### THE GROUND STATE ENERGY OF THE POLARON

#### 4.1 Introduction

The Feynman path integral formulation of quantum mechanics provides the following upper bound for the ground-state energy of a system:

$$E_G \leq E_{trial} + \lim_{\beta \rightarrow \infty} \frac{\langle S_{pol} - S_{trial} \rangle_{trial}}{\beta} \quad (4.1)$$

if  $S_{pol}$  and  $S_{trial}$  are real. In Eq(4.1),  $E_{trial}$  is the ground state energy of some “trial” model with action functional  $S_{trial}$  for imaginary values of the variable.  $S_{pol}$  is the action functional of the system under study. The path integral average  $\langle \dots \rangle_{trial}$  is defined with a probability density  $exp(S_{trial}) / \int D[\mathbf{r}_\tau] exp(S_{trial})$ :

$$\langle \dots \rangle_{trial} = \frac{\int D[\mathbf{r}_\tau] (\dots) e^{S_{trial}}}{\int D[\mathbf{r}_\tau] e^{S_{trial}}} \quad (4.2)$$

where the denominator is the path integral ( for imaginary time variables ) of the “trial” model. The condition that  $S_{pol}$  and  $S_{trial}$  are real implies the applicability of the Jensen inequality  $\langle e^X \rangle \geq e^{\langle X \rangle}$  of probability theory (often called the Jensen-Feynman inequality in its path integral application), which is valid for real random variables  $X$  with some normalized probability density.

The requirement that the actions (both  $S_{pol}$  and  $S_{trial}$ ) are real after the transformation to imaginary time variables presents a conceptual difficulty. For example, in the case where the Lagrangian describes a system of (charged) particles in a magnetic field, there is an imaginary term in the action. This difficulty was already recognized by Feynman and Hibbs [12], who suspected that only a “minor modification” in the formulation of the Feynman inequality is required for its application to a system which contains charged particles in a non-zero magnetic field.

The problem of the extension of the Feynman inequality Eq(4.1) to the case of a non-zero magnetic field has attracted particular attention with polarons, precisely because Feynman's variational treatment of the Fröhlich polaron, which is superior for  $\omega_c = 0$  (with  $\omega_c$  the cyclotron frequency of a charged particle in a magnetic field) and arbitrary coupling strength-is in general not justified for  $\omega_c \neq 0$ . The Jensen-Feynman inequality has been shown [32] to remain valid if the difference  $S_{pol} - S_{trial}$  is real, as is an example, the case in the study of the diamagnetic properties of the Fröhlich polaron in reference [16].

Despite the lack of a justification of the Feynman inequality for a non-zero magnetic field, approximation schemes have been developed [21,31] for the free energy of a polaron in a magnetic field, based on the working hypothesis that the Feynman inequality remains valid for  $\omega_c \neq 0$ . For a polaron in two dimensions subjected to a magnetic field it has been argued [23,33] that at least in the asymptotic limit  $\omega_c \rightarrow \infty$  this working hypothesis leads to an approximation for free energy which lies below the exact free energy. Although the argument of reference [23] might be questionable [34], the Jensen-Feynman inequality indeed has no variational justification for a particle subjected to a magnetic field, and does not a priori provide an upper bound to the ground state for non-zero magnetic field.

References [35,36] have given an unambiguous analytical proof that the Feynman-Jensen inequality in its unmodified form does not hold in the limit of a free particle in a magnetic field, and would yield an estimate of the ground state energy which lies below the exact value.

Recently DB [24] have extended the Feynman inequality to the case of a charged particle in a magnetic field. They used four adjustable parameters:  $v_{\perp}, w_{\perp}, v_{\parallel}, w_{\parallel}$ . The parameters are the natural generalizations of the parameters  $v$  and  $w$  in Feynman's upper bound to the ground-state energy of a polaron with out a magnetic field. In the Feynman model,  $w$  accounts for the retardation effect due to the elimination of the phonons, and  $v$  is the frequency of the couple harmonic oscillators of the trial

system.

Reference [24] has derived the analytic results but no numerical data was presented. In this chapter we would like to present some numerical result for the upper bound of the ground-state energy of the polaron in a magnetic field.

## 4.2 An upper bound for the ground-state energy of a particle in a magnetic field

In this section we briefly summarize how to get the upper bound for the ground-state energy. For the study of the Fröhlich polaron in a magnetic field  $\mathbf{B}$ , DB first consider the more general Hamiltonian:

$$H_{pol} = H_{pol}^0 + \sum_{\mathbf{k}} \left( C_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}} + C_{\mathbf{k}}^* e^{-i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}}^\dagger \right) \quad (4.3)$$

where

$$H_{pol}^0 = \frac{1}{2m} \left( \mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \quad (4.4)$$

or, in the gauge  $\mathbf{A} = (-By, Bx, 0)$  with the  $z$  axis in the direction of the magnetic field:

$$H_{pol}^0 = \frac{1}{2m} \left[ (p_x - m\omega_c y)^2 + (p_y + m\omega_c x)^2 \right] + \frac{1}{2m} p_z^2 + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \quad (4.5)$$

In analog with Feynman's quadratic action  $S_{trial}$  in his treatment of the polaron, DB propose the Hamiltonian  $H_{trial}$  as

$$H_{trial} = H_{\perp} + H_{\parallel} \quad (4.6)$$

$$H_{\perp} = \frac{1}{2m} \left[ (p_x - m\omega_c y)^2 + (p_y + m\omega_c x)^2 \right] + \sum_{i=x,y} \left[ \frac{P_i^2}{2m'} + \frac{1}{2} \kappa_{\perp} (r_i - R_i)^2 \right] \quad (4.7)$$

$$H_{\parallel} = \frac{p_z^2}{2m} + \frac{P_Z^2}{2m'} + \frac{1}{2} \kappa_{\parallel} (z - Z)^2 \quad (4.8)$$

This Hamiltonian describes an electron with coordinates  $(\mathbf{r}, \mathbf{p})$  and mass  $m$ , subjected to a magnetic field  $\mathbf{B} = B\hat{z}$  and interacting with a second particle, called the fictitious particle, with coordinates  $(\mathbf{R}, \mathbf{P})$ .

To obtain the upper bound of the ground-state energy Eq(3.17) in reference [24], they need to diagonalize the Hamiltonian Eq(4.6) by using standard techniques

[21], resulting in the Hamiltonian of these independent harmonic oscillators:

$$H_{\perp} = -\hbar w_{\perp} + \sum_{j=1}^3 \hbar s_j \left( b_j^{\dagger} b_j + \frac{1}{2} \right) \quad (4.9)$$

where  $b_j$  and  $b_j^{\dagger}$  are boson annihilation and creation operators. The eigenfrequencies  $s_j$  are the solutions of the equations:

$$s_j \left( s_j^2 - \Omega^2 - w_{\perp}^2 \right) = (-1)^{j+1} \omega_c \left( s_j^2 - w_{\perp}^2 \right); \quad j = 1, 2, 3 \quad (4.10)$$

where

$$\Omega^2 = \frac{4C_{\perp}}{\hbar w_{\perp}} \quad (4.11)$$

In the process of diagonalization of Eq(4.9) two canonically conjugate constructs of motion  $\Pi, Q$  enter, which satisfy the commutation relation  $[\Pi, Q] = \hbar/i$ . They are related to the classical orbit center [21], but do not appear in the Hamiltonian. The explicit transformations of the position and momentum operators into the creation and annihilation operators  $b_j, b_j^{\dagger}$  for this diagonalization also involve the expectation coefficients  $c_j$ , given by

$$c_j^2 = \frac{\hbar}{2m} \frac{s_j^2 - w_{\perp}^2}{s_j} \frac{1}{3s_j^2 - 2(-1)^{j+1} \omega_c s_j - \Omega^2 - w_{\perp}^2} \quad (4.12)$$

which play an important role in the further treatment.

Using the above result and calculating the matrix elements of Eq(3.17) in reference [24], it can be shown that the upper bound for the ground-state energy of a polaron in a magnetic field is: (see more detail in reference [24])

$$E_G^{DB} = \hbar \frac{\omega_c}{2} + \hbar \frac{(v_{\parallel} - w_{\parallel})^2}{4v_{\parallel}} + \hbar \frac{(s_2 - w_{\perp})^2 (s_2^2 - \omega_c w_{\perp})}{2s_2^3 + \omega_c s_2^2 + \omega_c w_{\perp}^2} + E_b \quad (4.13)$$

Introducing

$$D_{\parallel}(\tau) = \frac{\hbar \tau}{2m} \frac{w_{\parallel}^2}{v_{\parallel}^2} \left( 1 + \frac{v_{\parallel}^2 - w_{\parallel}^2}{w_{\parallel}^2} \frac{1 - e^{-v_{\parallel} \tau}}{v_{\parallel} \tau} \right) \quad (4.14)$$

$$D_{\perp}(\tau) = \sum_{j=1}^3 c_j^2 (1 - e^{-s_j \tau}) \quad (4.15)$$

$E_b$  can be rewritten as

$$E_b = -\frac{1}{\hbar} \sum_{\mathbf{k}} |C_{\mathbf{k}}|^2 \int_0^{\infty} d\tau e^{-\omega_{\mathbf{k}} \tau} e^{-k_{\perp}^2 D_{\perp}(\tau)} e^{-k_{\parallel}^2 D_{\parallel}(\tau)} \quad (4.16)$$

and the summation over the wave vectors can be done analytically:

$$E_b = -\frac{\alpha\hbar\omega_{\mathbf{k}}}{2\sqrt{\pi}}\sqrt{\frac{\hbar\omega_{\mathbf{k}}}{2m}}\int_0^\infty d\tau\frac{e^{-\omega_{\mathbf{k}}\tau}}{\sqrt{D_{\parallel}(\tau)}}F\left(\frac{D_{\parallel}(\tau)}{D_{\perp}(\tau)}\right) \quad (4.17)$$

with

$$F(x) = 2\sqrt{\frac{x}{x-1}}\ln\left(\sqrt{x} + \sqrt{x-1}\right) \quad (4.18)$$

Note that in the limit  $\omega_c = 0$  one immediately recovers the Feynman result for the Fröhlich polaron in the absence of a magnetic field.

To do numerical work it is useful to express the frequencies  $s_1$  and  $s_3$  in terms of  $s_2$  with the help of Eq(4.7) in reference [24].

$$s_{1,3} = \frac{\omega_c + s_2 \pm 2W}{2} \quad (4.19)$$

$$W = \sqrt{\left(\frac{\omega_c + s_2}{2}\right)^2 - \frac{\omega_c w_{\perp}^2}{s_2}} \quad (4.20)$$

and similarly

$$c_1^2 = \frac{\hbar}{2m\omega_c}\frac{s_3 - \omega_c}{s_3 - s_1} + \frac{s_3 + s_2}{s_3 - s_1}c_2^2 \quad (4.21)$$

$$c_3^2 = \frac{\hbar}{2m\omega_c}\frac{\omega_c - s_3}{s_3 - s_1} - \frac{s_3 + s_2}{s_3 - s_1}c_2^2 \quad (4.22)$$

Using Eqs(4.19)-(4.22), the function  $D_{\perp}(\tau)$  can also be completely expressed in  $s_2$  and  $w_{\perp}$ :

$$D_{\perp}(\tau) = \left(\frac{\hbar}{2m\omega_c} + c_2^2\right)T_1(\tau) + c_2^2T_2(\tau) \quad (4.23)$$

where

$$T_1(\tau) = 1 - e^{-(\omega_c + s_2)\tau/2} \left( \cosh W\tau + \frac{s_2 - \omega_c}{2W} \sinh W\tau \right) \quad (4.24)$$

$$T_2(\tau) = 1 - e^{-s_2\tau} - e^{-(\omega_c + s_2)\tau/2} \frac{s_2 + \omega_c}{W} \sinh W\tau \quad (4.25)$$

In Table 4.1-4.2 we show the numerical results of Eq(4.13) for  $\alpha = 1$   $\alpha = 3$ . To obtain the results in the tables we use a Fortran 90 programme which is given in Appendix C.

In Table 4.1-4.2 the ground-state energies obtained by different assumptions ( $E_G^{DB}$  and  $E_G^{PD}$  [22]) are compared as a function of the magnetic field for several values

$\omega_c$	$E_G^{DB}$	$E_G^{PD}$	$v_{\parallel}$	$w_{\parallel}$	$v_{\perp}$	$w_{\perp}$
0.2	-0.92925	-0.92920	2.973	2.7266	3.0700	2.8149
0.4	-0.84495	-0.84492	2.8589	2.6048	3.1024	2.8300
0.6	-0.76017	-0.76015	2.7645	2.5025	3.2342	2.9445
0.8	-0.67490	-0.67488	2.6864	2.4164	3.5186	3.2140
1	-0.58918	-0.58914	2.6211	2.3429	4.0243	3.7097
1.2	-0.50305	-0.50300	2.5655	2.2791	4.7834	4.4649
1.4	-0.41650	-0.41648	2.5182	2.2234	5.7648	5.4473
1.6	-0.32960	-0.32957	2.4785	2.1752	6.9216	6.6083
1.8	-0.24235	-0.24232	2.4456	2.1337	8.2211	7.9133
2	-0.15476	-0.15442	2.4188	2.0981	9.6422	9.3407
3	0.28801	0.28806	2.3392	1.9764	3.9607	3.9607
5	1.19337	1.1930	2.3335	1.8903	3.0144	3.0112
10	3.52007	3.5201	2.4416	1.8390	3.0164	3.0112

Table 4.1: The upper bound on the ground-state energy of polaron in a magnetic field for  $\alpha = 1$  for the following assumptions: Devreese and Brosens( $E_G^{DB}$ ), Peeters and Devreese( $E_G^{PD}$ ).

of the electron-phonon coupling constant ( $\alpha$ ). To obtain the ground-state energy, DB used the Rayleigh-Ritz variational principle, based on the maximum principle. At any stage in the calculation this corresponds to the Feynman path integral method. However, PD worked on the hypothesis that the Feynman-Jensen inequality is valid for  $\omega_c \neq 0$ . So, the  $E_G^{DB}$  has a higher upper bound than  $E_G^{PD}$ .

$\omega_c$	$E_G^{DB}$	$E_G^{PD}$	$v_{\parallel}$	$w_{\parallel}$	$v_{\perp}$	$w_{\perp}$
0.2	-3.08291	-3.080	3.3482	2.4612	3.4077	2.5027
0.4	-3.02716	-3.025	3.2892	2.3758	3.4214	2.4706
0.6	-2.97047	-2.969	3.2424	2.3021	3.4621	2.4645
0.8	-2.91466	-2.912	3.2057	2.2385	3.5334	2.4812
1	-2.85599	-2.853	3.1774	2.1831	3.6459	2.5566
1.2	-2.79414	-2.793	3.1558	2.1346	3.8263	2.6965
1.4	-2.73525	-2.732	3.1384	2.0909	4.1479	2.9887
1.6	-2.67356	-2.671	3.1210	2.0487	4.8071	3.6456
1.8	-2.61170	-2.609	3.0988	2.0024	6.0243	4.8991
2	-2.54840	-2.546	3.0775	1.9039	7.6063	6.5311
3	-2.23330	-2.231	3.0684	1.7788	17.2926	16.3963
5	-1.56921	-1.558	3.2632	1.6142	6.2213	6.2213
10	0.31405	0.3141	3.9339	1.4668	5.5890	5.5889

Table 4.2: The upper bound on the ground-state energy of polaron in a magnetic field for  $\alpha = 3$  for the following assumptions: Devreese and Brosens( $E_G^{DB}$ ), Peeters and Devreese( $E_G^{PD}$ ).

## CHAPTER 5

### POLARON MOTION IN APPLIED FIELDS

#### 5.1 Introduction

In this chapter we treat the motion of an electron in a polarizable crystal at arbitrary temperature subjected to a time dependent electric field and a constant magnetic field. The coupling of the electron to the lattice is also arbitrary. Many authors have already treated other aspects of the polaron problem [14–20]. Here we find a rather simple explicit relationship between the electric field and magnetic field strength in the lattice and the expectation value of the velocity of the electron.

In carrying out the solution, we maintain the standard polaron model of the electron coupled only to the optical phonons. The crystal with electric field and magnetic field is assumed to be initially in thermal equilibrium, and the steady-state, translational motion of the electron subsequent to its injection into the lattice is determined. Phonons emitted from (or absorbed in) the polaron are assumed to propagate away to infinity without interacting with the phonons already present in thermal equilibrium. If the electric field is so strong as to alter the frequency of the optical modes, it is these new frequencies that we must use in our expressions.

Using this model we present two approaches for the solution of the problem. In the first approach we find the expectation value of the displacement of the electron using Feynman's path integral method. The coordinates of the lattice oscillators are exactly eliminated, but since we cannot perform the path integrals over electron coordinates exactly, we approximate the effective lattice potential by an arbitrary distribution of oscillators, and then carry out a perturbation approach similar to that of Feynman-Hellwarth-Iddings-Platzman [15](hereafter referred to as FHIP) .

We emphasize that this perturbation approach does not involve an expansion in the electric field : the electric field term is never approximated. Having obtained

the expectation value of the displacement, that of velocity follows immediately from differentiation.

The second approach involves calculating the steady-state by using a single path integral based on the minimization principle of the ground state energy. In contrast to Thornber's method, we utilize the steady-state condition in the single path integral representation which it is much simpler and more straightforward than Thornber's.

Finally, we then consider the self-consistent influence functional for the impedance problem of FHIP and find that the Feynman one-oscillator model approximates a distribution of oscillator. We also comment on mobility and effective mass for the Fröhlich polaron in electric and magnetic fields.

## **5.2 First approach: the double path integral**

### **5.2.1 Outline of the method**

To determine the displacement in time of an electron in a polarizable crystal in a uniform, static, electric field, constant magnetic field, we proceed as follows. First the expectation value of the displacement of the electron is cast into the form of a Feynman path integral, from which all the coordinates associated with the lattice can be eliminated exactly, leaving only the coordinates of the electron. Then the action in the path integral is approximated by a distribution of harmonic oscillators, which enables us to expand the displacement in a power series in terms of the difference between the exact and approximate actions. Using an expansion motivated by an exact summation of such a series for a similar problem, we rewrite our series expansion in a form which more accurately represents the physics of the problem. Finally, a comparison of this result with various special cases can be solved by other means and leads directly to the final expression.

