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# สถาบนวิทยบริการ

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#### APPLICATION OF FEYNMAN PATH INTEGRATION TO THE GROUND STATE OF PLASMARON

Mr.Alongkorn Khudwilat

## สถาบนวทยบริการ

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วิทยานิพนธ์ฉบับนี้ได้ประยุกต์การอินทิเกรตตามวิถีของฟายน์แมนกับพลาสมารอนซึ่งเป็นรูป แบบอันตรกิริยาของอิเล็กตรอนและพลาสมอนโดยสามารถเขียนอยู่ในรูปแฮมิลโทเนียนอันตรกิริยา แบบโฟรห์ลิชซึ่งมีลักษณะคล้ายคลึงกับปัญหาของโพลารอน เราได้ทำการคำนวณตัวแผ่กระจายและ เมทริกซ์ความหนาแน่นซึ่งรวมส่วนของเมทริกซ์ไม่ทแยงมุมเอาไว้ด้วย จากนั้นจึงหาพลังงานสถานะพื้น และมวลยังผลแบบคริโวกลาซ-เปการ์จากส่วนเมทริกซ์ทแยงมุม สำหรับส่วนเมทริกซ์ไม่ทแยงมุมนั้นนำ มาคำนวณหามวลยังผลแบบฟายน์แมน ในที่นี้จะใช้โปรแกรมแมทธีมาทิคา หาผลเชิงตัวเลขและได้นำ ผลที่ได้มาเปรียบเทียบกับค่าที่คำนวณจากวิธีอินทิเกรตตามวิถีแบบทั่วไปในช่วงขอบเขตอันตรกิริยา แบบอ่อนและแบบแรง นอกจากนั้นพฤติกรรมของมวลยังผลยังอาจสามารถนำไปเชื่อมโยงกับปรากฏ การณ์ที่เรียกว่าการตกผลึกแบบวิกเนอร์

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KEY WORD: FRÖHLICH-TYPE HAMILTONIAN / PATH INTEGRAL / PLASMARON / GROUND STATE ENERGY / EFFECTIVE MASS

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In this thesis, the Fröhlich-type electron-plasmon Hamiltonian of the plasmaron which is the dressing of an electron by plasmons has been investigated using Feynman's path integral approach. The full form including the off-diagonal part of the plasmaron propagator and density matrix are derived. Then the ground state energy and the Krivoglaz-Pekar effective mass can be obtained from the diagonal part of the density matrix while the Feynman effective mass is evaluated from the off-diagonal part. The MATHEMATICA program has been used to find these quantities numerically. They are compared with those from the generalized path integral method in the weak coupling and strong coupling limits. Furthermore, the behaviour of the effective mass shows an interesting characteristic which may be connected to the phenomenon known as Wigner crystallization.

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## Chapter 1 Introduction

Progress in many-particle problems is generally associated with a successful model approach. In recent years, there have been intense research efforts on one-particle self-consistent treatments of many-particle systems. In the case of a charged test particle interacting with an electron gas, the single-particle spectrum was investigated in an approximation with a particle coupled to plasmons. This kind of coupling in solids has been discussed by many authors since the pioneering work by Bohm-Pines [1]. The Bohm-Pines results have been extended in various directions using the perturbation-theoretical method developed by Gell-Mann and Brueckner [2], the dielectric formulation of Nozieres and Pines [3], and the powerful many-body techniques [4].

In metal, Lundqvist [5] showed that the interaction of an individual electron with plasmons, in the random phase approximation (RPA), can be described in terms of the Fröhlich-type interaction Hamiltonian in analogy with the polaron problem [6]. This form of the electron-plasmon interaction may be called the **plasmaron coupling**.

In this thesis, we would like to study the behaviour of the ground state energy and the effective mass of the plasmaron by using Feynman's path integral approach [7]. Path integral is a very powerful method applied very successfully to the polaron problem [6], since it can be used for all ranges of coupling constants and gives the best results for intermediate values of the coupling interaction. The outlines of this work will be presented as follows: the next chapter will be devoted to the basic background of the Bohm-Pines theory of an electron gas with Coulomb interaction which leads to the concept of plasmon and screening effect. The electron-plasmon interaction Fröhlich-type Hamiltonian, proposed by Lundqvist, will also be discussed in details. In chapter 3, Feynman's path integration is presented. The propagator and density matrix including the offdiagonal part will be calculated by the variational method using the two-particle model trial action introduced by Samathiyakanit [8] in chapter 4. In chapter 5, the ground state energy and the effective mass of the plasmaron will be extracted from the density matrix obtained in the previous chapter with the numerical results and discussions. Conclusions for the application and the implication of the present theory will be given in the last chapter.



## Chapter 2 Theoretical Reviews

In this chapter the theory of an electron gas, developed by D. Bohm and D. Pines, will be discussed in details. This leads to the concept of plasmon and screening effect in solids. And next, Lundqvist's Fröhlich-type electron-plasmon interaction, which is very important in this work, will be presented.

### 2.1 The Bohm-Pines theory

Consider a system of electrons moving in a uniform positive charged background in which these electrons interact with each other and the positive background via the Coulomb potential. The Hamiltonian of this system can be written as

$$H = \sum_{i} \frac{\mathbf{p}_{i}^{2}}{2m} + \frac{1}{2} \sum_{\substack{ij \\ i \neq j}} \frac{e^{2}}{|\mathbf{x}_{i} - \mathbf{x}_{j}|} + H_{+}, \qquad (2.1)$$

where  $\mathbf{x}_i$  and  $\mathbf{p}_i$  denote the coordinate and momentum of the *i*th electron respectively,  $H_+$  represents the interaction between electrons and the positive background.

To calculate the ground state energy, the perturbation theory will be applied to this problem by trying to treat the Coulomb interaction as a perturbation. Unfortunately, it has been found that the second-order perturbation term **diverges**. This is because of the long-range nature of the Coulomb interaction. Thus it is not generally possible to simplify the calculation by considering only a small region of space surrounding any given particle. In the Bohm-Pines treatment [1, 9, 10] an extra approximation, just as extreme but opposite to that of the individual electron model, is introduced such that the behaviour of the entire electron gas is considered as a whole. Thus, besides the degrees of freedom associated with the motion of the individual particles, extra degrees of freedom associated with the collective behaviour of the electron gas are introduced. These give rise to a description in which electrons, beyond some screening radius  $r_c$  of any given electron, act cooperatively on that electron, while the individual-particle aspects are important for radii smaller than  $r_c$ . The collective modes of behaviour of the electron gas are associated with plasma oscillations with characteristic frequencies  $\omega_p$ , and their energy quanta ( $\hbar \omega_p$ ) are commonly called **plasmons**.