### 5.2.2 The expectation value of the displacement of the electron

If we let  $\rho$  be the density matrix of an electron-lattice system and  $\mathbf{r}$  be the position operator, then the expectation value of the displacement of the electron at time  $t$ ,  $\langle \mathbf{r}_t \rangle$ , given that its value at  $t = 0$  is zero, is

$$\langle \mathbf{r}_t \rangle = Tr(\mathbf{r}\rho_t) \tag{5.1}$$

For thermal equilibrium problems, one can use  $\rho = e^{-\beta H}$ , where  $\beta = 1/kT$  and  $H$  is the Hamiltonian of the system. In our problem, however, we only have  $\rho_0 = e^{-\beta H}$ . We have assume thermal equilibrium initially. To determine the density matrix for  $t > 0$ , we solve its time-evolution equation

$$i\hbar \frac{\partial \rho}{\partial \tau} = [H, \rho] \tag{5.2}$$

and therefore

$$\rho_t = e^{-\frac{i}{\hbar} \int_0^t H(\sigma) d\sigma} \rho_0 e^{+\frac{i}{\hbar} \int_0^t H'(\sigma) d\sigma} \tag{5.3}$$

Here the time-ordered operator notation is used: unprimed operators to the left and ordered right to left with increasing time, and primed operators to the right and ordered left to right with increasing time.

The Hamiltonian appropriate for an electron interacting with the longitudinal optical modes of an ionically bound crystal in an oscillating electric-field ( $\mathbf{E}_\tau = \mathbf{E}_0 e^{i\omega\tau}$ ), which preserves the essential physics of the problem, is

$$H_{pol} = \frac{1}{2m} \left( \mathbf{p} - q \frac{\mathbf{A}}{c} \right)^2 - q \mathbf{E}_\tau \cdot \mathbf{r}_\tau + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \left( C_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}_\tau} + C_{\mathbf{k}}^* a_{\mathbf{k}}^\dagger e^{i\mathbf{k} \cdot \mathbf{r}_\tau} \right) \tag{5.4}$$

To evaluate Eq(5.1) we note that since the energy of the electron and its interaction with the lattice is completely negligible compared with that of the heat bath, we may set

$$\rho_0 = \exp \left( -\beta \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \right) \tag{5.5}$$

as in Feynman [14], FHIP and TF. (If one questions the validity of this approximation, or in fact the entire approach, for zero temperature, we may compute the expectation

value directly without resorting to statistical means, because in this case the initial wave function for the lattice as well as for the electron is known. The result of such a computation gives the  $\beta \rightarrow \infty$  limit of our solution here)

The problem of integrating  $Tr\rho_t$  over the crystal oscillator coordinates has been solved in chapter 2. We now calculate

$$\langle \mathbf{r}_{t_2} \rangle = \frac{1}{i} \frac{\partial}{\partial \gamma} Tr\rho_{t_2} \Big|_{\gamma=0} \quad (5.6)$$

As the first step in evaluating the expectation value of Eq(5.6), we then eliminate the phonon coordinates exactly, cast the problem into the path-integral method, transform to a frame of reference drifting [TF] with the expectation value of the electron's velocity  $\mathbf{v}$ , and then  $Tr\rho_{t_2}$  assumes the form

$$Tr\rho_{t_2} = \int \int e^{i\Phi_e} D[\mathbf{y}_\tau] D[\mathbf{y}'_\tau] \quad (5.7)$$

where

$$\begin{aligned} \Phi_e = & \int_0^{t_2} d\tau \left\{ \frac{m}{2} \dot{\mathbf{y}}_\tau^2 + \mathbf{F}_\tau \cdot \mathbf{y}_\tau + \frac{1}{2} \dot{\mathbf{y}}_\tau \cdot \mathbf{B} \cdot \mathbf{y}_\tau \right\} - \int_0^{t_2} d\tau \left\{ \frac{m}{2} \dot{\mathbf{y}}'_\tau{}^2 + \mathbf{F}'_\tau \cdot \mathbf{y}'_\tau + \frac{1}{2} \dot{\mathbf{y}}'_\tau \cdot \mathbf{B} \cdot \mathbf{y}'_\tau \right\} \\ & + i \sum_{\mathbf{k}} |C_{\mathbf{k}}|^2 \int_0^{t_2} d\tau \int_0^\tau d\sigma \left\{ S_{\omega_{\mathbf{k}}}(\tau - \sigma) e^{-i\mathbf{k} \cdot (\mathbf{y}'_\tau - \mathbf{y}'_\sigma)} + S_{\omega_{\mathbf{k}}}^*(\tau - \sigma) e^{i\mathbf{k} \cdot (\mathbf{y}_\tau - \mathbf{y}_\sigma)} \right. \\ & \left. - S_{\omega_{\mathbf{k}}}(\tau - \sigma) e^{i\mathbf{k} \cdot (\mathbf{y}'_\tau - \mathbf{y}_\sigma)} - S_{\omega_{\mathbf{k}}}^*(\tau - \sigma) e^{-i\mathbf{k} \cdot (\mathbf{y}'_\tau - \mathbf{y}_\sigma)} \right\} \end{aligned} \quad (5.8)$$

and

$$\mathbf{F}_\tau = \mathbf{E}_\tau + \mathbf{v} \times \mathbf{B} \quad (5.9)$$

$$S_{\omega_{\mathbf{k}}}(\tau) = T_{\omega_{\mathbf{k}}}(\tau) e^{-i\mathbf{k} \cdot \mathbf{v}\tau} \quad (5.10)$$

$$T_{\omega_{\mathbf{k}}}(\tau) = \frac{e^{i\omega_{\mathbf{k}}\tau}}{1 - e^{-\beta\omega_{\mathbf{k}}}} + \frac{e^{-i\omega_{\mathbf{k}}\tau}}{e^{\beta\omega_{\mathbf{k}}} - 1} \quad (5.11)$$

Although Eq(5.8) represents quite a simplification in that the oscillator coordinates have been eliminated from Eq(5.1) and (5.4) exactly. We know of no way to perform the last two path-integrals. For these we must use an approximation method.

### 5.2.3 The method of approximation

The method of approximation that is physically a very reasonable one and that has worked particularly well on two priori occasions [14,15] is to replace  $\sum_{\mathbf{k}} |C_{\mathbf{k}}|^2 e^{i\mathbf{k}\cdot\mathbf{r}_\tau}$ , which is a  $\frac{1}{\mathbf{r}}$  potential for the Fröhlich Hamiltonian, by a harmonic oscillator potential  $\mathbf{r}_\tau^2$ . This means replacing, for example, the term  $\sum_{\mathbf{k}} |C_{\mathbf{k}}|^2 S_{\omega_{\mathbf{k}}}(\tau - \sigma) e^{-i\mathbf{k}\cdot(\mathbf{y}'_\tau - \mathbf{y}'_\sigma)}$  in the exact action  $\Phi_e$ , which is  $\frac{\alpha}{\sqrt{2}} S_{\omega_{\mathbf{k}}}(\tau - \sigma) |\mathbf{y}'_\tau - \mathbf{y}'_\sigma|^{-1}$  for the Frohlich case, by  $(\mathbf{y}'_\tau - \mathbf{y}'_\sigma) \cdot \vec{\mathbf{G}}_{\tau-\sigma} \cdot (\mathbf{y}'_\tau - \mathbf{y}'_\sigma)$ , where

$$\vec{\mathbf{G}}_{\tau-\sigma} = \int_{-\infty}^{\infty} d\Omega \vec{\mathbf{G}}(\Omega) e^{-i\Omega(\tau-\sigma)} \quad (5.12)$$

where  $\vec{\mathbf{G}}(\Omega)$  is the distribution function which is proposed in references [15, 17, 20].

We now write  $\vec{\mathbf{G}}(\Omega)$  in the symmetric form as

$$\vec{\mathbf{G}}(\Omega) = \begin{pmatrix} G_+(\Omega) & 0 & 0 \\ 0 & G_-(\Omega) & 0 \\ 0 & 0 & G_{\parallel}(\Omega) \end{pmatrix} \quad (5.13)$$

If we use the Feynman one-oscillator approximation, we write

$$G_+(\Omega) = G_-(\Omega) = C_{\perp} \delta(\Omega - w_{\perp}) \quad (5.14)$$

$$G_{\parallel}(\Omega) = C_{\parallel} \delta(\Omega - w_{\parallel}) \quad (5.15)$$

Thus let us set

$$\begin{aligned} \Phi_0 &= \int_0^{t_2} d\tau \left\{ \frac{m}{2} \dot{\mathbf{y}}_\tau^2 + \mathbf{F}_\tau \cdot \mathbf{y}_\tau + \frac{1}{2} \dot{\mathbf{y}}_\tau \cdot \mathbf{B} \cdot \mathbf{y}_\tau \right\} - \int_0^{t_2} d\tau \left\{ \frac{m}{2} \dot{\mathbf{y}}'_\tau{}^2 + \mathbf{F}'_\tau \cdot \mathbf{y}'_\tau + \frac{1}{2} \dot{\mathbf{y}}'_\tau \cdot \mathbf{B} \cdot \mathbf{y}'_\tau \right\} \\ &\quad - i \int_0^{t_2} d\tau \int_0^{\tau} d\sigma \left\{ (\mathbf{y}'_\tau - \mathbf{y}'_\sigma) \cdot \vec{\mathbf{G}}_{\tau-\sigma} \cdot (\mathbf{y}'_\tau - \mathbf{y}'_\sigma) + (\mathbf{y}_\tau - \mathbf{y}_\sigma) \cdot \vec{\mathbf{G}}_{\tau-\sigma}^* \cdot (\mathbf{y}_\tau - \mathbf{y}_\sigma) \right. \\ &\quad \left. + (\mathbf{y}'_\tau - \mathbf{y}_\sigma) \cdot \vec{\mathbf{G}}_{\tau-\sigma} \cdot (\mathbf{y}'_\tau - \mathbf{y}_\sigma) + (\mathbf{y}_\tau - \mathbf{y}'_\sigma) \cdot \vec{\mathbf{G}}_{\tau-\sigma}^* \cdot (\mathbf{y}_\tau - \mathbf{y}'_\sigma) \right\} \end{aligned} \quad (5.16)$$

and expand Eq(5.7) as follows:

$$\begin{aligned} \int \int e^{i\Phi_e} &= \int \int e^{i\Phi_0} e^{i(\Phi_e - \Phi_0)} \\ &= \int \int e^{i\Phi_0} (1 + i(\Phi_e - \Phi_0) + \dots) \end{aligned} \quad (5.17)$$

While each term in the power series expansion Eq(5.17) can be evaluated knowing the one basic path integral evaluated in the Appendix A, this approach would be algebraically unwieldy. We therefore make use of another argument motivated in FHIP, which gives us a means to obtain what we believe to be a physically accurate estimate for the sum in Eq(5.17).

It turns out that for our problem where we are interested only in the expectation value of the velocity in the limit  $t_2 \rightarrow \infty$  (steady-state), that only the zero-order and first-order terms in Eq(5.17) need be calculated in order to sum the series. (The other terms are not zero, however)

To present this more clearly we refer to the following expansion:

$$\langle \mathbf{y}_{t_2} \rangle_e = \langle \mathbf{y}_{t_2} \rangle_0 + e \langle \mathbf{y}_{t_2} \rangle_1 - e^2 \langle \mathbf{y}_{t_2} \rangle_2 + \dots \quad (5.18)$$

where

$${}_j \langle \mathbf{y}_{t_2} \rangle_k = \frac{1}{i} \frac{\partial}{\partial \gamma} \int \int i \Phi_j e^{i \Phi_k} D[\mathbf{y}_\tau] D[\mathbf{y}'_\tau] \quad (5.19)$$

$$\langle \mathbf{y}_{t_2} \rangle_k = \frac{1}{i} \frac{\partial}{\partial \gamma} \int \int e^{i \Phi_k} D[\mathbf{y}_\tau] D[\mathbf{y}'_\tau] \quad (5.20)$$

Also

$${}_j \mathbf{v}_k = \lim_{t_2 \rightarrow \infty} \frac{d}{dt_2} {}_j \langle \mathbf{y}_{t_2} \rangle_k \quad (5.21)$$

$$\mathbf{v}_k = \lim_{t_2 \rightarrow \infty} \frac{d}{dt_2} \langle \mathbf{y}_{t_2} \rangle_k \quad (5.22)$$

The  $\mathbf{v}$ 's represent the several velocities we must calculate. Upon evaluating the four terms in Eq(5.18) and determining Eq(5.21) and Eq(5.22) we find

$$\frac{1}{\mathbf{v}_e} = \frac{1}{\mathbf{v}_0} - \frac{e \mathbf{v}_0 - {}_0 \mathbf{v}_0}{\mathbf{v}_0^2} \quad (5.23)$$

to be an exact expansion of the velocity  $\mathbf{v}_e$ . This is nothing more than the first order expansion of the reciprocal of  $\mathbf{v}_e \simeq \mathbf{v}_0 + (e \mathbf{v}_0 - {}_0 \mathbf{v}_0)$ , as would be found by retaining only the first order terms in Eq(5.18). This correspondence, supplemented by the physical reasoning for using such an expansion for this type of problem is given in FHIP. The

consistency between this approach and their of reference [20] is also reassuring. Also it turns out, moreover, that  $\frac{1}{\mathbf{v}_0} = -\frac{0\mathbf{v}_0}{\mathbf{v}_0^2}$  which reduces Eq(5.23) to

$$\mathbf{v}_e = -\frac{\mathbf{v}_0^2}{e\mathbf{v}_0} \quad (5.24)$$

This expression represents another step towards our  $\mathbf{E} - \mathbf{B} - \mathbf{v}$  relationship.

#### 5.2.4 The evaluation of the velocity

Once  $\int \int e^{i\Phi_0}$  Eq(5.20) has been evaluated, various algebraic manipulations may be used to determine the  $\mathbf{v}_0$  and  ${}_e\mathbf{v}_0$  for Eq(5.24). The calculation of this path integral is long and is outlined in Appendix A. Using the result and calculating the Eq(5.20) by substitute  $\mathbf{F}_\tau \longrightarrow \mathbf{F}_\tau + \gamma\delta(\tau - t_2)$  and  $\mathbf{F}'_\tau \longrightarrow \mathbf{F}'_\tau$  in Eq(5.16), and differentiate with respect to  $\gamma$ . We may at once find  $\langle \mathbf{y}_{t_2} \rangle_0$

$$\langle \mathbf{y}_{t_2} \rangle_0 = -i \int_0^{t_2} d\tau \left\{ \vec{\mathbf{L}}(\tau) - \vec{\mathbf{L}}^*(\tau) \right\} \cdot \mathbf{F}_\tau \quad (5.25)$$

where

$$\vec{\mathbf{L}}(\tau) - \vec{\mathbf{L}}^*(\tau) = \int_{-\infty}^{\infty} \frac{d\nu}{2\pi i} \left( \frac{1}{\vec{\mathbf{Z}}_\nu} - \frac{1}{\vec{\mathbf{Z}}_\nu^\dagger} \right) e^{-i\nu\tau} \quad (5.26)$$

and

$$\vec{\mathbf{Z}}_\nu = -m(\nu + i\varepsilon)^2 \mathbf{I} - i(\nu + i\varepsilon) \mathbf{E} \cdot \mathbf{B} - 4(\nu + i\varepsilon) \int_{-\infty}^{\infty} \frac{d\Omega}{\Omega} \frac{\vec{\mathbf{G}}(\Omega)}{\Omega^2 - (\nu + i\varepsilon)^2} \quad (5.27)$$

For zero frequency( $\mathbf{E}_\tau \longrightarrow \mathbf{E}_0$ ), we find

$$\mathbf{v}_0 \equiv \langle \dot{\mathbf{y}}_{t_2} \rangle_0 = -2(\mathbf{E}_0 + \mathbf{v} \times \mathbf{B}) \text{Im} \vec{\mathbf{L}}(t_2) \quad (5.28)$$

which  $\text{Im} \vec{\mathbf{L}}(t_2)$  is independent of the temperature. The results express the fact that in zero order, where we consider a weak coupling of the electron to a distribution of harmonic oscillator potentials in place of the more correct Coulomb interaction. The oscillators capable of contributing to the D.C. mobility are those of lowest frequency. For Eq(5.28) is valid for all values of electric field and magnetic field, and the relationship is linear as one would expect.

The calculation of  $\int \int i\Phi_e e^{i\Phi_0}$  Eq(5.20) to obtain  ${}_e\mathbf{v}_0$  can be performed using

$$\begin{aligned} \int \int i\Phi_e e^{i\Phi_0} &= -\sum_{\mathbf{k}} |C_{\mathbf{k}}|^2 \int_{-\infty}^{\infty} d\theta \int_{-\infty}^{\theta} d\eta \left\{ S_{\omega_{\mathbf{k}}}(\theta - \eta) \int \int (1) + S_{\omega_{\mathbf{k}}}^*(\theta - \eta) \int \int (2) \right. \\ &\quad \left. - S_{\omega_{\mathbf{k}}}(\theta - \eta) \int \int (3) - S_{\omega_{\mathbf{k}}}^*(\theta - \eta) \int \int (4) \right\} \end{aligned} \quad (5.29)$$

As a shorter notation, we designate the solution of  $\int \int e^{i\Phi_0}$  by  $\int \int \{\mathbf{F}_{\tau}, \mathbf{F}'_{\tau}\}$  where we specify the forces to be inserted into  $\int \int e^{i\Phi_0}$ . with

$$\int \int (1) = \int \int \{\mathbf{F}_{\tau} + \gamma\delta(\tau - t_2), \mathbf{F}'_{\tau} + \mathbf{k}(\delta(\tau - \theta) - \delta(\tau - \eta))\} \quad (5.30)$$

$$\int \int (2) = \int \int \{\mathbf{F}_{\tau} + \gamma\delta(\tau - t_2) + \mathbf{k}(\delta(\tau - \theta) - \delta(\tau - \eta)), \mathbf{F}'_{\tau}\} \quad (5.31)$$

$$\int \int (3) = \int \int \{\mathbf{F}_{\tau} + \gamma\delta(\tau - t_2) + \mathbf{k}\delta(\tau - \theta), \mathbf{F}'_{\tau} + \mathbf{k}\delta(\tau - \eta)\} \quad (5.32)$$

$$\int \int (4) = \int \int \{\mathbf{F}_{\tau} + \gamma\delta(\tau - t_2) + \mathbf{k}\delta(\tau - \eta), \mathbf{F}'_{\tau} + \mathbf{k}\delta(\tau - \theta)\} \quad (5.33)$$

Again, doing the algebra and inserting the result for  ${}_e\mathbf{v}_0$  into Eq(5.23) yields

$$\frac{1}{\mathbf{v}_e} = -\frac{1}{\mathbf{v}_0^2} \left( -\frac{\mathbf{v}_0}{\mathbf{F}} \int_{-\infty}^{\infty} d\xi \sum_{\mathbf{k}} |C_{\mathbf{k}}|^2 \mathbf{k} S_{\omega_{\mathbf{k}}}(\xi) e^{-\mathbf{k} \cdot \vec{\mathbf{L}}_{\beta}(\xi) \cdot \mathbf{k}} \right) \quad (5.34)$$

where

$$\mathbf{F} = \mathbf{E}_0 + \mathbf{v} \times \mathbf{B} \quad (5.35)$$

$$\begin{aligned} \vec{\mathbf{L}}_{\beta}(\xi) &= \vec{\mathbf{L}}(\xi) - \vec{\mathbf{L}}(0) \\ &= \int_{-\infty}^{\infty} \frac{d\nu}{2\pi i} \left( \frac{1}{\vec{\mathbf{Z}}_{\nu}} - \frac{1}{\vec{\mathbf{Z}}_{\nu}^{\dagger}} \right) \frac{1 - e^{-i\nu\xi}}{e^{\beta\nu} - 1} \end{aligned} \quad (5.36)$$

The result obtained in Eq(5.34) for the approximate velocity  $\mathbf{v}_e$  as a function of  $\mathbf{E}_0$  and  $\mathbf{B}$ , is unsatisfactory in one respect. The critical dependence through  $\mathbf{v}_0$  of the result for the weak coupling of the electron to the fictitious particle. To remedy this we are motivated to replace  $\mathbf{v}_0$  and  $\mathbf{v}_e$  in Eq(5.34) by  $\mathbf{v}$ , the expectation, steady-state velocity. The result is

$$\mathbf{E}_0 + \mathbf{v} \times \mathbf{B} = \int_{-\infty}^{\infty} d\xi \sum_{\mathbf{k}} |C_{\mathbf{k}}|^2 \mathbf{k} T_{\omega_{\mathbf{k}}}(\xi) e^{-i\mathbf{k} \cdot \mathbf{v}\xi} e^{-\mathbf{k} \cdot \vec{\mathbf{L}}_{\beta}(\xi) \cdot \mathbf{k}} \quad (5.37)$$

and this is our fundamental equation relating the velocity to the electromagnetic fields.

Eq(5.37) agrees with Eq(12) in reference [20] which they used the method of rates.

### 5.3 Second approach: the single path integral

In section(5.2.1), the conservation of the energy and momentum in the steady-state was utilized in finding relationships between electromagnetic fields and velocity for weak coupling. In this section we propose the single path integral approach to obtain the steady-state condition.

With the Hamiltonian Eq(5.4) we can calculate expectation values of any operator  $\hat{Q}$  at time  $t$  as follows:

$$\langle \hat{Q}_t \rangle = \int_0^0 D[\mathbf{r}_\tau] \hat{Q} e^{\frac{i}{\hbar} S_{pol}} |_{force=0} \quad (5.38)$$

where the polaron action  $S_{pol}$  was obtained after the exact elimination of the phonon coordinates (chapter 2) and thus is a functional of the electron coordinates only. It is given by

$$\begin{aligned} S_{pol} = & \int_0^{t_2} d\tau \left( \frac{m}{2} \dot{\mathbf{r}}_\tau^2 + \frac{1}{2} \dot{\mathbf{r}}_\tau \cdot \mathbf{B} \times \mathbf{r}_\tau + \mathbf{E}_\tau \cdot \mathbf{r}_\tau \right) \\ & + \sum_{\mathbf{k}} |C_{\mathbf{k}}|^2 \int_0^{t_2} d\tau \int_0^{t_2} d\sigma \frac{\cos \omega_{\mathbf{k}} (|\tau - \sigma| - t_2/2)}{\sin \omega_{\mathbf{k}} t_2/2} e^{i\mathbf{k} \cdot (\mathbf{r}_\tau - \mathbf{r}_\sigma)} \end{aligned} \quad (5.39)$$

#### 5.3.1 The equation of motion

Using Eq(5.39) we can express the equation of motion of the polaron as

$$m \ddot{\mathbf{r}}_\tau - \dot{\mathbf{r}}_\tau \times \mathbf{B} - \mathbf{E}_\tau = i \sum_{\mathbf{k}} |C_{\mathbf{k}}|^2 \mathbf{k} \int_0^{t_2} d\sigma \frac{\cos \omega_{\mathbf{k}} (|\tau - \sigma| - t_2/2)}{\sin \omega_{\mathbf{k}} t_2/2} e^{i\mathbf{k} \cdot (\mathbf{r}_\tau - \mathbf{r}_\sigma)} \quad (5.40)$$

The expectation values of Eq(5.40) at time  $t_2$  is

$$m \langle \ddot{\mathbf{r}}_{t_2} \rangle - \langle \dot{\mathbf{r}}_{t_2} \rangle \times \mathbf{B} - \mathbf{E}_{t_2} = i \sum_{\mathbf{k}} |C_{\mathbf{k}}|^2 \mathbf{k} \int_0^{t_2} d\sigma \frac{\cos \omega_{\mathbf{k}} (t_2/2 - \sigma)}{\sin \omega_{\mathbf{k}} t_2/2} \langle e^{i\mathbf{k} \cdot (\mathbf{r}_\tau - \mathbf{r}_\sigma)} \rangle_{t_2} \quad (5.41)$$

From Eq(5.38),we can write

$$\langle e^{i\mathbf{k} \cdot (\mathbf{r}_\tau - \mathbf{r}_\sigma)} \rangle_{t_2} = \int_0^0 D[\mathbf{r}_\tau] e^{i\mathbf{k} \cdot (\mathbf{r}_{t_2} - \mathbf{r}_\sigma)} e^{\frac{i}{\hbar} S_{pol}} \quad (5.42)$$

The difficulty with the above path integral is that the polaron action  $S_{pol}$  is not quadratic in  $\mathbf{r}_\tau$  and  $\dot{\mathbf{r}}_\tau$ . So, we now introduce the trial action  $S_0$  which allows to

approximately evaluate the path integrals. We now write

$$\begin{aligned} \left\langle e^{i\mathbf{k}\cdot(\mathbf{r}_\tau-\mathbf{r}_\sigma)} \right\rangle_{t_2} &= \int_0^0 D[\mathbf{r}_\tau] e^{i\mathbf{k}\cdot(\mathbf{r}_{t_2}-\mathbf{r}_\sigma)} e^{\frac{i}{\hbar}(S_{pol}-S_0)} e^{\frac{i}{\hbar}S_0} \\ &= \int_0^0 D[\mathbf{r}_\tau] e^{i\mathbf{k}\cdot(\mathbf{r}_{t_2}-\mathbf{r}_\sigma)} \left\{ e^{\frac{i}{\hbar}S_0} + \frac{i}{\hbar}(S_{pol}-S_0) e^{\frac{i}{\hbar}S_0} + \dots \right\} \end{aligned} \quad (5.43)$$

where

$$S_0 = \int_0^{t_2} d\tau \left( \frac{m}{2} \dot{\mathbf{r}}_\tau^2 + \frac{1}{2} \dot{\mathbf{r}}_\tau \cdot \mathbf{B} \times \mathbf{r}_\tau \right) - \int_0^{t_2} d\tau \int_0^{t_2} d\sigma (\mathbf{r}_\tau - \mathbf{r}_\sigma) \cdot \vec{\mathbf{G}}_{|\tau-\sigma|} \cdot (\mathbf{r}_\tau - \mathbf{r}_\sigma) \quad (5.44)$$

with the diagonal matrix  $\vec{\mathbf{G}}_{\tau-\sigma}^{ij}$  defined in Eq(3.11). The physical meaning of this action is that of two-particle model system in which an electron is coupled to a second fictitious particle in the magnetic field where the position of the fictitious particle has been eliminated. The Hamiltonian for this two particle model system is defined in Eq(4.6).

We now consider only the first term of Eq(5.43), and

$$\left\langle e^{i\mathbf{k}\cdot(\mathbf{r}_\tau-\mathbf{r}_\sigma)} \right\rangle_{t_2} = \int_0^0 D[\mathbf{r}_\tau] e^{\frac{i}{\hbar}S'_0} \quad (5.45)$$

where

$$S'_0 = \int_0^{t_2} d\tau \left( \frac{m}{2} \dot{\mathbf{r}}_\tau^2 + \frac{1}{2} \dot{\mathbf{r}}_\tau \cdot \mathbf{B} \times \mathbf{r}_\tau + \mathbf{f}_\tau \cdot \mathbf{r}_\tau \right) - \int_0^{t_2} d\tau \int_0^{t_2} d\sigma (\mathbf{r}_\tau - \mathbf{r}_\sigma) \cdot \vec{\mathbf{G}}_{|\tau-\sigma|} \cdot (\mathbf{r}_\tau - \mathbf{r}_\sigma) \quad (5.46)$$

with

$$\mathbf{f}_\tau = \mathbf{k} (\delta(\tau - t_2) - \delta(\tau - \sigma)) \quad (5.47)$$

The path integral for Eq(5.46) can be solved exactly and we use the results of Eq(3.15) and Eq(3.89) in chapter 3. We obtain for Eq(5.45)

$$\left\langle e^{i\mathbf{k}\cdot(\mathbf{r}_\tau-\mathbf{r}_\sigma)} \right\rangle_{t_2} = e^{-\frac{i}{2m} \int_0^{t_2} d\tau \int_0^{t_2} d\sigma \mathbf{f}_\tau \cdot (\Delta_0^{-1} \cdot \Delta_\tau \cdot \Delta_{t_2-\sigma} - \Delta_{|\tau-\sigma|}) \cdot \mathbf{f}_\sigma} \quad (5.48)$$

where

$$\Delta_0^{-1} \cdot \Delta_\tau \cdot \Delta_{t_2-\sigma} - \Delta_{|\tau-\sigma|} = \frac{1}{2} \begin{pmatrix} \Delta_{\tau-\sigma}^{++} & -\Delta_{\tau-\sigma}^{--} & 0 \\ \Delta_{\tau-\sigma}^{--} & \Delta_{\tau-\sigma}^{++} & 0 \\ 0 & 0 & \Delta_{\tau-\sigma}^{33} \end{pmatrix} \quad (5.49)$$

and

$$\Delta_{\tau-\sigma}^{++} = -2 \sum_{j=1}^3 c_j^2 \left( \frac{\cos s_j \left( \frac{\tau-\sigma}{2} \right) \sin s_j \frac{\sigma}{2} \sin s_j \left( \frac{t_2-\tau}{2} \right)}{\sin s_j \frac{t_2}{2}} \right) \quad (5.50)$$

$$\Delta_{\tau-\sigma}^{--} = -2 \sum_{j=1}^3 c_j^2 \left( \frac{\sin s_j \left( \frac{\tau-\sigma}{2} \right) \sin s_j \frac{\sigma}{2} \sin s_j \left( \frac{t_2-\tau}{2} \right)}{\sin s_j \frac{t_2}{2}} \right) \quad (5.51)$$

$$\Delta_{\tau-\sigma}^{33} = 2 \left( \frac{v_{\parallel}^2 - w_{\parallel}^2}{v_{\parallel}^3} \right) \frac{\cos v_{\parallel} \left( \frac{\tau-\sigma}{2} \right) \sin v_{\parallel} \frac{\sigma}{2} \sin v_{\parallel} \left( \frac{t_2-\tau}{2} \right)}{\sin v_{\parallel} \frac{t_2}{2}} + \frac{w_{\parallel}^2}{v_{\parallel}^2} \frac{\sigma}{t_2} (t_2 - \sigma) \quad (5.52)$$

Inserting Eq(5.47) into Eq(5.48), we find

$$\left\langle e^{i\mathbf{k} \cdot (\mathbf{r}_{\tau} - \mathbf{r}_{\sigma})} \right\rangle_{t_2} = e^{-\frac{i}{2m} \mathbf{k} \cdot (\mathbf{\Delta}_0^{-1} \cdot \mathbf{\Delta}_{t_2-\sigma} \cdot \mathbf{\Delta}_{\sigma} - \mathbf{\Delta}_0) \cdot \mathbf{k}} \quad (5.53)$$

Thus equation of motion becomes

$$m \langle \ddot{\mathbf{r}}_{t_2} \rangle - \langle \dot{\mathbf{r}}_{t_2} \rangle \times \mathbf{B} - \mathbf{E}_{t_2} = i \sum_{\mathbf{k}} |C_{\mathbf{k}}|^2 \mathbf{k} \int_0^{t_2} d\sigma \frac{\cos \omega_{\mathbf{k}} (t_2/2 - \tau)}{\sin \omega_{\mathbf{k}} t_2/2} e^{-\frac{i}{2m} \mathbf{k} \cdot (\mathbf{\Delta}_0^{-1} \cdot \mathbf{\Delta}_{t_2-\sigma} \cdot \mathbf{\Delta}_{\sigma} - \mathbf{\Delta}_0) \cdot \mathbf{k}} \quad (5.54)$$

### 5.3.2 An alternative derivative of the steady-state condition of Thornber

In reference [17,20], the equation of motion is transformed to a reference frame moving with the electron. This change of reference frame leads to another difference which should be included in the approximation, the change of variables  $\mathbf{r}_{\tau} = \mathbf{y}_{\tau} + \mathbf{v}\tau$  leading to a modification of the frequency  $\omega_{\mathbf{k}} \rightarrow \omega_{\mathbf{k}} \pm \mathbf{k} \cdot \mathbf{v}$ . Hence, now Eq(5.54) with  $m = 1$  reads

$$\begin{aligned} \langle \ddot{\mathbf{y}}_{t_2} \rangle - \langle \dot{\mathbf{y}}_{t_2} \rangle \times \mathbf{B} - \mathbf{v} \times \mathbf{B} - \mathbf{E}_{t_2} &= i \sum_{\mathbf{k}} |C_{\mathbf{k}}|^2 \mathbf{k} \int_0^{t_2} d\tau \frac{\cos \omega_{\mathbf{k}} (t_2/2 - \tau)}{\sin \omega_{\mathbf{k}} t_2/2} \\ &\times e^{i\mathbf{k} \cdot \mathbf{v}\tau} e^{-\frac{i}{2m} \mathbf{k} \cdot (\mathbf{\Delta}_0^{-1} \cdot \mathbf{\Delta}_{t_2-\tau} \cdot \mathbf{\Delta}_{\tau} - \mathbf{\Delta}_0) \cdot \mathbf{k}} \end{aligned} \quad (5.55)$$

where  $\langle \ddot{\mathbf{y}}_{t_2} \rangle$  and  $\langle \dot{\mathbf{y}}_{t_2} \rangle$  are the expectation values of the velocity and acceleration of the linear response to the small probe electric field [20,37]. We now change the real time variables to the imaginary time ( $t_2 \rightarrow -i\beta$ ), and when the steady-state is reached, we find

$$\mathbf{E}_0 + \mathbf{v} \times \mathbf{B} = \sum_{\mathbf{k}} |C_{\mathbf{k}}|^2 \mathbf{k} \int_{-\infty}^{\infty} d\xi \frac{\cos \omega_{\mathbf{k}} \xi}{\sinh \omega_{\mathbf{k}} \beta/2} e^{-i\mathbf{k} \cdot \mathbf{v}(\xi+i\beta/2)} e^{-\frac{1}{2}(k_x^2+k_y^2)\Delta_{\perp}(\xi)} e^{-\frac{1}{2}k_z^2\Delta_{\parallel}(\xi)} \quad (5.56)$$

where

$$\Delta_{\perp}(\xi) = \sum_{j=1}^3 c_j^2 \left( \frac{\cosh s_j \frac{\beta}{2} - \cos s_j \xi}{\sinh s_j \frac{\beta}{2}} \right) \quad (5.57)$$

$$\Delta_{\parallel}(\xi) = \frac{w_{\parallel}^2}{v_{\parallel}^2} \left[ \left( \frac{v_{\parallel}^2 - w_{\parallel}^2}{v_{\parallel} w_{\parallel}^2} \right) \frac{\cosh v_{\parallel} \frac{\beta}{2} - \cos v_{\parallel} \xi}{\sinh v_{\parallel} \frac{\beta}{2}} + \frac{\xi^2}{\beta} + \frac{\beta}{4} \right] \quad (5.58)$$

Eq(5.56) agrees with Eq(23a) of Thornber [20] for the steady-state condition. The correspondence between our notation and that of Thornber is  $\Delta_{\perp}(\xi) \rightarrow K'_+(\xi) + K'_-(\xi)$ ,  $\Delta_{\parallel}(\xi) \rightarrow K'_0(\xi)$ . The left hand side of Eq(5.56) is the rate of increase of electron momentum and the right hand side may be interpreted as the net rate of emission of longitudinal optical phonons of wave vector  $\mathbf{k}$ , and  $\mathbf{k}$  may be interpreted as the change of momentum of the electron. So Eq(5.56) expresses the fact that in steady-state the gain and loss just balance.