The plasma itself may be treated in terms of the equations of motion of the particle density fluctuations of the system. In order to predict the equations of motion of density fluctuations in plasma, it is convenient, because of the periodic boundary conditions imposed on the electron wave functions, to describe our system in  $\mathbf{k}$  space rather than  $\mathbf{x}$  space. The potential energy for the interaction between the *i*th and *j*th electrons may be expanded in a Fourier series, then we obtain

$$\phi\left(|\mathbf{x}_{i} - \mathbf{x}_{j}|\right) = \frac{e^{2}}{|\mathbf{x}_{i} - \mathbf{x}_{j}|} = \frac{4\pi e^{2}}{V} \sum_{\mathbf{k}} \frac{1}{k^{2}} e^{i\mathbf{k}\cdot(\mathbf{x}_{i} - \mathbf{x}_{j})},$$
(2.2)

where V denotes volume of the system.

In the same way, the particle density  $\rho(\mathbf{x})$  is Fourier-decomposed with the corresponding Fourier coefficients or density fluctuations given by

$$\rho_k = \int d\mathbf{x} \rho\left(\mathbf{x}\right) e^{-i\mathbf{k}\cdot\mathbf{x}}.$$
(2.3)

If it is now assumed that we are dealing with point particles, then

$$\rho\left(\mathbf{x}\right) = \sum_{i} \delta\left(\mathbf{x} - \mathbf{x}_{i}\right). \tag{2.4}$$

Therefore the equation of motion of  $\rho_k$ , with the help of the equation  $m\ddot{\mathbf{x}}_i = -\nabla\phi$ , is

$$\ddot{\rho}_{k} = -\sum_{i} \left(\mathbf{k} \cdot \mathbf{v}_{i}\right)^{2} e^{-i\mathbf{k} \cdot \mathbf{x}_{i}} - \frac{4\pi e^{2}}{mV} \sum_{\mathbf{k}', ij} \frac{\left(\mathbf{k} \cdot \mathbf{k}'\right)}{k^{2}} e^{i\left(\mathbf{k}' - \mathbf{k}\right) \cdot \mathbf{x}_{i}} e^{-i\mathbf{k} \cdot \mathbf{x}_{j}}, \qquad (2.5)$$

where  $\mathbf{v}_i$  is the velocity of the *i*th electron.

When  $\mathbf{k} = \mathbf{k}'$ , the sum over *i* is independent of  $\mathbf{x}_i$  and gives *N*, the number of electrons in the system. When  $\mathbf{k} \neq \mathbf{k}'$ , there is indeed a dependence of the sum on  $\mathbf{x}_i$ . This involves the phase factors  $e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{x}_i}$ . Since there is a very large number of particles at random locations, these terms (summed over  $\mathbf{k} \neq \mathbf{k}'$ ) tend to cancel each other and, in the first approximation, the Bohm-Pines treatment neglects them. This is called the random phase approximation (RPA). Thus the equation of motion of Eq. (2.5) takes the approximate form as

$$\ddot{\rho}_k = -\sum_i \left(\mathbf{k} \cdot \mathbf{v}_i\right)^2 e^{-i\mathbf{k} \cdot \mathbf{x}_i} - \omega_p^2 \rho_k, \qquad (2.6)$$

where  $\omega_p = \sqrt{4\pi n e^2/m}$  = plasma frequency and n = N/V = mean electron density.

The first term on the right-hand side of Eq. (2.6) does not describe collective behaviour; rather it corresponds to the contribution of the thermal motion of individual particles to the density fluctuations. On the other hand, the second term on the right-hand side of Eq. (2.6) describes each constituent electron of the entire gas, to contribute the same frequency  $\omega_p$  to the density fluctuations. Thus the latter is a collective behaviour whereas the former is an individual-particle behaviour. They are both, in principle, present at all times. However, we may use the criteria of the relative magnitudes of their average values to determine when one or the other will predominate. If

$$\frac{4\pi n e^2}{m} \gg \left\langle \left( \mathbf{k} \cdot \mathbf{v}_i \right)^2 \right\rangle_{av}, \qquad (2.7)$$

the electron gas will tend to behave collectively, whereas the individual-particle aspects become important if this inequality is reversed.

Thus far, we have described the electron gas in a metal in terms of the density fluctuations  $\rho_k$ , and we have seen that these **field coordinates** incorporate both collective and individual-particle features of the electron gas. Thus they would not properly serve as pure collective coordinates. The Bohm-Pines treatment attempts to transform the Hamiltonian of the system (in terms of these coordinates), by means of canonical transformation from the appropriate set of field coordinates that represent extra degrees of freedom in the system, to the normal coordinates which describe the independent modes of collective behaviour separately from the individual-particle behaviour of the gas.

The Hamiltonian of Eq. (2.1) can be rewritten in terms of field coordinates,  $\rho_k$ , as

$$H = \sum_{i} \frac{\mathbf{p}_{i}^{2}}{2m} + \frac{2\pi e^{2}}{V} \sum_{\mathbf{k}\neq\mathbf{0}} \frac{\rho_{k}\rho_{k}^{*}}{k^{2}} - 2\pi n e^{2} \sum_{\mathbf{k}\neq\mathbf{0}} \frac{1}{k^{2}}.$$
 (2.8)

It is noted that  $\mathbf{k} = \mathbf{0}$  term cancels  $H_+$ , the interaction between electrons and the positive background, to zero.

By canonical transformation mentioned above, this Hamiltonian can be transformed into the equivalent one expressed in the approximate form as

$$H = T + H_{coll} + H_I + H_{sr} + H_{se}, (2.9)$$

where  $T = \sum_{i} \frac{\mathbf{p}_{i}^{2}}{2m}$  is the total kinetic energy of the electrons. The second term,

$$H_{coll} = -\frac{1}{2} \sum_{k < k_c} \left( \left| p_{\mathbf{k}} \right|^2 + \omega_p^2 \left| q_{\mathbf{k}} \right|^2 \right)$$
(2.10)

represents the collective modes of the system which is responsible for the longrange Coulomb interaction, where  $k_c$  is the critical wave number. The third term,

$$H_I = \sqrt{\frac{4\pi}{V}} \frac{e}{m} \sum_{k < k_c} \hat{\varepsilon}_{\mathbf{k}} \cdot \left( \mathbf{p}_i - \frac{\hbar}{2} \mathbf{k} \right) q_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{x}_i}, \qquad (2.11)$$

describes a coupling of each electron with the collective field of the remaining electrons, and

$$H_{sr} = \frac{2\pi e^2}{V} \sum_{k>k_c, i\neq j} \frac{e^{i\mathbf{k}\cdot(\mathbf{x}_i - \mathbf{x}_j)}}{k^2}$$
(2.12)

is a short-range interaction to the Coulomb potential which has a nature similar to the screening potential as shown in Fig. (2.1). The last term

$$H_{se} = -2\pi n e^2 \sum_{k < k_c} \frac{1}{k^2}$$
(2.13)

is the self-energy, when i = j .

The presence of the interaction term  $H_I$  in H means that, unless this term can be neglected, we have not yet provide a purely collective description. The final transformation to independent collective modes is carried out by Bohm and Pines [1] with the use of perturbation theoretic canonical transformation theory. The final form of the Hamiltonian can be transformed into

$$H_{new} = T\left(1 - \frac{\gamma^3}{6}\right) + H_{coll} + H_{se} + H_{sr} + H_{el-el}, \qquad (2.14)$$

where  $H_{el-el}$  represents the electron-electron interaction which is small compared with the other terms and  $\gamma = k_c/k_F$ . Note that the new frequency of the collective oscillations, denoted by  $\omega$ , is given by the dispersion relation

$$1 = \frac{4\pi n e^2}{m} \sum_{i} \frac{1}{\left[\omega\left(k\right) \left(\mathbf{k} \cdot \mathbf{p}_i\right) / m\right]^2 - \left(\hbar k^2 / 2m\right)^2},$$
(2.15)



Figure 2.1: The Coulomb potential and its division into a short-range component  $(k > k_c)$  and a long-range component  $(k < k_c)$ . For comparison an exponentially screened potential  $[\sim \exp(-k_c r)]$  is also shown [11].

which leads to

$$\omega^{2}(k) = \omega_{p}^{2} + \frac{3}{5} \left(\frac{\hbar k_{F}}{m}\right)^{2} k^{2} + \left(\frac{\hbar k^{2}}{2m}\right)^{2} + \dots \quad (2.16)$$

It is interesting that the kinetic energy term in Eq. (2.14) implies that the electron mass has been increased to

$$m' = \frac{m}{(1 - \gamma^3/6)}.$$
 (2.17)

This may be interpreted as the inertial property of a bare electron surrounded by a plasmon field.

The correlation energy, the total energy subtracted by the Hartree-Fock energy, of this system has been calculated by Pines [10, 12], it gives

$$E_{corr} = E_{BP} - E_{HF}$$
  
=  $(E_{sr} + E_{lr}) - E_{HF}$   
=  $-0.114 + 0.0313 \ln r_s - 0.0005 r_s$  Ry, (2.18)

where

$$E_{corr} = \text{correlation energy,}$$

$$E_{BP} = \text{Bohm-Pines total energy,}$$

$$E_{HF} = \text{Hartree-Fock energy} = \frac{2.21}{r_s^2} - \frac{0.916}{r_s} \text{ Ry,}$$

$$E_{sr} = \text{short-range energy,}$$

$$E_{lr} = \text{long-range energy,}$$

 $r_s$  = the interparticle distance in the unit of the Bohr radius. (2.19)

Before going into a more discussion, let us survey the regimes of different electron density [13]. We may characterize the electron density by  $r_s$  that is

$$\frac{4}{3}\pi r_s^3 a_0^3 = \frac{1}{n},\tag{2.20}$$

where  $a_0 = \hbar^2 / m e^2$ .

For actual metals  $r_s$  varies between about 2 and 5.5, if we regard the valence electrons as making up our free electron gas. There are for the general problem three regions of interest:

1) High densities	$r_s \ll 1$
2) Metallic densities	$2 \leq r_s \lesssim 5.5$
3) Low densities	$r_s \gg 10.$

In the high density case, the electronic kinetic energy dominates the scene, and the interaction between the electrons is relatively weak. In this domain the Coulomb interaction can be handled rigorously, and this is Gell-Mann and Brueckner [2] have done to evaluate the energy. The basic idea of the method is to examine the increasingly divergent terms of the perturbation series and to notice that they fall into subseries that can be summed under the integral sign to give convergent results. The summation is performed by a technique similar to Feynman's method in field theory. They find that the total energy per electron can be written as a power series in  $r_s$ , which has the form

$$E_{total}^{GM-B} = \frac{a}{r_s^2} + \frac{b}{r_s} + c + d\ln r_s + er_s + fr_s \ln r_s + \dots$$
 Ry, (2.21)

where the first two terms represent the average kinetic energy and the exchange energy, and the remaining terms are the correlation energy. We might add that the basic approximation which they make is the random phase approximation, which is rigorously satisfied in the very high density limit.

The very low density regime presents a quite different picture. Here, as Wigner [14] who first pointed out, the electron will be found in a regular array. The total energy per electron may be written as

$$E_{total}^{Wig} = \frac{a'}{r_s} + \frac{b'}{r_s^{3/2}} + \frac{c'}{r_s^2} + \dots \quad \text{Ry},$$
(2.22)

where the first term represents the exchange energy plus the leading term in the correlation energy, the second term represents the zero-point energy of the electrons oscillating about their equilibrium positions, and the third term arises from the van der Waals interaction between the electrons. In this case, the interaction between electrons is all important and actually forces them into a regular array. Of course the random phase approximation is no longer valid here, since the electrons are now in a periodic array.

# 2.2 Lundqvist's Fröhlich-type electron-plasmon interaction

In Lundqvist's model of the interacting electron gas [5], he views the system as a continuous medium or dielectric medium and studies the behaviour of a single electron added into this system by the Green function technique. We will now discuss his model in more details.