#### 5.4 Low-frequency limit of impedance and self-consistency

Another check on our results is to find the zero-frequency limit of the real part of the impedance calculated in FHIP[Eq(4)]. This limit gives the electronic mobility for arbitrary coupling and temperature, and agrees with the low-velocity limit of our result Eq(5.32)[B=0]. As was stressed in FHIP, careful attention had to be given to this limit because the approach used to sum the expansion of the impedance was subject to question for zero frequency. It can be derived using our approach which avoids the zero-frequency problem. From section 5.2.4 we can show that

$$\langle \mathbf{r}_{t_2} \rangle = -i \int_0^{t_2} d\tau \vec{\mathbf{Y}}_0(t_2 - \tau) \cdot \mathbf{E}_{\tau} \quad (5.59)$$

Using  $\mathbf{E}_{\tau} = \mathbf{E}_0 e^{-i\omega\tau}$ , we have

$$\langle \mathbf{r}_{t_2} \rangle = i \int_0^{t_2} d\xi \vec{\mathbf{Y}}_0(\xi) e^{i\omega\xi} \cdot \mathbf{E}_0 e^{-i\omega t_2} \quad (5.60)$$

Taking the Fourier transform of Eq(5.60) we obtain

$$\mathbf{r}_{\omega} = \vec{\mathbf{Y}}_0(\omega) \cdot \mathbf{E}_{\omega} \quad (5.61)$$

where  $\vec{\mathbf{Y}}_0(\omega)$  is the Fourier transform of the response function given by

$$\vec{\mathbf{Y}}_0(\omega) = \int_0^\infty d\xi e^{i\omega\xi} \int_0^{t_2} \frac{d\nu}{2\pi i} \left[ \frac{1}{\vec{\mathbf{Z}}_\nu} - \frac{1}{\vec{\mathbf{Z}}_\nu^\dagger} \right] e^{-i\nu\xi} \equiv \frac{1}{\vec{\mathbf{Z}}_\omega} \quad (5.62)$$

We now derive for  $\vec{\mathbf{Z}}_\omega$  from the equation of motion without imposing the steady-state restriction and we have

$$\mathbf{E}_{t_2} + \langle \dot{\mathbf{r}}_{t_2} \rangle \times \mathbf{B} = \sum_{\mathbf{k}} \mathbf{k} \langle R_{\mathbf{k}} \rangle_{t_2} + m \langle \ddot{\mathbf{r}}_{t_2} \rangle \quad (5.63)$$

where  $R_{\mathbf{k}}$  defined in Eq(8b) of reference [17] and make a change of variables  $\mathbf{r}_\tau = \mathbf{y}_\tau + \bar{a}e^{-i\omega\tau}$ , where  $\bar{a}$  is the amplitude of the vibration, and  $e^{-i\omega\tau}$  is the time-dependence of the oscillator of frequency  $\omega$  [FHIP use  $e^{+i\nu\tau}$ ]. Calculating the  $\langle R_{\mathbf{k}} \rangle_{t_2}$  as in section 5.2, and expanding this result for  $\bar{a}$  small, we obtain

$$\vec{\mathbf{Z}}_\omega = -m\omega^2 \vec{\mathbf{I}} - i\omega \in \cdot \mathbf{B} + \int_0^\infty d\xi \left(1 - e^{i\omega\xi}\right) \text{Im} \vec{\mathbf{S}}(\xi) \quad (5.64)$$

where

$$\vec{\mathbf{S}}(\xi) = \sum_{\mathbf{k}} |C_{\mathbf{k}}|^2 \mathbf{k} \mathbf{k} 2T_{\omega_{\mathbf{k}}}(\xi) e^{-\mathbf{k} \cdot \vec{\mathbf{L}}_\beta(\xi) \cdot \mathbf{k}} \quad (5.65)$$

and

$$\vec{\mathbf{L}}_\beta(\xi) = \int_{-\infty}^\infty \frac{d\nu}{2\pi i} \left[ \frac{1}{\vec{\mathbf{Z}}_\nu} \left( 4\pi i \vec{\mathbf{G}}(\Omega) \right) \frac{1}{\vec{\mathbf{Z}}_\nu^\dagger} \right] \left( 1 - e^{-i\nu\xi} \right) \quad (5.66)$$

Next, using the identity

$$\left( 1 - e^{i\omega\xi} \right) = 4\omega^2 \int_{-\infty}^\infty \frac{d\Omega}{4\pi i} \frac{e^{-i\Omega\xi}}{\Omega} \frac{1}{\Omega^2 - \omega^2} \quad (5.67)$$

it is straight forward to verify that

$$\int_0^\infty d\xi \left( 1 - e^{i\omega\xi} \right) \text{Im} \vec{\mathbf{S}}(\xi) = -4\omega^2 \int_{-\infty}^\infty \frac{d\Omega}{\Omega} \frac{\vec{\mathbf{G}}(\Omega)}{\Omega^2 - \omega^2} \quad (5.68)$$

where

$$\vec{\mathbf{G}}(\Omega) \equiv \frac{1}{2} \sum_{\mathbf{k}} |C_{\mathbf{k}}|^2 \mathbf{k} \mathbf{k} \int_{-\infty}^\infty \frac{d\xi}{2\pi} e^{-i\Omega\xi} T_{\omega_{\mathbf{k}}}(\xi) e^{-\mathbf{k} \cdot \vec{\mathbf{L}}_\beta(\xi) \cdot \mathbf{k}} \quad (5.69)$$

Eq(5.68) and Eq(5.64) gives  $\vec{\mathbf{Z}}_\omega$  in terms of  $\vec{\mathbf{G}}(\Omega)$ , Eq(5.69) gives  $\vec{\mathbf{G}}(\Omega)$  in terms of  $\vec{\mathbf{L}}_\beta(\xi)$ , and Eq(5.66) gives  $\vec{\mathbf{L}}_\beta(\xi)$  in terms of  $\vec{\mathbf{G}}(\Omega)$  and  $\vec{\mathbf{Z}}_\omega$ . This set of equations describes a self-consistent relationship from which  $\vec{\mathbf{G}}, \vec{\mathbf{Z}}$  and  $\vec{\mathbf{L}}_\beta$  may be determined

for arbitrary magnetic field  $\mathbf{B}$ , reciprocal-lattice temperature  $\beta$ , and electron-phonon interaction  $|C_{\mathbf{k}}|^2$ . We now write

$$\vec{\mathbf{Z}}_{\omega} = -m\omega^2\vec{\mathbf{I}} - i\omega \in \cdot \mathbf{B} + \vec{\chi}(\omega) \quad (5.70)$$

where

$$\vec{\chi}(\omega) \equiv \int_0^{\infty} d\xi (1 - e^{i\omega\xi}) \text{Im}\vec{\mathbf{S}}(\xi) \quad (5.71)$$

For numerical work it is convenient to use  $\vec{\mathbf{S}}$  in the form (using the results in Appendix B)

$$\vec{\mathbf{S}}(\xi) = \int \frac{d^3k}{(2\pi)^3} |C_{\mathbf{k}}|^2 \mathbf{k} \mathbf{k} 2T_{\omega_{\mathbf{k}}}(\xi) e^{-k_{\perp}^2 K_{\beta}^{\perp}(\xi)} e^{-k_z^2 K_{\beta}^{\parallel}(\xi)} \quad (5.72)$$

where

$$K_{\beta}^{\perp}(\xi) = \sum_{j=1}^3 c_j^2 \left( \frac{\cosh s_j \beta/2 - \cos s_j (\xi - i\beta/2)}{\sinh s_j \beta/2} \right) \quad (5.73)$$

$$K_{\beta}^{\parallel}(\xi) = \frac{1}{2m} \frac{w_{\parallel}^2}{v_{\parallel}^2} \left[ \left( \frac{v_{\parallel}^2 - w_{\parallel}^2}{v_{\parallel} w_{\parallel}^2} \right) \frac{\cosh v_{\parallel} \beta/2 - \cos v_{\parallel} (\xi - i\beta/2)}{\sinh v_{\parallel} \beta/2} - i\xi + \frac{\xi^2}{\beta} \right] \quad (5.74)$$

The first two terms on the right-hand side of Eq(5.70) represent a particle in a magnetic field, while  $\vec{\chi}(\omega)$  contains all of the corrections due to the interaction with phonons. The entire dependence of our results Eq(5.70) on the trial action  $\Phi_0$  is in  $K_{\beta}^{\perp}$  and  $K_{\beta}^{\parallel}$ .

## 5.5 Zero temperature; effective mass

Reference [15] discusses in more details the behavior of the impedance. In this section, for Fröhlich's case we firstly consider the case  $\omega < 1$ ,  $\beta = \infty$ . Then the path of integration along the real axis may be rotated to a path along the positive or negative imaginary axis  $\xi \cong 0$  to  $\pm i\infty$  [15]. The resulting expression is

$$\begin{aligned} \vec{\mathbf{Z}}_{\omega} &= -m\omega^2\vec{\mathbf{I}} - i\omega \in \cdot \mathbf{B} - 2 \int_0^{\infty} e^{-u} (1 - \cosh \omega u) \\ &\quad \times \int \frac{d^3k}{(2\pi)^3} |C_{\mathbf{k}}|^2 \mathbf{k} \mathbf{k} e^{-k_{\perp}^2 K_{\perp}(u)} e^{-k_z^2 K_{\parallel}(u)} \end{aligned} \quad (5.75)$$

where

$$K_{\parallel}(u) = \frac{1}{2m} \frac{w_{\parallel}^2}{v_{\parallel}^2} \left[ \left( \frac{v_{\parallel}^2 - w_{\parallel}^2}{v_{\parallel} w_{\parallel}^2} \right) (1 - e^{-v_{\parallel} u}) + u \right] \quad (5.76)$$

$$K_{\perp}(u) = \sum_{j=1}^3 c_j^2 (1 - e^{-s_j u}) \quad (5.77)$$

For extremely low frequencies  $\omega$  we can approximate  $(1 - \cosh \omega u) = -\omega^2 u^2/2$ . The result is that for the impedance in the direction parallel with the magnetic field

$$Z_{\parallel} = -\omega^2 \left\{ 1 + \frac{\alpha}{\sqrt{\pi}} \int_0^{\infty} du \frac{u^2 e^{-u}}{(K_{\parallel} - K_{\perp})^{\frac{3}{2}}} \left\{ \ln \left[ \frac{\sqrt{K_{\parallel}} + \sqrt{K_{\parallel} - K_{\perp}}}{\sqrt{K_{\parallel}} + \sqrt{K_{\parallel} - K_{\perp}}} \right] - \frac{2\sqrt{K_{\parallel} - K_{\perp}}}{\sqrt{K_{\parallel}}} \right\} \right\} \quad (5.78)$$

We now introduce

$$Z = -\omega^2 - \frac{\alpha}{\sqrt{\pi}} \int_0^{\infty} du \frac{\omega^2 u^2 e^{-u}}{\sqrt{K_{\parallel} K_{\perp}}} \quad (5.79)$$

We now obtain for the impedance in the direction perpendicular to the magnetic field

$$\begin{aligned} Z_{\perp} &= \frac{Z - Z_{\parallel}}{2} \\ &= -\omega^2 \left\{ 1 + \frac{\alpha}{2\sqrt{\pi}} \int_0^{\infty} du u^2 e^{-u} \left[ \frac{1}{\sqrt{K_{\parallel} K_{\perp}}} - \frac{1}{(K_{\parallel} - K_{\perp})^{\frac{3}{2}}} \right] \right. \\ &\quad \times \left. \left\{ \ln \left[ \frac{\sqrt{K_{\parallel}} + \sqrt{K_{\parallel} - K_{\perp}}}{\sqrt{K_{\parallel}} + \sqrt{K_{\parallel} - K_{\perp}}} \right] - \frac{2\sqrt{K_{\parallel} - K_{\perp}}}{\sqrt{K_{\parallel}}} \right\} \right\} \quad (5.80) \end{aligned}$$

From Eq(5.78) and Eq(5.80), we can see that the polaron behaves like a free particle with an effective mass

$$m_{\parallel}^* = 1 + \frac{\alpha}{\sqrt{\pi}} \int_0^{\infty} du \frac{u^2 e^{-u}}{(K_{\parallel} - K_{\perp})^{\frac{3}{2}}} \left\{ \ln \left[ \frac{\sqrt{K_{\parallel}} + \sqrt{K_{\parallel} - K_{\perp}}}{\sqrt{K_{\parallel}} + \sqrt{K_{\parallel} - K_{\perp}}} \right] - \frac{2\sqrt{K_{\parallel} - K_{\perp}}}{\sqrt{K_{\parallel}}} \right\} \quad (5.81)$$

$$\begin{aligned} m_{\perp}^* &= 1 + \frac{\alpha}{2\sqrt{\pi}} \int_0^{\infty} du u^2 e^{-u} \left[ \frac{1}{\sqrt{K_{\parallel} K_{\perp}}} - \frac{1}{(K_{\parallel} - K_{\perp})^{\frac{3}{2}}} \right] \\ &\quad \times \left\{ \ln \left[ \frac{\sqrt{K_{\parallel}} + \sqrt{K_{\parallel} - K_{\perp}}}{\sqrt{K_{\parallel}} + \sqrt{K_{\parallel} - K_{\perp}}} \right] - \frac{2\sqrt{K_{\parallel} - K_{\perp}}}{\sqrt{K_{\parallel}}} \right\} \quad (5.82) \end{aligned}$$

It is very easily to show that for zero magnetic field  $K_{\perp} \rightarrow K_{\parallel}$  and

$$m_{\perp}^* \rightarrow m_{\parallel}^* = 1 + \frac{\alpha}{3\sqrt{\pi}} \int_0^{\infty} du \frac{u^2 e^{-u}}{K_{\parallel}^{\frac{3}{2}}} \quad (5.83)$$

which is the result of Feynman [14, 15]

### 5.5.1 The mobility for Fröhlich's polaron

The analytic properties of  $\vec{\mathbf{S}}(\xi)$  outlined in reference [15] allows one to rewrite the expression for  $\text{Im}\vec{\chi}(\omega)$  in a form more convenient for computation. We may write Eq(5.71) as

$$\text{Im}\vec{\chi}(\omega) = \text{Im} \int_0^{\infty} \sin \omega u \vec{\mathbf{S}}(u) du \quad (5.84)$$

We may change the contour of integration in Eq(5.84) as in reference [15]. The contribution from the remaining part of the contour gives

$$\text{Im}\vec{\chi}(\omega) = \sinh(\beta\omega/2) \int_0^{\infty} \cos(\omega u) \vec{\Sigma}(u) du \quad (5.85)$$

where  $\vec{\Sigma}(u) = \vec{\mathbf{S}}(u + i\beta/2)$  is given by;  $\omega_{\mathbf{k}} = 1$

$$\vec{\Sigma}(u) = \int \frac{d^3k}{(2\pi)^3} |C_{\mathbf{k}}|^2 \mathbf{k} \mathbf{k}^2 \frac{\cos(u)}{\sinh(\beta/2)} e^{-k_{\perp}^2 D_{\perp}(u)} e^{-k_z^2 D_{\parallel}(u)} \quad (5.86)$$

with  $D_{\perp, \parallel}(u) = K_{\beta}^{\perp, \parallel}(u + i\beta/2)$

$$D_{\perp}(u) = \sum_{j=1}^3 c_j^2 \left( \frac{\cosh s_j \beta/2 - \cos s_j(u)}{\sinh s_j \beta/2} \right) \quad (5.87)$$

$$D_{\parallel}(u) = \frac{1}{2m} \frac{w_{\parallel}^2}{v_{\parallel}^2} \left[ \left( \frac{v_{\parallel}^2 - w_{\parallel}^2}{v_{\parallel} w_{\parallel}^2} \right) \frac{\cosh v_{\parallel} \beta/2 - \cos v_{\parallel}(u)}{\sinh v_{\parallel} \beta/2} + \frac{\beta}{4} + \frac{u^2}{\beta} \right] \quad (5.88)$$

The dc mobility for the polaron is given by

$$\begin{pmatrix} 1/\mu_{\perp} \\ 1/\mu_{\parallel} \end{pmatrix} = \lim_{\omega \rightarrow 0} \begin{pmatrix} \frac{\text{Im}\chi_{\perp}(\omega)}{\omega} \\ \frac{\text{Im}\chi_{\parallel}(\omega)}{\omega} \end{pmatrix} \quad (5.89)$$

Our result Eq(5.85), therefore, gives the mobility in the direction parallel and perpendicular with the magnetic field as

$$\begin{pmatrix} 1/\mu_{\perp} \\ 1/\mu_{\parallel} \end{pmatrix} = \frac{\beta}{2} \int_0^{\infty} \begin{pmatrix} \Sigma_{\perp}(u) du \\ \Sigma_{\parallel}(u) du \end{pmatrix} \quad (5.90)$$

where

$$\text{Im}\chi_{\parallel}(\omega) = \sinh(\beta\omega/2) \int_0^{\infty} \cos(\omega u) \Sigma_{\parallel}(u) du \quad (5.91)$$

$$\Sigma_{\parallel}(u) = \int \frac{d^3k}{(2\pi)^3} |C_{\mathbf{k}}|^2 k_z^2 \frac{\cos(u)}{\sinh(\beta/2)} e^{-k_{\perp}^2 D_{\perp}(u)} e^{-k_z^2 D_{\parallel}(u)}$$

$$\begin{aligned}
 &= \frac{2\alpha}{\sqrt{\pi}} \frac{\cos(u)}{\sinh(\beta/2)} \frac{1}{\left(D_{\parallel}(u) - D_{\perp}(u)\right)^{3/2}} \\
 &\quad \left\{ \ln \left[ \frac{\sqrt{D_{\parallel}(u)} + \sqrt{D_{\parallel}(u) - D_{\perp}(u)}}{\sqrt{D_{\parallel}(u)} - \sqrt{D_{\parallel}(u) - D_{\perp}(u)}} \right] - 2 \frac{\sqrt{D_{\parallel}(u) - D_{\perp}(u)}}{\sqrt{D_{\parallel}(u)}} \right\} \quad (5.92)
 \end{aligned}$$

We now introduce

$$\text{Im}\chi(\omega) = \sinh(\beta\omega/2) \int_0^{\infty} \cos(\omega u) \Sigma(u) du \quad (5.93)$$

where

$$\begin{aligned}
 \Sigma(u) &= \int \frac{d^3k}{(2\pi)^3} |C_{\mathbf{k}}|^2 k^2 2 \frac{\cos(u)}{\sinh(\beta/2)} e^{-k_{\perp}^2 D_{\perp}(u)} e^{-k_{\parallel}^2 D_{\parallel}(u)} \\
 &= \frac{2\alpha}{\sqrt{\pi}} \frac{\cos(u)}{\sinh(\beta/2)} \frac{1}{D_{\perp}(u) \sqrt{D_{\parallel}(u)}} \quad (5.94)
 \end{aligned}$$

and

$$\text{Im}\chi_{\perp}(\omega) = \frac{\text{Im}\chi(\omega) - \text{Im}\chi_{\parallel}(\omega)}{2} \quad (5.95)$$

It is very easily to show that in the limit of zero magnetic field  $D_{\perp} \rightarrow D_{\parallel}$  and correspondingly  $\text{Im}\chi(\omega) \rightarrow \frac{3}{2}\text{Im}\chi_{\parallel}(\omega)$ . This implies

$$\text{Im}\chi_{\perp}(\omega) \rightarrow \text{Im}\chi_{\parallel}(\omega) = \frac{2\alpha}{3\sqrt{\pi}} \frac{\sinh(\beta\omega/2)}{\sinh(\beta/2)} \int_0^{\infty} \frac{\cos(\omega u) \cos u du}{D_{\parallel}^{3/2}(u)} \quad (5.96)$$

which is the result of FHIP.