The single-particle properties, i.e. the properties of the electron system, when one electron has been added or subtracted, are described by the electron Green function or propagator  $G(\mathbf{q}, \varepsilon) = G(q)$  [15, 16]. This propagator satisfies the Dyson equation

$$G(q) = G_0(q) + G_0(q) M(q) G(q).$$
(2.23)

Here the energy spectrum of the non-interacting electrons, described by the propagator

$$G_0(q) = \frac{1}{\varepsilon - \varepsilon(\mathbf{q}) + i(q_F - |\mathbf{q}|)\xi}$$
(2.24)

with  $\varepsilon \left( \mathbf{q} \right) = \hbar^2 \mathbf{q}^2 / 2m$ , is modified by a self-energy

$$M(q) = ie^{2}\hbar \int \frac{d^{4}k}{(2\pi)^{4}} e^{-i\xi\omega} G(q-k) \Gamma(q,k) V(k).$$
 (2.25)

This self-energy depends on the propagator  $V(k) = V(\mathbf{k}, \omega)$  for the effective interaction,

$$V(k) = \frac{v_{\mathbf{k}}}{\epsilon(k)} \equiv \frac{v_{\mathbf{k}}}{(1 - v_{\mathbf{k}}P(k))},$$
(2.26)

where  $v_{\mathbf{k}} = 4\pi/\mathbf{k}^2$  is the Coulomb potential in  $\mathbf{k}$  space and P(k) is the polarization

$$P(k) = -2ie^{2}\hbar \int \frac{d^{4}q}{\left(2\pi\right)^{4}} e^{i\xi\varepsilon} G(q) \Gamma(q,k) G(q-k). \qquad (2.27)$$

In his work,  $q_F$  is the Fermi wave number and  $\xi$  a positive infinitesimal constant. The vertex part  $\Gamma$  involves the coupling to the hierarchy of many-particle equations.

The expression for the self-energy may be written as a sum of a generalized exchange term ( it reduces to the Hartree-Fock exchange potential, if  $\Gamma$  is approximated by 1 and G by  $G_0$  ),

$$M_e(q) = ie^2 \hbar \int \frac{d^4k}{(2\pi)^4} e^{-i\xi\omega} G(q-k) \Gamma(q,k) v_{\mathbf{k}}, \qquad (2.28)$$

and a term involving the single-particle coupling to the density fluctuations [17],

$$M_{d}(q) = ie^{2}\hbar \int \frac{d^{4}k}{(2\pi)^{4}} G(q-k) \Gamma(q,k) S(k) v_{\mathbf{k}}^{2}, \qquad (2.29)$$

where

$$S(k) \equiv \frac{P(k)}{\left(1 - v_{\mathbf{k}}P(k)\right)} = \frac{1}{v_{\mathbf{k}}} \left(\frac{1}{\epsilon(k)} - 1\right)$$
(2.30)

is the propagator for the density fluctuations.

The collective excitations, the plasmons [1], appear in low approximations as poles of the density fluctuation propagator S(k). For instance, in random phase approximation

$$S(\mathbf{k},\omega) = e^{2} \int \frac{d^{3}q}{(2\pi)^{3}} \frac{2\left(\varepsilon\left(\mathbf{q}+\mathbf{k}\right)-\varepsilon\left(\mathbf{q}\right)\right)}{\omega^{2}-\left(\varepsilon\left(\mathbf{q}+\mathbf{k}\right)-\varepsilon\left(\mathbf{q}\right)\right)^{2}} \frac{\Theta\left(q_{F}-q\right)\Theta\left(|\mathbf{q}+\mathbf{k}|-q_{F}\right)}{|\varepsilon\left(\mathbf{k},\varepsilon\left(\mathbf{q}+\mathbf{k}\right)-\varepsilon\left(\mathbf{q}\right)\right)|^{2}} -\frac{1}{v_{\mathbf{k}}} \frac{1}{\partial\epsilon\left(\mathbf{k},\omega\left(k\right)\right)/\partial\omega} \frac{2\omega\left(k\right)\Theta\left(k_{c}-|\mathbf{k}|\right)}{\omega^{2}-\left(\omega\left(k\right)-i\xi\right)^{2}},$$
(2.31)

where  $\Theta(x)$  is the unit step function.

The first term expresses the propagation of the continuum of electron-hole pair states, and the second the propagation of the plasmon state, which exists as a pole only for k smaller than a critical momentum  $k_c$ . For long wavelength the plasmon frequency  $\omega(k)$  approaches  $\omega_p = \sqrt{4\pi n e^2/m}$ .

With an effective coupling

$$\left|g_{k}\right|^{2} = \frac{e^{2}v_{\mathbf{k}}}{\partial\epsilon\left(\mathbf{k},\omega\left(k\right)\right)/\partial\omega}$$
(2.32)

and a Bose propagator

$$D(k) \equiv D(\mathbf{k}, \omega) = \frac{2\omega(k)}{\omega^2 - \omega^2(k) + i\xi}$$
(2.33)

for the plasmon, the contribution to the self-energy from only the last term of Eq. (2.31) is

$$M_{p}(q) = i\hbar \int \frac{d^{4}k}{(2\pi)^{4}} |g_{k}|^{2} D(k) G(q-k)$$
(2.34)

in an approximation that neglects vertex corrections and the electron-hole pair excitation appeared in the first term of Eq. (2.31), or mathematically by taking  $k_c$  approach infinity. This is just the self-energy in the lowest self-consistent approximation for a fermion coupled to a boson field.

Eq. (2.34) can be derived from the following Hamiltonian:

$$H_{eff} = \sum_{\mathbf{q}} \varepsilon \left(\mathbf{q}\right) c_{\mathbf{q}}^{+} c_{\mathbf{q}} + \sum_{\mathbf{k}} \hbar \omega \left(k\right) b_{\mathbf{k}}^{+} b_{\mathbf{k}} + \sum_{\mathbf{q},\mathbf{k}} \sqrt{\frac{\hbar}{V}} g_{k} c_{\mathbf{q}+\mathbf{k}}^{+} c_{\mathbf{q}} \left(b_{\mathbf{k}} + b_{-\mathbf{k}}^{+}\right). \quad (2.35)$$

Here  $c_{\mathbf{q}}^{+}$ ,  $c_{\mathbf{q}}$  and  $b_{\mathbf{k}}^{+}$ ,  $b_{\mathbf{k}}$  are creation and annihilation operators for fermions and bosons, respectively, and V is the volume of the system. For the electron gas problem this effective Hamiltonian is applicable only to determine the dressing of the fermions due to the fermion-boson coupling. The source of both of the two last terms of Eq. (2.35) is the electron-electron interaction term of the exact Hamiltonian.

By using the relation [18]

$$\sum_{\mathbf{q}} c^+_{\mathbf{q}+\mathbf{k}} c_{\mathbf{q}} = e^{i\mathbf{k}\cdot\mathbf{x}}$$
(2.36)

for only one electron, this Hamiltonian can be rewritten, with the zero-point energy of plasmons, as

$$H_{eff} = \frac{\mathbf{p}^2}{2m} + \sum_{\mathbf{k}} \hbar \omega \left(k\right) \left(b_{\mathbf{k}}^+ b_{\mathbf{k}} + \frac{1}{2}\right) + \sum_{\mathbf{k}} \sqrt{\frac{\hbar}{V}} g_k \left(b_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} + b_{\mathbf{k}}^+ e^{-i\mathbf{k}\cdot\mathbf{x}}\right), \quad (2.37)$$

which is in the form of Fröhlich-type Hamiltonian similar to the polaron problem [6]. We will call this form of coupling **the plasmaron coupling**.

For Lundqvist's model [19], a simple interpolation formula for the dielectric function has been used. It can be expressed as

$$\epsilon \left( \mathbf{k}, \omega \right) = \frac{\omega^2 \left( k \right) - \omega^2}{\omega^2 \left( k \right) - \omega_p^2 - \omega^2}.$$
(2.38)

The form of the dielectric function given in Eq. (2.38) is chosen to produce the following sum rules:

$$\int_{0}^{\infty} d\omega \omega Im \left(1/\epsilon \left(\mathbf{k}, \omega + i\xi\right)\right) = -\frac{\pi}{2}\omega_{p}^{2}$$

$$\int_{0}^{\infty} d\omega \omega Im \left(\epsilon \left(\mathbf{k}, \omega + i\xi\right)\right) = \frac{\pi}{2}\omega_{p}^{2}.$$
(2.39)

The plasmon dispersion law is taken as

and

$$\omega^2(k) = \omega_p^2 + \frac{1}{3} \left(\frac{\hbar k_F}{m}\right)^2 k^2 + \left(\frac{\hbar k^2}{2m}\right)^2.$$
(2.40)

The coefficient in front of the  $k^2$  term in Eq. (2.40) is a factor 5/9 smaller than the RPA coefficient of Eq. (2.16). It is chosen in order to give the correct Thomas-Fermi potential in the static long wavelength limit [18]

$$v_{\mathbf{k}} \xrightarrow{\omega \longrightarrow 0} \frac{4\pi}{k^2 + k_{TF}^2},\tag{2.41}$$

where  $k_{TF} = 6\pi ne^2/E_F$  being the Thomas-Fermi screening constant.

As pointed out by Lundqvist, that the  $k^2$  term is not as important as the  $k^4$  term determining the contributions from short wavelength fluctuations. From the information given above, the electron-plasmon coupling constant  $g_k$  defining in Eq. (2.32) can be expressed by the equation

$$|g_k|^2 = \frac{4\pi e^2}{k^2} \left(\frac{1}{\partial \epsilon \left(\mathbf{k}, \omega\left(k\right)\right) / \partial \omega}\right)_{\omega = \omega_p} = \frac{2\pi e^2 \omega_p^2}{k^2 \omega\left(k\right)}.$$
 (2.42)

In the later chapters, Feynman path integral method will be applied to this model for some quantities of our interest, i.e. the ground state energy and the effective mass of the plasmaron.



## Chapter 3 Feynman's path integration

In this chapter we would like to discuss the path integral formulation of quantum mechanics [7], first proposed by R.P. Feynman, which is based on Lagrangian instead of Hamiltonian. For simplicity, we shall restrict ourselves to the case of a particle moving in one dimension. Thus the position at any time can be specified by a coordinate x, a function of  $\tau$ . By the path, then, we mean a function  $x(\tau)$ . Before we go on to give the rule for the quantum-mechanical case, let us remind ourselves of the situation in classical mechanics.

#### 3.1 The classical action

One of the most elegant ways of expressing the condition that determines the particular classical path  $\overline{x}(\tau)$  out of all the possible paths for a particle, from an initial point  $x_a$  at time  $t_a$  to a final point  $x_b$  at time  $t_b$ , is the principle of least action. That is, there exists a certain quantity S which can be computed for each path. The classical path  $\overline{x}$  is that for which S is a minimum. Actually, the real condition is that S be merely an extremum. That is to say, the value of S is unchanged in the first order if the path  $\overline{x}(\tau)$  is modified slightly. The quantity S is given by the expression

$$S = \int_{t_a}^{t_b} L\left(\dot{x}, x, \tau\right) d\tau, \qquad (3.1)$$

where L is the Lagrangian for the system. For a particle of mass m moving in a potential  $V(x, \tau)$ , which is a function of position and time, the Lagrangian is

$$L = \frac{m}{2}\dot{x}^{2} - V(x,\tau).$$
 (3.2)

The form of the extremum path  $\overline{x}(\tau)$  is determined with the usual procedures of the calculus of variations. Thus, suppose the path is varied away from  $\overline{x}$  by the amount  $\delta x(\tau)$ ; the condition that the end points of  $\overline{x}$  are fixed requires

$$\delta x\left(t_{a}\right) = \delta x\left(t_{b}\right) = 0. \tag{3.3}$$

The condition that  $\overline{x}$  be an extremum of S means

$$\delta S = S\left[\overline{x} + \delta x\right] - S\left[\overline{x}\right] = 0 \tag{3.4}$$

to first order in  $\delta x$ . Using the definition of Eq. (3.1) we may write

$$S[x + \delta x] = \int_{t_a}^{t_b} L(\dot{x} + \delta \dot{x}, x + \delta x, \tau) d\tau$$
  
$$= \int_{t_a}^{t_b} \left[ L(\dot{x}, x, \tau) + \delta \dot{x} \frac{\partial L}{\partial \dot{x}} + \delta x \frac{\partial L}{\partial x} \right] d\tau$$
  
$$= S[x] + \int_{t_a}^{t_b} \left( \delta \dot{x} \frac{\partial L}{\partial \dot{x}} + \delta x \frac{\partial L}{\partial x} \right) d\tau.$$
(3.5)

Upon integration by parts, the variation in S becomes

$$\delta S = \delta x \frac{\partial L}{\partial \dot{x}} \Big|_{t_a}^{t_b} - \int_{t_a}^{t_b} \delta x \left[ \frac{d}{d\tau} \left( \frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} \right] d\tau.$$
(3.6)

Since  $\delta x$  is 0 at the end points, the first term on the right-hand of this equation is 0. Between the end points,  $\delta x$  can take on any arbitrary value. Thus the extremum is that curve along which the following condition is always satisfied:

$$\frac{d}{d\tau} \left( \frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} = 0. \tag{3.7}$$

This is, of course, the classical Lagrangian equation of motion.