For zero magnetic field, FHIP calculated  $\text{Im}\chi(\omega)$  at  $\beta = 100$ . By contrast the  $\alpha = 3$  and  $\alpha = 5$  results show that  $\text{Im}\chi(\omega)$  is relatively smooth in  $\omega$ , whereas for  $\alpha = 7$ , relatively sharp peaks occur at  $\omega \simeq m\nu + 1$ ,  $m = 0, 1, 2, 3, \dots$ . For  $m = 0$  these correspond to the absorption of quanta by the polaron and the subsequent emission of a optical phonon, the polaron remaining in the ground state. For  $m = 1$ , the series might represent the polaron excited in addition to the emission of a phonon, etc (see more details in reference [38]). This result is reproduced by F.M. Peeters and J.T. Devreese [39] with the Heisenberg operator method.

For non-zero magnetic field, our expressions  $\chi_{\parallel}(\omega)$  and  $\chi_{\perp}(\omega)$  agree with reference [40] where they are called memory functions. In this reference three independent configurations were of interest.

- i) Voigt configuration: The corresponding memory function is denoted by  $\chi_{\parallel}(\omega)$  and gives the linear response to an electric field parallel to the magnetic field.
- ii) Faraday configuration for the cyclotron resonance active mode( $+\omega_c$ ): The memory function in this case  $\chi_{\perp}(\omega)$  describes the response to circular polarized light along the z-axis (which leads to an electric field perpendicular to the  $\mathbf{B}$  field)
- iii) Faraday configuration for the cyclotron resonance inactive mode( $-\omega_c$ ): The memory function in this case is given by  $-\chi_{\perp}(-\omega)$ .

They also obtained the numerical results for the imaginary part of these functions as in FHIP. To compute the imaginary part of the memory functions Eq(5.91) and Eq(5.95), they suggested that the integrand of the integral of Eq(5.91) and Eq(5.95) consists of a factor which decreases slowly where  $u \rightarrow \infty$  superimposed on a rapidly oscillating component. As a consequence this representation for the imaginary part of the memory functions  $\text{Im}\chi_{\parallel}(\omega)$  and  $\text{Im}\chi_{\perp}(\omega)$  is not suitable for numerical programming. They presented another representation which it is more suitable for numerical work.

## CHAPTER 6

### CONCLUSION

We derived the propagator for a particle subjected to a local oscillator, an electromagnetic field and being under the influence of a one non-local oscillator (memory potential). For the exact calculations of the corresponding path integral the classical paths were determined explicitly.

In reference [24], it was shown that the Feynman-Jensen inequality failed to apply for a particle in a magnetic field. An alternative method was proposed by J.D. Devreese and F. Brosens. They derived the analytic result. We compared some of our numerical results which were better than PD [21].

For the polaron motion in an applied field, we treated the motion of an electron in a polarizable crystal under the influence of an electric field and a magnetic field. Starting with the crystal in thermal dynamic equilibrium, the electron was injected with zero velocity, and its subsequent steady-state motion was determined using two methods. For the first approach, in contrast to Thornber method (the method of rates), we started from the expectation value of displacement of the electron and then carry out a perturbation approach similar to that of FHIP. The time derivative gave the steady-state velocity. In the other approach, we used a single path integral to obtain the steady-state condition. The essential approximation to derive this lied in the procedure to calculate  $\langle S_{pol} - S_{trial} \rangle$ . In both cases no approximation regarding the field strength, velocity, lattice coupling constant, or temperature was ever made. However, the part of the action describing the electron-lattice interaction was approximated as close as possible to physical reality, and an expansion in the difference of the exact and approximate actions were combined in manners suggested by the exact solution of similar problems.

At low-frequency of the electric field, we did not impose the steady-state. We found the self-consistent relationship between  $\vec{\mathbf{G}}$ ,  $\vec{\mathbf{L}}$  and  $\vec{\mathbf{Z}}$  that agrees with Thornber [20]. We also expressed the effective mass and the mobility of the polaron in the magnetic field.

Finally, we also calculated the dissipation as in FHIP for the polaron in the magnetic field which agreed with that of reference [40]. We may improve the accuracy of the numerical results in reference [40] by using our numerical data  $(v_{\perp}, w_{\perp}, v_{\parallel}, w_{\parallel})$  which were got from minimizing the upper bound ground-state energy based on Devreese's assumption.

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## APPENDIX A

### THE CALCULATION OF THE DOUBLE PATH

In this Appendix we evaluate

$$I = \int \int e^{\tilde{\Phi}_0(\dot{\mathbf{r}}, \mathbf{r}, \dot{\mathbf{r}}', \mathbf{r}', \tau)} D[\mathbf{r}_\tau] D[\mathbf{r}'_\tau] \quad (\text{A.1})$$

where

$$\tilde{\Phi}_0(\dot{\mathbf{r}}, \mathbf{r}, \dot{\mathbf{r}}', \mathbf{r}', \tau) = S_0(\dot{\mathbf{r}}, \mathbf{r}, \tau) - S'_0(\dot{\mathbf{r}}', \mathbf{r}', \tau) - \tilde{\Phi}(\mathbf{r}, \mathbf{r}', \tau, \sigma), \quad (\text{A.2})$$

$$S_0(\dot{\mathbf{r}}, \mathbf{r}, \tau) = \int_{-\infty}^{\infty} d\tau \left( \frac{m}{2} \dot{\mathbf{r}}_\tau \cdot \dot{\mathbf{r}}_\tau - \frac{m\omega_0^2}{2} \mathbf{r}_\tau \cdot \mathbf{r}_\tau + \frac{1}{2} \dot{\mathbf{r}}_\tau \cdot \boldsymbol{\epsilon} \cdot \mathbf{B} \cdot \mathbf{r}_\tau + \mathbf{f}_\tau \cdot \mathbf{r}_\tau \right), \quad (\text{A.3})$$

$$S'_0(\dot{\mathbf{r}}', \mathbf{r}', \tau) = \int_{-\infty}^{\infty} d\tau \left( \frac{m}{2} \dot{\mathbf{r}}'_\tau \cdot \dot{\mathbf{r}}'_\tau - \frac{m\omega_0^2}{2} \mathbf{r}'_\tau \cdot \mathbf{r}'_\tau + \frac{1}{2} \dot{\mathbf{r}}'_\tau \cdot \boldsymbol{\epsilon} \cdot \mathbf{B} \cdot \mathbf{r}'_\tau + \mathbf{f}'_\tau \cdot \mathbf{r}'_\tau \right), \quad (\text{A.4})$$

$$\tilde{\Phi}(\mathbf{r}, \mathbf{r}', \tau, \sigma) = \tilde{\Phi}_1(\mathbf{r}'_\tau, \mathbf{r}'_\sigma) + \tilde{\Phi}_2(\mathbf{r}_\tau, \mathbf{r}_\sigma) + \tilde{\Phi}_3(\mathbf{r}_\tau, \mathbf{r}'_\sigma) + \tilde{\Phi}_4(\mathbf{r}'_\tau, \mathbf{r}_\sigma), \quad (\text{A.5})$$

$$\tilde{\Phi}_1(\mathbf{r}'_\tau, \mathbf{r}'_\sigma) = i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\tau} d\sigma \left( (\mathbf{r}'_\tau - \mathbf{r}'_\sigma) \cdot \vec{\mathbf{G}}(\Omega) \cdot (\mathbf{r}'_\tau - \mathbf{r}'_\sigma) \right) e^{i\Omega(\tau-\sigma)}, \quad (\text{A.6})$$

$$\tilde{\Phi}_2(\mathbf{r}_\tau, \mathbf{r}_\sigma) = i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\tau} d\sigma \left( (\mathbf{r}_\tau - \mathbf{r}_\sigma) \cdot \vec{\mathbf{G}}(\Omega) \cdot (\mathbf{r}_\tau - \mathbf{r}_\sigma) \right) e^{-i\Omega(\tau-\sigma)} \quad (\text{A.7})$$

$$\tilde{\Phi}_3(\mathbf{r}_\tau, \mathbf{r}'_\sigma) = i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\tau} d\sigma \left( (\mathbf{r}_\tau - \mathbf{r}'_\sigma) \cdot \vec{\mathbf{G}}(\Omega) \cdot (\mathbf{r}_\tau - \mathbf{r}'_\sigma) \right) e^{i\Omega(\tau-\sigma)}, \quad (\text{A.8})$$

$$\tilde{\Phi}_4(\mathbf{r}'_\tau, \mathbf{r}_\sigma) = i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\tau} d\sigma \left( (\mathbf{r}'_\tau - \mathbf{r}_\sigma) \cdot \vec{\mathbf{G}}(\Omega) \cdot (\mathbf{r}'_\tau - \mathbf{r}_\sigma) \right) e^{-i\Omega(\tau-\sigma)} \quad (\text{A.9})$$

$\boldsymbol{\epsilon}$  is the third-rank totally antisymmetric tensor. The expression  $\mathbf{a} \cdot \boldsymbol{\epsilon} \cdot \mathbf{b} \cdot \mathbf{c}$  is defined in perfect analogy to  $\mathbf{a} \cdot \mathbf{b} \times \mathbf{c} = a_i \epsilon_{ijk} b_j c_k$ . Now we express  $\mathbf{r}_\tau$ ,  $\mathbf{r}'_\tau$ ,  $\mathbf{f}_\tau$  and  $\mathbf{f}'_\tau$  by their Fourier transform

$$\mathbf{r}_\nu = \int_{-\infty}^{\infty} d\tau \mathbf{r}_\tau e^{i\nu\tau} \quad , \quad \mathbf{f}_\nu = \int_{-\infty}^{\infty} d\tau \mathbf{f}_\tau e^{i\nu\tau} \quad (\text{A.10})$$

and

$$\mathbf{r}_\tau = \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \mathbf{r}_\nu e^{-i\nu\tau} \quad , \quad \mathbf{f}_\tau = \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \mathbf{f}_\nu e^{-i\nu\tau} \quad (\text{A.11})$$

Consider

$$\begin{aligned}
& S_0(\dot{\mathbf{r}}, \mathbf{r}, \tau) \\
&= \int_{-\infty}^{\infty} d\tau \left\{ \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} \frac{d\nu'}{2\pi} \nu\nu' m\mathbf{r}_\nu \cdot \mathbf{r}_{\nu'} e^{i(\nu+\nu')\tau} - \frac{\omega_0^2}{2} \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} \frac{d\nu'}{2\pi} m\mathbf{r}_\nu \cdot \mathbf{r}_{\nu'} e^{i(\nu+\nu')\tau} \right. \\
&\quad \left. + \frac{i}{2} \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} \frac{d\nu'}{2\pi} \nu\mathbf{r}_\nu \cdot \mathbf{B} \cdot \mathbf{r}_{\nu'} e^{i(\nu+\nu')\tau} + \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} \frac{d\nu'}{2\pi} \mathbf{f}_\nu \cdot \mathbf{r}_{\nu'} e^{i(\nu+\nu')\tau} \right\} \\
&= \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} d\nu' \int_{-\infty}^{\infty} \frac{d\tau}{2\pi} \left\{ \frac{\nu\nu'}{2} m\mathbf{r}_\nu \cdot \mathbf{r}_{\nu'} - \frac{m\omega_0^2}{2} \mathbf{r}_\nu \cdot \mathbf{r}_{\nu'} \right. \\
&\quad \left. + \frac{i\nu}{2} \mathbf{r}_\nu \cdot \mathbf{B} \cdot \mathbf{r}_{\nu'} + \mathbf{f}_\nu \cdot \mathbf{r}_{\nu'} \right\} e^{i(\nu+\nu')\tau} \\
&= \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} d\nu' \left\{ \frac{\nu\nu'}{2} m\mathbf{r}_\nu \cdot \mathbf{r}_{\nu'} - \frac{m\omega_0^2}{2} \mathbf{r}_\nu \cdot \mathbf{r}_{\nu'} \right. \\
&\quad \left. + \frac{i\nu}{2} \mathbf{r}_\nu \cdot \mathbf{B} \cdot \mathbf{r}_{\nu'} + \mathbf{f}_\nu \cdot \mathbf{r}_{\nu'} \right\} \delta(\nu + \nu') \\
&= \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \left\{ -\frac{\nu^2}{2} m\mathbf{r}_\nu \cdot \mathbf{r}_{-\nu} - \frac{m\omega_0^2}{2} \mathbf{r}_\nu \cdot \mathbf{r}_{-\nu} + \frac{i\nu}{2} \mathbf{r}_\nu \cdot \mathbf{B} \cdot \mathbf{r}_{-\nu} + \mathbf{f}_\nu \cdot \mathbf{r}_{-\nu} \right\} \quad (\text{A.12})
\end{aligned}$$

so that we can express  $S'_0$  as

$$S'_0(\mathbf{r}', \mathbf{r}', \tau) = \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \left\{ -\frac{\nu^2}{2} m\mathbf{r}'_\nu \cdot \mathbf{r}'_{-\nu} - \frac{m\omega_0^2}{2} \mathbf{r}'_\nu \cdot \mathbf{r}'_{-\nu} + \frac{i\nu}{2} \mathbf{r}'_\nu \cdot \mathbf{B} \cdot \mathbf{r}'_{-\nu} + \mathbf{f}'_\nu \cdot \mathbf{r}'_{-\nu} \right\} \quad (\text{A.13})$$

Next we consider

$$\begin{aligned}
\tilde{\Phi}_1(\mathbf{r}'_\tau, \mathbf{r}'_\sigma) &= i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\tau} d\sigma \left\{ \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} \frac{d\nu'}{2\pi} (\mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{\nu'}) e^{i(\nu+\nu')\tau} e^{i\Omega(\tau-\sigma)} \right. \\
&\quad - \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{\nu'} e^{i\nu'\tau} e^{i\nu\sigma} e^{i\Omega(\tau-\sigma)} - \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{\nu'} e^{i\nu\tau} e^{i\nu'\sigma} e^{i\Omega(\tau-\sigma)} \\
&\quad \left. + \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{\nu'} e^{i(\nu+\nu')\sigma} e^{i\Omega(\tau-\sigma)} \right\} \quad (\text{A.14})
\end{aligned}$$

Using the symmetry of  $\vec{\mathbf{G}}(\Omega)$ , eq(A.14) becomes

$$\begin{aligned}
&= i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\tau} d\sigma \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} \frac{d\nu'}{2\pi} \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{\nu'} \left\{ e^{i(\nu+\nu'+\Omega)\tau} e^{-i\Omega\sigma} \right. \\
&\quad \left. - 2e^{i(\nu-\Omega)\tau} e^{-i(\nu'+\Omega)\sigma} + e^{i(\nu+\nu'-\Omega)\sigma} e^{i\Omega\tau} \right\} \\
&= i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} \frac{d\nu'}{2\pi} \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{\nu'} \left\{ \frac{e^{i(\nu+\nu'+\Omega)\tau} e^{-i\Omega\sigma}}{-i\Omega} \right\} \Bigg|_{-\infty}^{\tau}
\end{aligned}$$

$$\begin{aligned}
 & - \frac{2e^{i(\nu-\Omega)\tau} e^{-i(\nu'+\Omega)\sigma}}{i(\nu-\Omega)} \Big|_{-\infty}^{\tau} + \frac{e^{i(\nu+\nu'-\Omega)\sigma} e^{i\Omega\tau}}{i(\nu+\nu'-\Omega)} \Big|_{-\infty}^{\tau} \Big\} \\
 = & i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} \frac{d\nu'}{2\pi} \mathbf{r}'_{\nu} \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{\nu'} e^{i(\nu+\nu)\tau} \left\{ -\frac{1}{\Omega} - \frac{2}{\nu-\Omega} \right. \\
 & \left. + \frac{1}{\nu+\nu'+\Omega} \right\} \\
 = & i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \mathbf{r}'_{\nu} \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{-\nu} \left\{ -\frac{1}{\Omega} - \frac{2}{\nu-\Omega} + \frac{1}{\Omega} \right\} \\
 = & 2 \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \mathbf{r}'_{\nu} \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{-\nu} \frac{\nu}{\Omega(\Omega-\nu)} \tag{A.15}
 \end{aligned}$$

A quick inspection shows that the integration has a pole at  $\nu = +\Omega$ . Therefore, we must specify a contour in the complex  $\nu$ -plane in order to evaluate the integral. We choose an enclosing the contour in the upper half plane above the real axis of  $\nu$ . So Eq(A.15) becomes

$$\tilde{\Phi}_1(\mathbf{r}'_{\tau}, \mathbf{r}'_{\sigma}) = 2 \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \mathbf{r}'_{\nu} \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{-\nu} \frac{\nu}{\Omega(\Omega-\nu+i\varepsilon)} \tag{A.16}$$

Next we consider

$$\begin{aligned}
 \tilde{\Phi}_2(\mathbf{r}_{\tau}, \mathbf{r}_{\sigma}) & = i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\tau} d\sigma \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} \frac{d\nu'}{2\pi} \mathbf{r}'_{\nu} \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{\nu'} \left\{ e^{i(\nu+\nu'-\Omega)\tau} e^{i\Omega\sigma} \right. \\
 & \left. - 2e^{i(\nu+\Omega)\tau} e^{-i(\nu'-\Omega)\sigma} + e^{i(\nu+\nu'+\Omega)\tau} e^{-i\Omega\sigma} \right\} \\
 & = i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} \frac{d\nu'}{2\pi} \mathbf{r}'_{\nu} \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{\nu'} \left\{ \frac{e^{i(\nu+\nu'-\Omega)\tau} e^{i\Omega\sigma}}{i\Omega} \Big|_{-\infty}^{\tau} \right. \\
 & \left. - \frac{2e^{i(\nu+\Omega)\tau} e^{-i(\nu'-\Omega)\sigma}}{i(\nu+\Omega)} \Big|_{-\infty}^{\tau} + \frac{e^{i(\nu+\nu'+\Omega)\sigma} e^{-i\Omega\tau}}{i(\nu+\nu'+\Omega)} \Big|_{-\infty}^{\tau} \right\} \\
 & = i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} \frac{d\nu'}{2\pi} \mathbf{r}'_{\nu} \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{\nu'} e^{i(\nu+\nu)\tau} \left\{ \frac{1}{\Omega} - \frac{2}{\nu+\Omega} \right. \\
 & \left. + \frac{1}{\nu+\nu'+\Omega} \right\} \\
 & = i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \mathbf{r}'_{\nu} \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{-\nu} \left\{ \frac{1}{\Omega} - \frac{2}{\nu+\Omega} + \frac{1}{\Omega} \right\} \\
 & = 2 \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \mathbf{r}'_{\nu} \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{-\nu} \frac{\nu}{\Omega(\Omega+\nu-i\varepsilon)} \tag{A.17}
 \end{aligned}$$