#### 3.2 The quantum-mechanical amplitude

The basic difference between classical mechanics and quantum mechanics should now be apparent. In classical mechanics the particular path of extremum action is associated with the particle's motion; in contrast, in quantum mechanics all possible paths must play roles including those which do not bear any resemblance to the classical path. There exists the amplitude, to go from an initial point ato a final point b, associated with each path. We must say how much each trajectory contributes to the total amplitude to go from a point a to a point b. Feynman conjectures that they contribute equal amounts to the total amplitude, but contribute at different phases. The phase of the contribution from a given path is the action S for that path in units of the quantum of action  $\hbar$ .

The propability P(b, a) to go from a point  $x_a$  at the time  $t_a$  to a point  $x_b$  at the time  $t_b$  is the absolute square of an amplitude G(b, a) to go from a to b

$$P(b,a) = |G(b,a)|^2$$
, (3.8)

where this amplitude is the sum of contribution  $\phi[x(\tau)]$  from each path.

$$G(b,a) = \sum_{\text{over all paths}} \phi[x(\tau)]. \qquad (3.9)$$

The contribution of a path has a phase proportional to the action S:

$$\phi[x(\tau)] = \text{const.} \exp\left(\frac{i}{\hbar}S[x(\tau)]\right).$$
(3.10)

The action is that for the corresponding classical system. The constant will be chosen to normalize G conveniently, and it will be taken up later when we discuss more mathematically just what we mean in Eq. (3.9) by a sum over paths.

#### 3.3 The sum over paths

We can follow through an analogous procedure of Riemann integral in defining the sum over all paths. To do this, we devide the independent variable time into steps of width  $\varepsilon$ . This gives us a set of values  $\tau_i$  spaced a distance  $\varepsilon$  apart between the value  $t_a$  and  $t_b$ . At each time  $\tau_i$  we select some special point  $x_i$ . We construct a path by connecting all the points so selected with straight lines. It is possible to define a sum over all paths constructed in this manner by taking a mutiple integral over all values of  $x_i$  for i between 1 and N - 1, where

$$N\varepsilon = t_b - t_a$$
  

$$\varepsilon = \tau_{i+1} - \tau_i$$
  

$$\tau_0 = t_a, \tau_N = t_b$$
  

$$x_0 = x_a, x_N = x_b.$$
(3.11)

The resulting equation is

$$G(b,a) = \int \int \dots \int \phi \left[ x\left(\tau\right) \right] dx_1 dx_2 \dots dx_{N-1}.$$
(3.12)

We do not integrate over  $x_0$  or  $x_N$  because these are the fixed end points  $x_a$  and  $x_b$ .

In the present case we can obtain a more representative sample of the complete set of all possible paths between a and b by making  $\varepsilon$  smaller. However, just as in the case of the Riemann integral, we cannot proceed to the limit of this process because the limit does not exist. Once again we must provide some normalizing factor which we expect will depend on  $\varepsilon$ .

Unfortunately, to define such a normalizing factor seems to be a very difficult problem and we do not know how to do it in general terms. But we



Figure 3.1: Diagram showing the sum over paths defined as a limit, in which at first the path is specified by giving only its coordinate x at a large number of specified times separated by very small intervals  $\epsilon$  [7].

do know how to give the definition for all situations which so far seem to have practical value. For example, take the case where the Lagrangian is given by Eq. (3.2). The normalizing factor turns out to be  $A^{-N}$ , where

$$A = \left(\frac{2\pi i\hbar\varepsilon}{m}\right)^{\frac{1}{2}}.$$
(3.13)

With this factor the limit exists and we may write

$$G(b,a) = \lim_{\varepsilon \to 0} \frac{1}{A} \int \int \dots \int \exp\left(\frac{i}{\hbar} S[b,a]\right) \frac{dx_1}{A} \frac{dx_2}{A} \dots \frac{dx_{N-1}}{A}, \quad (3.14)$$

where

$$S[b,a] = \int_{\tau_a}^{\tau_b} L(\dot{x}, x, \tau) d\tau \qquad (3.15)$$

is a line integral taken over the trajectory passing through the point  $x_i$  with straight sections in between, as in Fig. (3.1)

We shall write the sum over all paths in a less restrictive notation as

$$G(b,a) = \int_{a}^{b} \exp\left(\frac{i}{\hbar}S[b,a]\right) Dx(\tau), \qquad (3.16)$$

which we shall call a **path integral** and G(b, a) is named a **propagator**.

#### 3.4 Gaussian integrals

The simplest path integrals are those in which all of the variables appear up to the second degree in an exponent. We shall call them Gaussian integrals. In quantum mechanics this corresponds to a case in which the action S involves the path  $x(\tau)$  up to and including the second power.

To illustrate how the method works in such a case, consider a particle whose Lagrangian has the form

$$L = a(\tau) \dot{x}^{2} + b(\tau) \dot{x}x + c(\tau) x^{2} + d(\tau) \dot{x} + e(\tau) x + f(\tau).$$
(3.17)

The action is the integral of this function with respect to time between two fixed end points. Actually, in this form the Lagrangian is a little more general than necessary. The factor  $\dot{x}$  could be removed from those terms, in which it is linear through an integration by parts, but this fact is unimportant for our present propose. We wish to determine

$$G(b,a) = \int_{a}^{b} \exp\left[\frac{i}{\hbar} \int_{\tau_{a}}^{\tau_{b}} L(\dot{x}, x, \tau) d\tau\right] Dx(\tau), \qquad (3.18)$$

the integral over all paths which go from  $(x_a, t_a)$  to  $(x_b, t_b)$ .

Of course, it is possible to carry out this integral over all paths in the way which was first described by deviding the region into short time elements, and so on. That this will work follows from the fact that the integrand is an exponential of a quadratic form in the variables  $\dot{x}$  and x. Such an integral can always be carried out. We shall not go through this tedious calculation, since we can determine the most important characteristics of the propagator in the following manner.



Figure 3.2: Some possible alternative path in terms of the deviation  $y(\tau)$  from the classical path  $\bar{x}(\tau)$  [7].

Let  $\overline{x}(\tau)$  be the classical path between the specified end points. This is the path which is an extremum for the action S. In the notation we have been using

$$S_{cl}[b,a] = S\left[\overline{x}\left(\tau\right)\right]. \tag{3.19}$$

We can represent x in terms of  $\overline{x}$  and a new variable y:

$$x = \overline{x} + y. \tag{3.20}$$

That is to say, instead of defining a point on the path by its distance  $x(\tau)$  from and arbitrary coordinate axis, we measure instead the deviation  $y(\tau)$  from the classical path, as shown in Fig. (3.2).

At each  $\tau$  the variables x and y differ by the constant  $\overline{x}$ . (Of course, this is a different constant for each value of  $\tau$ .) Therefore, clearly,  $dx_i = dy_i$ for each specific point  $\tau_i$  in the subdivision of time. In general, we may say  $Dx(\tau) = Dy(\tau)$ . The integral for the action can be written

$$S[x(\tau)] = S[\overline{x}(\tau) + y(\tau)] = \int_{t_a}^{t_b} \left[ a(\tau) \left( \dot{x}^2 + 2\overline{\dot{x}}\dot{y} + \dot{y}^2 \right) + \dots \right] d\tau.$$
(3.21)

If all the terms which do not involve y are collected, the resulting integral is just  $S[\overline{x}(\tau)] = S_{cl}$ . If all the terms which contain y as a linear factor are collected, the resulting integral vanishes. This could be proved by actually carrying out the integration (some integration by parts would be involved); however, such a calculation is unnecessary, since we already know the result is true. The function  $\overline{x}(\tau)$  is determined by this very requirement. That is,  $\overline{x}$  is so chosen that there is no change in S, to first order, for variations of the path around  $\overline{x}$ . All that we can write

$$S[x(\tau)] = S_{cl}[b,a] + \int_{t_a}^{t_b} \left[ a(\tau) \dot{y}^2 + b(\tau) \dot{y}y + c(\tau) y^2 \right] d\tau.$$
(3.22)

The integral over paths does not depend upon the classical path, so the propagator can be written

$$G(b,a) = e^{(i/\hbar)S_{cl}[b,a]} \int_0^0 \left( \exp\left\{\frac{i}{\hbar} \int_{t_a}^{t_b} \left[a(\tau) \dot{y}^2 + b(\tau) \dot{y}y + c(\tau) y^2\right] d\tau \right\} \right) Dy(\tau) d\tau$$
(3.23)

Since all paths  $y(\tau)$  start from and return to the point y = 0, the integral over paths can be a function only of times at the end points. This means that the propagator can be written as

$$G(b,a) = F(t_b, t_a) \exp\left(\frac{i}{\hbar} S_{cl}[b,a]\right), \qquad (3.24)$$

where  $F(t_b, t_a)$  is called the prefactor which can be evaluated by using the Van Vleck-Pauli formula as follows

$$F(t_b, t_a) = \left[ \det \left( \frac{1}{2\pi\hbar} \frac{\partial^2}{\partial x_a \partial x_b} S_{cl} \right) \right]^{\frac{1}{2}}.$$
 (3.25)

It is interesting to note that the approximate expression  $G \sim \exp\left(\frac{i}{\hbar}S_{cl}\right)$  is exact for the case that S is a quadratic form.

### 3.5 The path integral formulation of density matrices

If a quantum-mechanical system is described by a complete set of wave function  $\phi_i(x)$ , the density matrix can be written in the form

$$\rho(x',x) = \sum_{i} \phi_i(x') \phi_i^*(x) e^{-\beta E_i}, \qquad (3.26)$$

where  $\beta = \frac{1}{kT}$  and T is the absolute temperature.

It is remarkable that Eq. (3.26) bears a close resemblance to the general expression for the propagator written as

$$G(x_2, t_2; x_1, t_1) = \sum_j \phi_j(x_2) \phi_j^*(x_1) e^{-(i/\hbar)E_j(t_2 - t_1)}.$$
(3.27)

The validity of this expression is restricted to situations in which the Hamiltonian is constant in time and  $t_2 > t_1$ . However, this situation is implied in statistical mechanics; for only if the Hamiltonian is constant in time can equilibrium be achieved. The difference between the form of Eq. (3.26) and that of Eq. (3.27) is in the argument of the exponential. If the time difference  $t_2 - t_1$  of Eq. (3.27) is replaced by  $-i\beta\hbar$ , we see that the expression for the density matrix is formally identical to the expression for the propagator corresponding to an imaginary negative time interval.

We can develop the similarity between these two expressions from another point of view. Suppose we write the density matrix in a way which makes it look a little bit more like a propagator, thus,  $k(x_2, u_2; x_1, u_1)$  for  $\rho(x_2, x_1)$ , where

$$k(x_2, u_2; x_1, u_1) = \sum_{i} \phi_i(x_2) \phi_i^*(x_1) e^{-[(u_2 - u_1)/\hbar]E_i}.$$
(3.28)

Then if  $x_2 = x'$ ,  $x_1 = x$ ,  $u_2 = \hbar\beta$ , and  $u_1 = 0$ , Eq. (3.28) becomes identical with Eq. (3.26).