Next we consider

$$\begin{aligned}
\tilde{\Phi}_3(\mathbf{r}_\tau, \mathbf{r}'_\sigma) &= i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\tau} d\sigma \left\{ \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} \frac{d\nu'}{2\pi} (\mathbf{r}_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{\nu'} e^{i(\nu+\nu'+\Omega)\tau} e^{-i\Omega\sigma} \right. \\
&\quad \left. - 2\mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{\nu'} e^{i(\nu'-\Omega)\tau} e^{i(\nu-\Omega)\sigma} + \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{\nu'} e^{i(\nu+\nu'-\Omega)\tau} e^{i\Omega\sigma} \right\} \\
&= i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} \frac{d\nu'}{2\pi} \left\{ \mathbf{r}_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{\nu'} \frac{e^{i(\nu+\nu'+\Omega)\tau} e^{-i\Omega\sigma}}{-i\Omega} \Big|_{-\infty}^{\tau} \right. \\
&\quad \left. + \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{\nu'} \frac{e^{i(\nu+\nu'-\Omega)\tau} e^{i\Omega\sigma}}{i(\nu+\nu'-\Omega)} \Big|_{-\infty}^{\tau} \right\} \\
&\quad - 2i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} d\sigma \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} \frac{d\nu'}{2\pi} \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{\nu'} e^{i(\nu-\Omega)\sigma} e^{i(\nu'+\Omega)\tau} \\
&= \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \left\{ -\mathbf{r}_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{-\nu} \frac{1}{\Omega} - \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{-\nu} \frac{1}{\Omega} \right\} \\
&\quad - 2i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} d\sigma \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} \frac{d\nu'}{2\pi} \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{\nu'} \delta(\nu' + \Omega) e^{i(\nu-\Omega)\sigma} \\
&= - \int_{-\infty}^{\infty} \frac{d\Omega}{\Omega} \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \left\{ \mathbf{r}_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{-\nu} + \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{-\nu} \right\} \\
&\quad - 2i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} d\sigma \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} d\nu' \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{\nu'} e^{i(\nu+\nu')\sigma} \\
&= - \int_{-\infty}^{\infty} \frac{d\Omega}{\Omega} \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \left\{ \mathbf{r}_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{-\nu} + \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{-\nu} \right\} \\
&\quad - 2i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} d\nu \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{\nu'} \delta(\nu + \nu') \\
&= - \int_{-\infty}^{\infty} \frac{d\Omega}{\Omega} \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \left\{ \mathbf{r}_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{-\nu} + \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{-\nu} \right\} \\
&\quad - 4\pi i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{-\nu} \delta(\nu - \Omega) \tag{A.18}
\end{aligned}$$

and

$$\begin{aligned}
\tilde{\Phi}_4(\mathbf{r}'_\tau, \mathbf{r}_\sigma) &= i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\tau} d\sigma \left\{ \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} \frac{d\nu'}{2\pi} (\mathbf{r}_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{\nu'} e^{i(\nu+\nu'-\Omega)\tau} e^{i\Omega\sigma} \right. \\
&\quad \left. - 2\mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{\nu'} e^{i(\nu'+\Omega)\tau} e^{i(\nu+\Omega)\sigma} + \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{\nu'} e^{i(\nu+\nu'+\Omega)\tau} e^{-i\Omega\sigma} \right\} \\
&= \int_{-\infty}^{\infty} \frac{d\Omega}{\Omega} \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \left\{ \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{-\nu} + \mathbf{r}_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{-\nu} \right\}
\end{aligned}$$

$$+4\pi i \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \mathbf{r}'_{\nu} \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{-\nu} \delta(\nu + \Omega) \quad (\text{A.19})$$

Using Eqs(A.12), (A.13), (A.17), (A.18), (A.19) and (A.20), Eq (A.1) becomes

$$I = \iint e^{i\tilde{\Phi}'_0(\mathbf{r}_{\nu}, \mathbf{r}_{-\nu}, \mathbf{r}'_{\nu}, \mathbf{r}'_{-\nu})} D[\mathbf{r}_{\nu}] D[\mathbf{r}_{-\nu}] D[\mathbf{r}'_{\nu}] D[\mathbf{r}'_{-\nu}] \quad (\text{A.20})$$

where

$$\begin{aligned} \tilde{\Phi}'_0(\mathbf{r}_{\nu}, \mathbf{r}_{-\nu}, \mathbf{r}'_{\nu}, \mathbf{r}'_{-\nu}) &= \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \{L_0(\mathbf{r}_{\nu}, \mathbf{r}_{-\nu}) - L'_0(\mathbf{r}_{\nu}, \mathbf{r}_{-\nu})\} \\ &+ 2 \int_{-\infty}^{\infty} d\Omega \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \Xi(\mathbf{r}_{\nu}, \mathbf{r}_{-\nu}, \mathbf{r}'_{\nu}, \mathbf{r}'_{-\nu}) \end{aligned} \quad (\text{A.21})$$

and

$$L_0(\mathbf{r}_{\nu}, \mathbf{r}_{-\nu}) = -\frac{m\nu^2}{2} \mathbf{r}_{\nu} \cdot \mathbf{r}_{-\nu} - \frac{m\omega_0^2}{2} \mathbf{r}_{\nu} \cdot \mathbf{r}_{-\nu} + \frac{i\nu}{2} \mathbf{r}_{\nu} \cdot \mathbf{E} \cdot \mathbf{r}_{-\nu} + \mathbf{f}_{\nu} \cdot \mathbf{r}_{-\nu} \quad (\text{A.22})$$

$$L'_0(\mathbf{r}_{\nu}, \mathbf{r}_{-\nu}) = -\frac{m\nu^2}{2} \mathbf{r}'_{\nu} \cdot \mathbf{r}'_{-\nu} - \frac{m\omega_0^2}{2} \mathbf{r}'_{\nu} \cdot \mathbf{r}'_{-\nu} + \frac{i\nu}{2} \mathbf{r}'_{\nu} \cdot \mathbf{E} \cdot \mathbf{r}'_{-\nu} + \mathbf{f}'_{\nu} \cdot \mathbf{r}'_{-\nu} \quad (\text{A.23})$$

$$\begin{aligned} \Xi(\mathbf{r}_{\nu}, \mathbf{r}_{-\nu}, \mathbf{r}'_{\nu}, \mathbf{r}'_{-\nu}) &= \mathbf{r}'_{\nu} \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_{-\nu} \frac{\nu}{\Omega(\Omega - \nu + i\varepsilon)} - \mathbf{r}_{\nu} \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{-\nu} \frac{\nu}{\Omega(\Omega + \nu - i\varepsilon)} \\ &- 2\pi i \mathbf{r}_{\nu} \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_{-\nu} (\delta(\nu - \Omega) + \delta(\nu + \Omega)) \end{aligned} \quad (\text{A.24})$$

We note that since  $\mathbf{r}_{\tau}, \mathbf{r}'_{\tau}, \mathbf{f}_{\tau}$  and  $\mathbf{f}'_{\tau}$  are real,  $\mathbf{r}_{\nu} \equiv \mathbf{r}_{-\nu}^*, \mathbf{f}_{\nu} \equiv \mathbf{f}_{-\nu}^*$ . Thus by changing

$\int_{-\infty}^{\infty} d\nu \rightarrow \int_0^{\infty} d\nu$ , we have

$$\begin{aligned} \tilde{\Phi}'_0(\mathbf{r}_{\nu}, \mathbf{r}_{-\nu}, \mathbf{r}'_{\nu}, \mathbf{r}'_{-\nu}) &= \int_{-\infty}^0 \frac{d\nu}{2\pi} L_0(\mathbf{r}_{\nu}, \mathbf{r}_{-\nu}) + \int_0^{-\infty} \frac{d\nu}{2\pi} L_0(\mathbf{r}_{\nu}, \mathbf{r}_{-\nu}) \\ &- \int_{-\infty}^0 \frac{d\nu}{2\pi} L'_0(\mathbf{r}_{\nu}, \mathbf{r}_{-\nu}) - \int_0^{-\infty} \frac{d\nu}{2\pi} L'_0(\mathbf{r}_{\nu}, \mathbf{r}_{-\nu}) \\ &+ 2 \int_{-\infty}^0 d\Omega \left( \int_{-\infty}^0 \frac{d\nu}{2\pi} \Xi(\mathbf{r}_{\nu}, \mathbf{r}_{-\nu}, \mathbf{r}'_{\nu}, \mathbf{r}'_{-\nu}) + \int_0^{\infty} \frac{d\nu}{2\pi} \Xi(\mathbf{r}_{\nu}, \mathbf{r}_{-\nu}, \mathbf{r}'_{\nu}, \mathbf{r}'_{-\nu}) \right) \\ &+ 2 \int_0^{\infty} d\Omega \left( \int_{-\infty}^0 \frac{d\nu}{2\pi} \Xi(\mathbf{r}_{\nu}, \mathbf{r}_{-\nu}, \mathbf{r}'_{\nu}, \mathbf{r}'_{-\nu}) + \int_0^{\infty} \frac{d\nu}{2\pi} \Xi(\mathbf{r}_{\nu}, \mathbf{r}_{-\nu}, \mathbf{r}'_{\nu}, \mathbf{r}'_{-\nu}) \right) \end{aligned} \quad (\text{A.25})$$

We consider

$$\begin{aligned}
\int_{-\infty}^0 \frac{d\nu}{2\pi} L_0(\mathbf{r}_\nu, \mathbf{r}_{-\nu}) &= \int_0^{\infty} \frac{d\nu}{2\pi} \left\{ -\frac{m\nu^2}{2} \mathbf{r}_\nu \cdot \mathbf{r}_{-\nu} - \frac{m\omega_0^2}{2} \mathbf{r}_\nu \cdot \mathbf{r}_{-\nu} + \frac{i\nu}{2} \mathbf{r}_\nu \cdot \in \cdot \mathbf{B} \cdot \mathbf{r}_{-\nu} \right. \\
&\quad \left. + \mathbf{f}_\nu \cdot \mathbf{r}_{-\nu} \right\}^* \\
&= \int_0^{\infty} \frac{d\nu}{2\pi} \left\{ -\frac{m\nu^2}{2} \mathbf{r}_{-\nu}^* \cdot \mathbf{r}_\nu^* - \frac{m\omega_0^2}{2} \mathbf{r}_{-\nu}^* \cdot \mathbf{r}_\nu^* + \frac{i\nu}{2} \mathbf{r}_{-\nu}^* \cdot \in \cdot \mathbf{B} \cdot \mathbf{r}_\nu^* \right. \\
&\quad \left. + \mathbf{r}_{-\nu}^* \cdot \mathbf{f}_\nu^* \right\} \\
&= \int_0^{\infty} \frac{d\nu}{2\pi} \left\{ -\frac{m\nu^2}{2} \mathbf{r}_\nu \cdot \mathbf{r}_\nu^* - \frac{m\omega_0^2}{2} \mathbf{r}_\nu \cdot \mathbf{r}_\nu^* + \frac{i\nu}{2} \mathbf{r}_\nu \cdot \in \cdot \mathbf{B} \cdot \mathbf{r}_\nu^* \right. \\
&\quad \left. + \mathbf{r}_\nu \cdot \mathbf{f}_\nu^* \right\} \tag{A.26}
\end{aligned}$$

and

$$\begin{aligned}
\int_{-\infty}^0 \frac{d\nu}{2\pi} \Xi(\mathbf{r}_\nu, \mathbf{r}_{-\nu}, \mathbf{r}'_\nu, \mathbf{r}'_{-\nu}) &= \int_0^{\infty} \frac{d\nu}{2\pi} \Xi^*(\mathbf{r}_\nu, \mathbf{r}_{-\nu}, \mathbf{r}'_\nu, \mathbf{r}'_{-\nu}) \\
&= \int_0^{\infty} \frac{d\nu}{2\pi} \left\{ \mathbf{r}'_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}'_\nu^* \frac{\nu}{\Omega(\Omega - \nu - i\varepsilon)} \right. \\
&\quad \left. - \mathbf{r}_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_\nu^* \frac{\nu}{\Omega(\Omega + \nu + i\varepsilon)} \right. \\
&\quad \left. + 2\pi i \mathbf{r}_\nu \cdot \vec{\mathbf{G}}(\Omega) \cdot \mathbf{r}_\nu^* (\delta(\nu - \Omega) + \delta(\nu + \Omega)) \right\} \tag{A.27}
\end{aligned}$$

Using the results of Eq(A.26) and Eq(A.27), we obtain

$$I = \int \int e^{i\tilde{\Phi}_0''(\mathbf{r}_\nu, \mathbf{r}_\nu^*, \mathbf{r}'_\nu, \mathbf{r}'_\nu^*)} D[\mathbf{r}_\nu] D[\mathbf{r}_\nu^*] D[\mathbf{r}'_\nu] D[\mathbf{r}'_\nu^*] \tag{A.28}$$

where

$$\begin{aligned}
\tilde{\Phi}_0''(\mathbf{r}_\nu, \mathbf{r}_\nu^*, \mathbf{r}'_\nu, \mathbf{r}'_\nu^*) &= \int_0^{\infty} \frac{d\nu}{2\pi} \left( \mathbf{r}_\nu^* \cdot \mathbf{f}_\nu + \mathbf{f}_\nu^* \cdot \mathbf{r}_\nu - \mathbf{r}'_\nu \cdot \mathbf{f}'_\nu - \mathbf{f}'_\nu \cdot \mathbf{r}'_\nu - \mathbf{r}'_\nu \cdot \left[ \vec{\mathbf{Z}}_+^* - \vec{\mathbf{Z}}_+ \right] \cdot \mathbf{r}_\nu \right. \\
&\quad \left. - \mathbf{r}_\nu^* \cdot \left[ \vec{\mathbf{Z}}_-^* - \vec{\mathbf{Z}}_- \right] \cdot \mathbf{r}' + \mathbf{r}_\nu^* \cdot \left[ -\vec{\mathbf{Z}}_+ - \vec{\mathbf{Z}}_- + i\nu \in \cdot \mathbf{B} \right] \cdot \mathbf{r}_\nu \right. \\
&\quad \left. - \mathbf{r}'_\nu \cdot \left[ -\vec{\mathbf{Z}}_+ - \vec{\mathbf{Z}}_- + i\nu \in \cdot \mathbf{B} \right] \cdot \mathbf{r}'_\nu \right) \tag{A.29}
\end{aligned}$$

and

$$\vec{\mathbf{Z}}_+ = -\frac{m}{2} \nu^2 \vec{\mathbf{I}} - \frac{m\omega_0^2}{2} \vec{\mathbf{I}} - 4\nu^2 \int_0^{\infty} \frac{d\Omega}{\Omega} \frac{\vec{\mathbf{G}}(\Omega)}{(\Omega - i\varepsilon)^2 - \nu^2} \tag{A.30}$$

$$\vec{\mathbf{Z}}_- = -\frac{m}{2} \nu^2 \vec{\mathbf{I}} - \frac{m\omega_0^2}{2} \vec{\mathbf{I}} - 4\nu^2 \int_{-\infty}^0 \frac{d\Omega}{\Omega} \frac{\vec{\mathbf{G}}(\Omega)}{(\Omega - i\varepsilon)^2 - \nu^2} \tag{A.31}$$

where  $\vec{\mathbf{I}}$  is the identity tensor. Next we perform the integral in Eq(A.28)

$$\begin{aligned}
 I &= \int \left\{ \exp \left( -i \int_0^\infty \frac{d\nu}{2\pi} (-\mathbf{r}'_{\nu^*} \cdot \mathbf{f}'_{\nu} - \mathbf{f}'_{\nu} \cdot \mathbf{r}'_{\nu} - \mathbf{r}'_{\nu^*} \cdot \vec{\mathbf{Z}}_2 \cdot \mathbf{r}'_{\nu}) \right) \right. \\
 &\quad \times \int \exp \left( i \int_0^\infty \frac{d\nu}{2\pi} (\mathbf{r}'_{\nu} \cdot \vec{\mathbf{Z}}_1 \cdot \mathbf{r}_{\nu} - [\mathbf{r}'_{\nu^*} \cdot (\vec{\mathbf{Z}}_+^* - \vec{\mathbf{Z}}_+) + \mathbf{f}'_{\nu^*}] \cdot \mathbf{r}_{\nu} \right. \\
 &\quad \left. \left. - \mathbf{r}'_{\nu^*} \cdot [(\vec{\mathbf{Z}}_-^* - \vec{\mathbf{Z}}_-) \cdot \mathbf{r}' - \mathbf{f}_{\nu}] \right) D[\mathbf{r}_{\nu}] D[\mathbf{r}'_{\nu}] \right\} D[\mathbf{r}'_{\nu}] D[\mathbf{r}'_{\nu^*}] \quad (\text{A.32})
 \end{aligned}$$

where

$$\vec{\mathbf{Z}}_1 = -\vec{\mathbf{Z}}_+ - \vec{\mathbf{Z}}_- + i\nu \in \cdot \mathbf{B} \quad (\text{A.33})$$

$$\vec{\mathbf{Z}}_2 = -\vec{\mathbf{Z}}_+^* - \vec{\mathbf{Z}}_-^* + i\nu \in \cdot \mathbf{B} \quad (\text{A.34})$$

$$\begin{aligned}
 &= \exp \left\{ i \int_0^\infty \frac{d\nu}{2\pi} \left( \mathbf{f}'_{\nu^*} \cdot \frac{1}{\vec{\mathbf{Z}}_+ + \vec{\mathbf{Z}}_-^* - i\nu \in \cdot \mathbf{B}} \cdot (\mathbf{f}'_{\nu} - \mathbf{f}_{\nu}) \right. \right. \\
 &\quad \left. \left. + \mathbf{f}'_{\nu} \cdot \frac{1}{\vec{\mathbf{Z}}_+^* + \vec{\mathbf{Z}}_- + i\nu \in \cdot \mathbf{B}} \cdot (\mathbf{f}'_{\nu^*} - \mathbf{f}_{\nu^*}) + (\mathbf{f}'_{\nu} - \mathbf{f}_{\nu}) \cdot \frac{1}{\vec{\mathbf{Z}}_+ + \vec{\mathbf{Z}}_-^* - i\nu \in \cdot \mathbf{B}} \right. \right. \\
 &\quad \left. \left. \times [\vec{\mathbf{Z}}_+ - \vec{\mathbf{Z}}_+^* + \vec{\mathbf{Z}}_- - \vec{\mathbf{Z}}_-^*] \cdot \frac{1}{\vec{\mathbf{Z}}_+ + \vec{\mathbf{Z}}_- - i\nu \in \cdot \mathbf{B}} \cdot (\mathbf{f}'_{\nu^*} - \mathbf{f}_{\nu^*}) \right) \right\} \quad (\text{A.35})
 \end{aligned}$$

Defining

$$\begin{aligned}
 \vec{\mathbf{Z}}_{\nu} &= \vec{\mathbf{Z}}_+ + \vec{\mathbf{Z}}_-^* - i\nu \in \cdot \mathbf{B} \\
 &= -m\nu^2 \vec{\mathbf{I}} - m\omega_0^2 \vec{\mathbf{I}} - i\nu \in \cdot \mathbf{B} - 4\nu^2 \int_{-\infty}^{\infty} \frac{d\Omega}{\Omega} \frac{\vec{\mathbf{G}}(\Omega)}{\Omega^2 - \nu^2 - i\varepsilon} \quad ; \nu \geq 0 \quad (\text{A.36})
 \end{aligned}$$

we replace  $\mathbf{f}_{\nu}$  and  $\mathbf{f}'_{\nu}$  by their integral representations

$$\mathbf{f}_{\nu} = \int_{-\infty}^{\infty} d\tau \mathbf{f}_{\tau} e^{-i\nu\tau} \quad , \quad \mathbf{f}'_{\nu} = \int_{-\infty}^{\infty} d\tau \mathbf{f}'_{\tau} e^{-i\nu\tau}$$

Then Eq(A.35) becomes

$$I = \exp \left\{ \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} d\sigma (\mathbf{f}_{\tau} - \mathbf{f}'_{\tau}) \cdot [\vec{\mathbf{L}}^*(\tau - \sigma) \cdot \mathbf{f}_{\sigma} - \vec{\mathbf{L}}(\tau - \sigma) \cdot \mathbf{f}'_{\sigma}] \right\} \quad (\text{A.37})$$

where

$$\vec{\mathbf{L}}(\xi) = \int_0^\infty \frac{d\nu}{2\pi} \frac{1}{\vec{\mathbf{Z}}_{\nu}} \cdot [\vec{\mathbf{Z}}_- - \vec{\mathbf{Z}}_-^*] \cdot \frac{1}{\vec{\mathbf{Z}}_{\nu}^*} e^{-i\nu\xi} + \int_0^\infty \frac{d\nu}{2\pi} \frac{1}{\vec{\mathbf{Z}}_{\nu}^*} \cdot [\vec{\mathbf{Z}}_+ - \vec{\mathbf{Z}}_+^*] \cdot \frac{1}{\vec{\mathbf{Z}}_{\nu}} e^{i\nu\xi} \quad (\text{A.38})$$

To pass from Eq(5.22) to Eq(5.23) in the text, we must calculate

$$\vec{\mathbf{L}}(\xi) - \vec{\mathbf{L}}^*(\xi) = \int_0^\infty \frac{d\nu}{2\pi i} \left[ \left( \frac{1}{\vec{\mathbf{Z}}_\nu} - \frac{1}{\vec{\mathbf{Z}}_\nu^\dagger} \right) e^{-i\nu\xi} + \left( \frac{1}{\vec{\mathbf{Z}}_\nu^*} - \frac{1}{\vec{\mathbf{Z}}_\nu} \right) e^{i\nu\xi} \right] \quad (\text{A.39})$$

which follows at once from Eq(A.38) and the symmetry of  $\vec{\mathbf{Z}}_\pm(\nu)$ . If as in TF we generalize  $\vec{\mathbf{Z}}_\nu$  to  $-\infty \leq \nu \leq \infty$  by writing  $\vec{\mathbf{Z}}_\nu$  as

$$\vec{\mathbf{Z}}_\nu = -m(\nu + i\varepsilon)^2 \vec{\mathbf{I}} - m\omega_0^2 \vec{\mathbf{I}} - i(\nu + i\varepsilon) \varepsilon \cdot \mathbf{B} - 4(\nu + i\varepsilon)^2 \int_{-\infty}^\infty \frac{d\Omega}{\Omega} \frac{\vec{\mathbf{G}}(\Omega)}{\Omega^2 - (\nu + i\varepsilon)^2} \quad (\text{A.40})$$

then  $\vec{\mathbf{Z}}_\nu = \vec{\mathbf{Z}}_{-\nu}^*$  and  $\vec{\mathbf{Z}}_\nu = \vec{\mathbf{Z}}_{-\nu}^\dagger$  and Eq(A.39) becomes

$$\vec{\mathbf{L}}(\xi) - \vec{\mathbf{L}}^*(\xi) = \int_{-\infty}^\infty \frac{d\nu}{2\pi i} \left( \frac{1}{\vec{\mathbf{Z}}_\nu} - \frac{1}{\vec{\mathbf{Z}}_\nu^\dagger} \right) e^{-i\nu\xi} \quad (\text{A.41})$$

as desired. In the text we also need to follow the relationships easily obtainable from Eqs(A.30), (A.31) and (A.36)

$$\vec{\mathbf{Z}}_+^* - \vec{\mathbf{Z}}_+ = \vec{\mathbf{Z}}_+^* - \vec{\mathbf{Z}}_+ = 4\pi i \vec{\mathbf{G}}(\nu) \quad (\text{A.42})$$

$$\vec{\mathbf{Z}}_-^* - \vec{\mathbf{Z}}_- = \vec{\mathbf{Z}}_-^\dagger - \vec{\mathbf{Z}}_- = 4\pi i \vec{\mathbf{G}}(-\nu) \quad (\text{A.43})$$

$$\vec{\mathbf{Z}}_\nu^\dagger - \vec{\mathbf{Z}}_\nu = \vec{\mathbf{Z}}_{-\nu} - \vec{\mathbf{Z}}_{-\nu}^* = 4\pi i [\vec{\mathbf{G}}(\nu) - \vec{\mathbf{G}}(-\nu)] \quad (\text{A.44})$$

## APPENDIX B

### THE CALCULATION OF THE $\vec{\mathbf{L}}_\beta(\xi)$

In this appendix we evaluate the function

$$\begin{aligned} \vec{\mathbf{L}}_\beta(\xi) &= \int_{-\infty}^{\infty} \frac{d\nu}{2\pi i} \left( \frac{1}{\vec{\mathbf{Z}}_\nu} - \frac{1}{\vec{\mathbf{Z}}_\nu^\dagger} \right) \frac{1 - e^{-i\nu\xi}}{e^{\beta\nu} - 1} \\ &= \begin{pmatrix} K_\beta^+(\xi) & -K_\beta^-(\xi) & 0 \\ K_\beta^-(\xi) & K_\beta^+(\xi) & 0 \\ 0 & 0 & K_\beta^\parallel(\xi) \end{pmatrix} \end{aligned} \quad (\text{B.1})$$

where

$$K_\beta^\pm(\xi) = \int_{-\infty}^{\infty} \frac{d\nu}{2\pi i} \left( \frac{1}{Z_+} \pm \frac{1}{Z_-} \right) \frac{1 - e^{-i\nu\xi}}{e^{\beta\nu} - 1} \quad (\text{B.2})$$

$$K_\beta^\parallel(\xi) = \int_{-\infty}^{\infty} \frac{d\nu}{2\pi i} \frac{1}{Z_\parallel} \left( \frac{1 - e^{i\nu\xi}}{1 - e^{-\beta\nu}} + \frac{1 - e^{-i\nu\xi}}{e^{\beta\nu} - 1} \right) \quad (\text{B.3})$$

$$Z_\pm = -m\nu^2 - m\omega_0^2 \pm \nu B - 4\nu^2 \int_{-\infty}^{\infty} \frac{d\Omega}{\Omega} \frac{G_\pm(\Omega)}{\Omega^2 - \nu^2 - i\varepsilon} \quad (\text{B.4})$$

$$Z_\parallel = -m\nu^2 - m\omega_0^2 - 4\nu^2 \int_{-\infty}^{\infty} \frac{d\Omega}{\Omega} \frac{G_\parallel(\Omega)}{\Omega^2 - \nu^2 - i\varepsilon} \quad (\text{B.5})$$

Using the Feynman one oscillator approximation

$$G_\pm(\Omega) = C_\perp \delta(\Omega - w_\perp) \quad (\text{B.6})$$

$$G_\parallel(\Omega) = C_\parallel \delta(\Omega - w_\parallel) \quad (\text{B.7})$$

Inserting  $G_\parallel(\Omega)$  into Eq(B.5), we have

$$\begin{aligned} -Z_\parallel &= m\nu^2 + m\omega_0^2 + \frac{4C_\parallel \nu^2}{w_\parallel(w_\parallel^2 - \nu^2 - i\varepsilon)} \\ &= \frac{m\nu^2(w_\parallel^2 + 4\frac{C_\parallel}{w_\parallel} + \omega_0^2) - m\nu^2 - m\nu^2 i\varepsilon + m\omega_0^2 w_\parallel^2 + m\omega_0^2 i\varepsilon}{(w_\parallel^2 - \nu^2 - i\varepsilon)} \\ Z_\parallel &= \frac{m\nu^4 - m\nu^2(\nu_\parallel^2 + \omega_0^2 + i\varepsilon) + m\omega_0^2 w_\parallel^2 - m\omega_0^2 i\varepsilon}{(w_\parallel^2 - \nu^2 - i\varepsilon)} \end{aligned}$$

$$\begin{aligned} & ; \quad v_{\parallel}^2 = w_{\parallel}^2 + \frac{4C_{\parallel}}{w_{\parallel}} \\ Z_{\parallel} & = m \frac{(z_1^2 - \nu^2)(z_2^2 - \nu^2)}{(w_{\parallel}^2 - \nu^2 - i\varepsilon)} \end{aligned} \quad (\text{B.8})$$

where

$$z_1^2 = \frac{(v_{\parallel}^2 + \omega_0^2 + i\varepsilon)}{2} + \frac{\sqrt{(v_{\parallel}^2 + \omega_0^2 + i\varepsilon)^2 + 4(w_{\parallel}^2 \omega_0^2 - \omega_0^2 i\varepsilon)}}{2} \quad (\text{B.9})$$

$$z_2^2 = \frac{(v_{\parallel}^2 + \omega_0^2 + i\varepsilon)}{2} - \frac{\sqrt{(v_{\parallel}^2 + \omega_0^2 + i\varepsilon)^2 + 4(w_{\parallel}^2 \omega_0^2 - \omega_0^2 i\varepsilon)}}{2} \quad (\text{B.10})$$

Substituting Eq(B.8) into Eq(B.3)

$$\begin{aligned} K_{\beta}^{\parallel}(\xi) & = \frac{1}{m} \int_{-\infty}^{\infty} \frac{d\nu}{2\pi i} \frac{(w_{\parallel}^2 - \nu^2 - i\varepsilon)}{(z_1^2 - \nu^2)(z_2^2 - \nu^2)} \left( \frac{1 - e^{i\nu\xi}}{1 - e^{-\beta\nu}} + \frac{1 - e^{-i\nu\xi}}{e^{\beta\nu} - 1} \right) \\ & = \frac{1}{m} \int_{-\infty}^{\infty} \frac{d\nu}{2\pi i} \frac{(w_{\parallel}^2 - \nu^2 - i\varepsilon)}{(z_1 - \nu)(z_1 + \nu)(z_2 - \nu)(z_2 + \nu)} \\ & \quad \times \left( \frac{1 - e^{i\nu\xi}}{1 - e^{-\beta\nu}} + \frac{1 - e^{-i\nu\xi}}{e^{\beta\nu} - 1} \right) \end{aligned} \quad (\text{B.11})$$

A quick inspection shows that the integration has poles at  $\pm z_1$  and  $\pm z_2$ , and

$$\begin{aligned} K_{\beta}^{\parallel}(\xi) & = \frac{1}{m} \frac{(w_{\parallel}^2 - z_1^2 - i\varepsilon)}{2z_1(z_2^2 - z_1^2)} \left( \frac{1 - e^{iz_1\xi}}{1 - e^{-\beta z_1}} + \frac{1 - e^{-iz_1\xi}}{e^{\beta z_1} - 1} \right) \\ & \quad + \frac{1}{m} \frac{(w_{\parallel}^2 - z_2^2 - i\varepsilon)}{2z_2(z_1^2 - z_2^2)} \left( \frac{1 - e^{iz_2\xi}}{1 - e^{-\beta z_2}} + \frac{1 - e^{-iz_2\xi}}{e^{\beta z_2} - 1} \right) \\ & = \frac{1}{m} \frac{(z_1^2 - w_{\parallel}^2 + i\varepsilon)}{2(z_1^2 - z_2^2)} \frac{\cosh\left(\frac{z_1\beta}{2}\right) - \cos z_1\left(\xi - \frac{i\beta}{2}\right)}{z_1 \sinh\left(\frac{z_1\beta}{2}\right)} \\ & \quad + \frac{1}{m} \frac{(z_2^2 - w_{\parallel}^2 + i\varepsilon)}{2(z_2^2 - z_1^2)} \frac{\cosh\left(\frac{z_2\beta}{2}\right) - \cos z_2\left(\xi - \frac{i\beta}{2}\right)}{z_2 \sinh\left(\frac{z_2\beta}{2}\right)} \end{aligned} \quad (\text{B.12})$$

So

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} K_{\beta}^{\parallel}(\xi) & = \frac{1}{m} \frac{(z_1^2 - w_{\parallel}^2)}{2(z_1^2 - z_2^2)} \frac{\cosh\left(\frac{z_1\beta}{2}\right) - \cos z_1\left(\xi - \frac{i\beta}{2}\right)}{z_1 \sinh\left(\frac{z_1\beta}{2}\right)} \\ & \quad + \frac{1}{m} \frac{(z_2^2 - w_{\parallel}^2)}{2(z_2^2 - z_1^2)} \frac{\cosh\left(\frac{z_2\beta}{2}\right) - \cos z_2\left(\xi - \frac{i\beta}{2}\right)}{z_2 \sinh\left(\frac{z_2\beta}{2}\right)} \end{aligned} \quad (\text{B.13})$$

For  $\omega_0 \rightarrow 0$ , then  $z_1 = v_{\parallel}$  and  $z_2 = 0$ , Eq(B.13) becomes

$$\begin{aligned} K_{\beta}^{\parallel}(\xi) & = \frac{1}{m} \frac{(v_{\parallel}^2 - w_{\parallel}^2)}{2v_{\parallel}^3} \frac{\cosh\left(\frac{v_{\parallel}\beta}{2}\right) - \cos v_{\parallel}\left(\xi - \frac{i\beta}{2}\right)}{\sinh\left(\frac{v_{\parallel}\beta}{2}\right)} - \frac{1}{2m} \frac{w_{\parallel}^2}{v_{\parallel}^2} \left( i\xi + \frac{\xi^2}{\beta} \right) \\ & = \frac{1}{2m} \frac{w_{\parallel}^2}{v_{\parallel}^2} \left( \left( \frac{v_{\parallel}^2 - w_{\parallel}^2}{v_{\parallel} w_{\parallel}^2} \right) \frac{\cosh\left(\frac{v_{\parallel}\beta}{2}\right) - \cos v_{\parallel}\left(\xi - \frac{i\beta}{2}\right)}{\sinh\left(\frac{v_{\parallel}\beta}{2}\right)} - i\xi + \frac{\xi^2}{\beta} \right) \end{aligned} \quad (\text{B.14})$$

Next we insert  $G_+(\Omega)$  into Eq(B.4), and we have

$$\begin{aligned}
 -Z_+ &= m\nu^2 + m\omega_0^2 + \nu B + \frac{4\nu^2 C_\perp}{w_\perp(w_\perp^2 - \nu^2 - i\varepsilon)} \\
 &= \frac{m\nu^2(v_\perp^2 + \omega_0^2 - i\varepsilon) - m\nu^4 + \nu^3 B + \nu(i\varepsilon - w_\perp^2)B + m\omega_0^2 w_\perp^2 - m\omega_0^2 i\varepsilon}{(w_\perp^2 - \nu^2 - i\varepsilon)} \\
 &\quad ; \quad v_\perp^2 = w_\perp^2 + \frac{4C_\perp}{w_\perp} \\
 Z_+ &= m \frac{(s_1 - \nu)(s_2 - \nu)(s_3 - \nu)(s_4 - \nu)}{(w_\perp^2 - \nu^2 - i\varepsilon)} \tag{B.15}
 \end{aligned}$$

where  $s_i$  is the solution of the polynomial degree four

$$m\nu^4 + \nu^3 B - m\nu^2(v_\perp^2 + \omega_0^2 - i\varepsilon) - \nu(i\varepsilon - w_\perp^2)B + m\omega_0^2 w_\perp^2 + m\omega_0^2 i\varepsilon \tag{B.16}$$

Next we insert  $G_-(\Omega)$  into Eq(B.4), and we have

$$\begin{aligned}
 -Z_- &= m\nu^2 + m\omega_0^2 - \nu B + \frac{4\nu^2 C_\perp}{w_\perp(w_\perp^2 - \nu^2 - i\varepsilon)} \\
 &= \frac{m\nu^2(v_\perp^2 + \omega_0^2 - i\varepsilon) - m\nu^4 - \nu^3 B - \nu(i\varepsilon - w_\perp^2)B + m\omega_0^2 w_\perp^2 - m\omega_0^2 i\varepsilon}{(w_\perp^2 - \nu^2 - i\varepsilon)} \\
 &\quad ; \quad v_\perp^2 = w_\perp^2 + \frac{4C_\perp}{w_\perp} \\
 Z_- &= m \frac{(s_1 + \nu)(s_2 + \nu)(s_3 + \nu)(s_4 + \nu)}{(w_\perp^2 + \nu^2 - i\varepsilon)} \tag{B.17}
 \end{aligned}$$

where  $-s_i$  is the solution of the polynomial degree four

$$m\nu^4 - \nu^3 B - m\nu^2(v_\perp^2 + \omega_0^2 - i\varepsilon) + \nu(i\varepsilon - w_\perp^2)B + m\omega_0^2 w_\perp^2 + m\omega_0^2 i\varepsilon \tag{B.18}$$

Inserting Eq(B.15) and Eq(B.17) into Eq(B.2), we find

$$\begin{aligned}
 K_\beta^+(\xi) &= \int_{-\infty}^{\infty} \frac{d\nu}{2\pi i} \left( \frac{1}{Z_+} + \frac{1}{Z_-} \right) \frac{1 - e^{-i\nu\xi}}{e^{\beta\nu} - 1} \\
 &= \int_{-\infty}^{\infty} \frac{d\nu}{2\pi i} \left( \frac{(w_\perp^2 - \nu^2 - i\varepsilon)}{(s_1 - \nu)(s_2 - \nu)(s_3 - \nu)(s_4 - \nu)} \right. \\
 &\quad \left. + \frac{(w_\perp^2 - \nu^2 - i\varepsilon)}{(\nu + s_1)(\nu + s_2)(\nu + s_3)(\nu + s_4)} \right) \frac{1 - e^{-i\nu\xi}}{e^{\beta\nu} - 1} \tag{B.19}
 \end{aligned}$$

A quick inspection shows that the integration has poles at  $\pm s_i$ , and Eq(B.19) becomes

$$\begin{aligned}
 K_\beta^+(\xi) &= \frac{1}{m} \left\{ -\frac{(w_\perp^2 - s_1^2 - i\varepsilon)}{(s_1 - s_2)(s_1 - s_3)(s_1 - s_4)} \frac{1 - e^{-is_1\xi}}{e^{\beta s_1} - 1} \right. \\
 &\quad \left. + \frac{(w_\perp^2 - s_1^2 - i\varepsilon)}{(s_1 - s_2)(s_1 - s_3)(s_1 - s_4)} \frac{1 - e^{is_1\xi}}{1 - e^{-\beta s_1}} \right\}
 \end{aligned}$$

$$\begin{aligned}
& - \frac{(w_\perp^2 - s_2^2 - i\varepsilon)}{(s_2 - s_1)(s_2 - s_3)(s_2 - s_4)} \frac{1 - e^{-is_2\xi}}{e^{\beta s_2} - 1} \\
& + \frac{(w_\perp^2 - s_2^2 - i\varepsilon)}{(s_2 - s_1)(s_2 - s_3)(s_2 - s_4)} \frac{1 - e^{is_2\xi}}{1 - e^{-\beta s_2}} \\
& - \frac{(w_\perp^2 - s_3^2 - i\varepsilon)}{(s_3 - s_1)(s_3 - s_2)(s_3 - s_4)} \frac{1 - e^{-is_3\xi}}{e^{\beta s_3} - 1} \\
& + \frac{(w_\perp^2 - s_3^2 - i\varepsilon)}{(s_3 - s_1)(s_3 - s_2)(s_3 - s_4)} \frac{1 - e^{is_3\xi}}{1 - e^{-\beta s_3}} \\
& - \frac{(w_\perp^2 - s_4^2 - i\varepsilon)}{(s_4 - s_1)(s_4 - s_2)(s_4 - s_3)} \frac{1 - e^{-is_4\xi}}{e^{\beta s_4} - 1} \\
& + \frac{(w_\perp^2 - s_4^2 - i\varepsilon)}{(s_4 - s_1)(s_4 - s_2)(s_4 - s_3)} \frac{1 - e^{is_4\xi}}{1 - e^{-\beta s_4}} \Big\} \tag{B.20}
\end{aligned}$$

Then

$$\begin{aligned}
K_\beta^+(\xi) &= \frac{1}{m} \sum_{j=1}^4 \frac{(s_j^2 - w_\perp^2 + i\varepsilon)}{\prod_{j \neq i} (s_j - s_i)} \left( \frac{1 - e^{-is_j\xi}}{e^{\beta s_j} - 1} - \frac{1 - e^{is_j\xi}}{e^{-\beta s_j} - 1} \right) \\
&= \frac{1}{m} \sum_{j=1}^4 \frac{(s_j^2 - w_\perp^2 + i\varepsilon)}{\prod_{j \neq i} (s_j - s_i)} \frac{\cosh\left(\frac{s_j\beta}{2}\right) - \cos s_j\left(\xi - \frac{i\beta}{2}\right)}{\sinh\left(\frac{s_j\beta}{2}\right)} \\
\lim_{\varepsilon \rightarrow 0} K_\beta^+(\xi) &= \frac{1}{m} \sum_{j=1}^4 \frac{(s_j^2 - w_\perp^2)}{\prod_{j \neq i} (s_j - s_i)} \frac{\cosh\left(\frac{s_j\beta}{2}\right) - \cos s_j\left(\xi - \frac{i\beta}{2}\right)}{\sinh\left(\frac{s_j\beta}{2}\right)} \tag{B.21}
\end{aligned}$$

For  $\omega_0 \rightarrow 0$ ,  $s_4 = 0$ , we get

$$K_\beta^+(\xi) = \frac{1}{m} \sum_{j=1}^3 \frac{(s_j^2 - w_\perp^2)}{s_j \prod_{j \neq i} (s_j - s_i)} \frac{\cosh\left(\frac{s_j\beta}{2}\right) - \cos s_j\left(\xi - \frac{i\beta}{2}\right)}{\sinh\left(\frac{s_j\beta}{2}\right)} \tag{B.22}$$

For convenience we will use the Devreese expression [24], so that Eq(B.22) becomes

$$K_\beta^+(\xi) = \sum_{j=1}^3 c_j^2 \frac{\cosh\left(\frac{s_j\beta}{2}\right) - \cos s_j\left(\xi - \frac{i\beta}{2}\right)}{\sinh\left(\frac{s_j\beta}{2}\right)} \tag{B.23}$$

where

$$c_j^2 = \frac{1}{2m} \frac{s_j^2 - w_\perp^2}{s_j} \frac{1}{3s_j^2 - 2(-1)^{j+1} \omega_c s_j - v_\perp^2} \tag{B.24}$$

Using the results of Eq(B.15) and Eq(B.17), we express  $K_\beta^-(\xi)$  as

$$K_\beta^-(\xi) = \sum_{j=1}^3 c_j^2 \frac{\sinh\left(\frac{s_j\beta}{2}\right) + i \sin s_j\left(\xi - \frac{i\beta}{2}\right)}{\sinh\left(\frac{s_j\beta}{2}\right)} \tag{B.25}$$

Finally it is very easy to show that

$$\mathbf{k} \cdot \vec{\mathbf{L}}_\beta(\xi) \cdot \mathbf{k} = k_\perp^2 K_\beta^\perp(\xi) + k_z^2 K_\beta^\parallel(\xi) \tag{B.26}$$

where

$$K_{\beta}^{\perp}(\xi) = K_{\beta}^{+}(\xi) \tag{B.27}$$

## APPENDIX C

GROUND STATE ENERGY CALCULATION  
PROGRAM

```
*****
c  program: Ground state energy of a polaron in a magnetic field
c  purpose: To minimize ground state energy of the polaron in a
c           magnetic field
*****

      program ground

      implicit real*8(a-h,o-z)

*****
c  Global-variable declaration
*****

      common/glob/v1,w1,s2,w2,c2,wb,wc,alpha,hold,tol,sta,fin,nst

      common/gruss/xi(48),wi(48)

      common/quad/nstrip

      common/range/scale

*****
c  Initialize default value to all parameter
*****

      call setpquad

      call setglob

      call initialvalue

      write(6,*)'tol',tol

      write(6,*)'sta',sta
```

```

write(6,*)'fin',fin
write(6,*)'nst',nst
total=0.d0
hold=e0()
write(6,*)'before search'
write(6,*)'v1',v1
write(6,*)'w1',w1
write(6,*)'s2',s2
v2=dsqrt(s2*s2+wc*s2-wc*w2*w2/s2)
write(6,*)'v2',v2
write(6,*)'w2',w2
write(6,*)'wc',wc
write(6,*)'(v1*v1)/(w1*w1)',(v1*v1)/(w1*w1)
write(6,*)'(v2*v2)/(w2*w2)',(v2*v2)/(w2*w2)
write(6,*)'energy',hold
high=hold
write(6,*)'alpha',alpha
write(6,*)'searching'

*****

c  Optiminze parameters;including v1,w1,v2,w2

*****

scale=1.d0*sta

40 l=0

10 call search()

l=l+1

if(l.lt.1000)goto 10

*****

c  Show energy and parameters after calculation 1000 times

```

\*\*\*\*\*

```

write(6,*)'energy',hold
write(6,*)'scale',scale
write(6,*)'V1',V1
write(6,*)'v1',v1
write(6,*)'w1',w1
write(6,*)'s2',s2
v2=dsqrt(s2*s2+wc*s2-wc*w2*w2/s2)
write(6,*)'v2',v2
write(6,*)'w2',w2
write(6,*)'wc',wc
write(6,*)'(v1*v1)/(w1*w1)',(v1*v1)/(w1*w1)
write(6,*)'(v2*v2)/(w2*w2)',(v2*v2)/(w2*w2)
diffen=abs(bigh-hold)
total=total+diffen
if(diffen.lt.tol)scale=.5d0*scale
bigh=hold
if(scale.ge.fin)goto 40
write(6,*)'total change is',total
28 write(6,*)'input nstrip for integral check'
read(5,*)nst
if(nst.eq.0)goto 29
hold=e0()
write(6,200)hold
goto 28
29 continue

```

\*\*\*\*\*

c Format of reading data from field'data.dat'

```
*****
200 format(3f23.15)
300 format(23x,2f23.15)
400 format(2f10.5,I4)

    stop

    end

*****

c  Subroutine search
*****

    subroutine search()
    implicit real*8 (a-h,o-z)
    real*4 urand

    common/glob/v1,w1,s2,w2,c2,wb,wc,alpha,hold,tol,sta,fin,nst
    common/range/scale
    data iseed/0/
    rand=(urand(iseed)-.5)*v1
    rand=scale*urand(iseed)*rand
    v1=v1+rand

        if(v1.ge.w1.and.v1.ge.1.d0)then
            e=e0()

                if(hold.gt.e)then
                    hold=e

                    goto 3

                endif

            endif

        v1=v1-rand
3  rand=(urand(iseed)-.5)*w1
    rand=scale*urand(iseed)*rand
```

```
w1=w1+rand
      if(w1.le.v1.and.w1.ge.1.d0)then
        e=e0()
        if(hold.gt.e)then
          hole=e
          goto 4
        endif
      endif
w1=w1-rand
4  rand=(urand(iseed)-.5)*s2
   rand=scale*urand(iseed)*rand
   s2=s2+rand
      if(s2.ge.w2.and.s2.gt.wc)then
        e=e0()
        if(hold.gt.e)then
          hole=e
          goto 4
        endif
      endif
s2=s2-rand
5  continue
   rand=(urand(iseed)-.5)*w2
   rand=scale*urand(iseed)*rand
w2=w2+rand
      if(w2.le.s2.and.w2.gt.wc)then
        e=e0()
        if(hold.gt.e)then
          hole=e
```

```
        goto 4
    endif
endif

w2=w2-rand
1 continue

return

end

*****
c  Set global variables by reading data from file'data.dat'
*****

subroutine setglob
implicit real*8 (a-h,o-z)
common/glob/v1,w1,s2,w2,c2,wb,wc,alpha,hold,tol,sta,fin,nst
open(1,file='variabledata.dat')
read(1,*)alpha
read(1,*)v1
read(1,*)w1
read(1,*)s2
read(1,*)w2
read(1,*)wc
close(1)

return

end

*****
c  Set global initial value by reading data from
file'inivalue.dat'
*****

subroutine initialvalue
```

```

implicit real*8 (a-h,o-z)

common/glob/v1,w1,s2,w2,c2,wb,wc,alpha,hold,tol,sta,fin,nst

open(2,file='inivalue.dat')

read(2,*)tol

read(2,*)sta

read(2,*)fin

read(2,*)nst

close(2)

return

end

```

```

*****

```

```

c Expression of energy of the polaron in a magnetic field

```

```

*****

```

```

function e0()

implicit real*8 (a-h,o-z)

common/glob/v1,w1,s2,w2,c2,wb,wc,alpha,hold,tol,sta,fin,nst

external f

pi=4.d0*datan(1.d0)

call integr1(g)

e0=2.d0*s2*s2*s2+wc*s2*s2+wc*w2*w2

e0=(s2-w2)*(s2-w2)*(s2*s2-wc*w2)/e0

e0=wc/2+(v1-w1)*(v1-w1)/(4.d0*v1)+e0

e0=e0-alpha-dsqrt(1.d0/(2.d0*pi))*alpha*g

return

end

```

```

*****

```

```

c Expression of t1(x)

```

\*\*\*\*\*

```

function t1(x)
implicit real*8 (a-h,o-z)
common/glob/v1,w1,s2,w2,c2,wb,wc,alpha,hold,tol,sta,fin,nst

wb=(wc+s2)*(wc+s2)/4.d0
wb=wb-(wc*w2*w2)/s2
wb=dsqrt(wb)

y=(wc+s2)*x/2.d0
c=wb*x
t1=cosh(c)+(s2-wc)*sinh(c)/wb/2.d0
t1=1.d0-t1*dexp(-y)
return
end

```

\*\*\*\*\*

c Expression of t2(x)

\*\*\*\*\*

```

function t2(x)
implicit real*8 (a-h,o-z)
common/glob/v1,w1,s2,w2,c2,wb,wc,alpha,hold,tol,sta,fin,nst

wb=(wc+s2)*(wc+s2)/4.d0
wb=wb-(wc*w2*w2)/s2
wb=dsqrt(wb)

a=s2*x
y=(wc+s2)*x/2.d0

```

```

c=wb*x

t2=(s2+wc)*dexp(-y)*sinh(c)/wb
t=1.d0-dexp(-a)-t2
return
end

*****
c Expression f(x)
*****

function f(x)
implicit real*8 (a-h,o-z)
common/glob/v1,w1,s2,w2,c2,wb,wc,alpha,hold,tol,sta,fin,nst
*****

c Expression di(x)
*****

r=v1*v1-w1*w1
y=v1*x

a=(1.d0-y-dexp(-y))/y
b=a/y

c=r*a/v1/v1
d=r*b/v1
di=c*(1.d0+c)/d/2.d0

*****

c Expression dh(x)
*****

c2=(2.d0*s2*s2*s2)+(s2*s2*wc)+(w2*w2*wc)

```

```
c2=(s2-w2)*(s2+w2)/c2
```

```
c2=dsqrt(c2)
```

```
dh=(1.d0/wc+c2*c2)*t1(x)
```

```
dh=dh+c2*c2*t2(x)
```

```
dh=dh/2.d0
```

```
*****
```

```
c Expression b(h)
```

```
*****
```

```
h=di/dh
```

```
if(h.lt.1.d0)then
```

```
b=dsqrt(h/(-h+1.d0))*dlog((dsqrt(h)+dsqrt(-h+1.d0)))
```

```
else
```

```
b=dsqrt(h/(h-1.d0))*dlog((dsqrt(h)+dsqrt(h-1.d0)))
```

```
endif
```

```
f=b/dsqrt(di)-dsqrt(2.d0/x)
```

```
f=f*dexp(-x)
```

```
return
```

```
end
```

```
*****
```

```
c Quadrature integration: g is return value
```

```
*****
```

```
subroutine intgr1(g)
```

```
implicit real*8 (a-h,o-z)
```

```
external f
```

```
common/quad/nstrip
```

```
cut=0.d0
```

```
1 cut=cut+1.d0
```

```
    if(f(cut).gt.1.d-15)goto 1
    d=1.d0/dfloat(nstrip)
    g=0.d0
    do 3 i=1,nstrip
    a=dfloat(nstrip-i+1)*d
    b=a-d
    a=-dlog(a)
        if(i.lt.nstrip)then
            b=-dlog(b)
        else
            b=cut
        endif
3  g=g+pquad(a,b,f)
    return
end

function pquad(a,b,fun)
real*8 pquad,a,b,xi,wi,c,d,yi,fun
external fun
parameter(n=48,n2=n*2)
dimension xi(n),wi(n),yi(n2)
common/guass/xi,wi
c=.5d0*(b-a)
d=.5d0*(b+a)
do 2 i=1,n
    yi(i)=c*xi(i)+d
2  yi(i+n)=-c*xi(i)+d
pquad=0.d0
```

```

do 1 i=1,n
  pquad=pquad+fun(yi(i)*wi(i)
1  pquad=pquad+fun(yi(i+n))*wi(i)
  pquad=pquad*c
  return
end

*****
c  Initialize pquad parameters
*****

subroutine setpquad
  implicit real*8 (a-h,o-z)
  common/gauss/xi(48),wi(48)
  common/quad/nstrip
  nstrip=5
  open(1,file='pquad.dat')
  read(1,100)(xi(i),wi(i),i=1,48)
100 format(2d24.17)
  close(1)
  return
end

*****
c  Random generator
*****

function urand(iy)
c  uniform random number generator\
c  initialize iy prior to first call.
c  calling program must not alter iy between call.\
c  values of urand are returned in the interval (0,1).\

```

```
real*8 halfm
data m2/0/,itwo/2/
if(m2.ne.0)goto 20
c  if first entry, compute machine integer word length.
m=1
10 m2=m
m=itwo*m2
if(m.gt.m2)goto 10
halfm=m2
c  compute multiplier and increment for linear congruential
method.\
ia=8*idint(halfm*datan(1.d0)/8.d0)+5
ic=2*idint(halfm*(.5d0-DSQRT(3.D0))/6.D0))+1
mic=(m2-ic)+m2
c  s is the scale factor for converting to floating point.
s=.5/halfm
c  compute next random number
20 iy=iy*ia

c  the following statement is for computers which do not allow
c  integer overflow on addition.
c  if(iy.gt.mic)iy=(iy-m2)-m2
iy=iy+ic
c  the following statement is for compute where the word length
c  for addition is greater than for multiplication.

c  if(iy/2.gt.m2)iy=(iy-m2)-m2
c  the following statement is for compute where integer overflow
```

```
c  affects the sign bit.  
  if(iy.lt.0)iy=(iy+m2)+m2  
  urand=flodt(iy)*s  
  return  
  end
```

## BIOGRAPHY

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