If we differentiate k partially with respect to  $u_2$ , we get

$$-\hbar \frac{\partial k}{\partial u_2} = \sum_i E_i \phi_i(x_2) \phi_i^*(x_1) e^{-[(u_2 - u_1)/\hbar]E_i}.$$
(3.29)

Now we recall that  $E_i\phi_i(x') = H\phi_i(x')$  and let  $H_2$  imply operations only upon the variables  $x_2$ , we can write

$$-\hbar \frac{\partial k\left(2,1\right)}{\partial u_2} = H_2 k\left(2,1\right) \tag{3.30}$$

or, to put the same thing another way,

$$-\frac{\partial\rho\left(2,1\right)}{\partial\beta} = H_2\rho\left(2,1\right) \tag{3.31}$$

with simple Hamiltonians involving only momenta and coordinates, we have been able to write the propagator as a path integral. For example, if the Hamiltonian is given by

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x), \qquad (3.32)$$

then the solution for the propagator over a very short time interval  $t_2 - t_1 = \varepsilon$  is

$$G(2,1) = \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{\frac{1}{2}} \exp\left[\frac{im\left(x_2 - x_1\right)^2}{\varepsilon} - \frac{i}{\hbar}\varepsilon V\left(\frac{x_2 + x_1}{2}\right)\right],\tag{3.33}$$

which can be directly verified by substitution into Eq. (3.32) By building up a product of many propagators of the form of Eq. (3.33) and taking the limit as the time interval  $\varepsilon$  goes to 0 and the number of terms in the product becomes infinite, we have produced a path integral describing the propagator over a finite period of time. We can produce a solution to Eq. (3.30) in the same manner.
The solution for an infinitesimal interval of  $u_2 - u_1 = \eta$  is given by substituting  $\varepsilon = -i\eta$  into Eq. (3.33). Thus

$$k(x_2,\eta;x_1,0) = \left(\frac{m}{2\pi\hbar\eta}\right)^{\frac{1}{2}} \exp\left[-\frac{(m/2\eta)(x_2-x_1)^2 + \eta V\left[(x_2+x_1)/2\right]}{\hbar}\right].$$
(3.34)

That this is a valid solution of Eq. (3.30) can be demonstrated by direct substitution of Eq. (3.34) into Eq. (3.30).

The rule for the combination of functions defined for successive values of u is the same as the rule for the combination of propagators for successive intervals of time. That is,

$$k(2,1) = \int k(2,3) k(3,1) dx_3.$$
(3.35)

That this result still holds follows from the fact that Eq. (3.29) is a first-order derivative in u. This rule can be used to obtain the path integral to define k(2, 1) as

$$k(x_{2}, u_{2}; x_{1}, u_{1}) = \int \left( \exp\left\{ -\sum_{i=0}^{N-1} \left[ \frac{m}{2\hbar\eta} \left( x_{i+1} - x_{i} \right)^{2} + \frac{\eta}{\hbar} V(x_{i}) \right] \right\} \right) \prod_{i=1}^{N-1} \frac{dx_{i}}{a}.$$
(3.36)

The normalizing constant a now becomes

$$a = \left(\frac{2\pi\hbar\eta}{m}\right)^{\frac{1}{2}} \tag{3.37}$$

and the integral is carried out over all paths going from  $x_1$  to  $x_2$  (that is,  $x_i$  is  $x_1$ for i = 0 and  $x_2$  for i = N) in the interval  $u_2 - u_1 = N\eta$ .

The result of this derivation is that if we consider a path x(u) as a function which gives a coordinate in terms of the parameter u, and if we call  $\dot{x}$  the derivative dx/du, then

$$\rho\left(x_{2}, x_{1}\right) = \int \left(\exp\left\{-\frac{1}{\hbar}\int_{0}^{\beta\hbar}\left[\frac{m}{2}\dot{x}^{2}\left(u\right) + V\left(x\right)\right]du\right\}\right)Dx\left(u\right).$$
(3.38)

It is noticed that Eq. (3.38) can be obtained by just substituting -iu and  $-i\beta\hbar$ into  $\tau$  and  $t_2$  respectively of the propagator  $G(x_2, t_2; x_1, t_1)$  as follows

$$\rho(x_2, x_1) \equiv G(x_2, t_2 = -i\hbar\beta; x_1, t_1 = 0).$$
(3.39)



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### Chapter 4 The plasmaron propagator

The purpose of this chapter is to formulate the plasmaron problem in terms of Feynman's path integral [7]. This method has been applied very successfully to several problems such as polarons [6], disordered system [20], etc. The full form, including the off-diagonal part, of the plasmaron propagator (the diagonal part has already been calculated by Sa-yakanit [21]) will be calculated from Lundqvist's Fröhlich-type electron-plasmon Hamiltonian which will be used to study the ground state energy and the effective mass in the next chapter.

#### 4.1 The plasmaron action

From chapter 2, the Hamiltonian of the Fröhlich-type electron-plasmon interaction can be written, in the second quantization form, as

$$H = \frac{\mathbf{p}^2}{2m} + \sum_{\mathbf{k}} \hbar\omega\left(k\right) \left(b_{\mathbf{k}}^+ b_{\mathbf{k}} + \frac{1}{2}\right) + \sum_{\mathbf{k}} \sqrt{\frac{\hbar}{V}} g_k \left(b_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} + b_{\mathbf{k}}^+ e^{-i\mathbf{k}\cdot\mathbf{x}}\right).$$
(4.1)

Since the Hamiltonian given in Eq. (4.1) is expressed in terms of the second quantization creation and annihilation operators which is not appropriate for use in the path integral method, it has to be transformed back to the first quantization form using the fact that the plasmaron coordinate q and its conjugate momentum p are

$$q_{\mathbf{k}} = \sqrt{\frac{\hbar}{2m\omega(k)}} \left( b_{\mathbf{k}} + b_{\mathbf{k}}^{+} \right)$$

$$p_{\mathbf{k}} = \sqrt{\frac{m\omega(k)\hbar}{2}} \frac{\left( b_{\mathbf{k}} - b_{\mathbf{k}}^{+} \right)}{i}.$$
(4.2)

Solve these two equations to obtain  $b_{\mathbf{k}}$ ,  $b_{\mathbf{k}}^+$  and substitute into Eq. (4.1), then the Hamiltonian becomes

$$H = \frac{\mathbf{p}^2}{2m} + \sum_{\mathbf{k}} \left( \frac{p_{\mathbf{k}}^2}{2m} + \frac{m}{2} \omega^2 \left( k \right) q_{\mathbf{k}}^2 \right) + \sum_{\mathbf{k}} \sqrt{\frac{2m\omega\left( k \right)}{V}} g_k q_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}.$$
 (4.3)

The Lagrangian corresponding to the Hamiltonian in Eq. (4.3) can be easily evaluated by using the relation from classical mechanics

$$L = \sum_{I} p_i \dot{q}_i - H. \tag{4.4}$$

Therefore

$$L = \frac{m}{2}\dot{\mathbf{x}}^2 + \sum_{\mathbf{k}} \frac{m}{2} \left( \dot{q}_{\mathbf{k}}^2 - \omega^2 \left( k \right) q_{\mathbf{k}}^2 \right) - \sum_{\mathbf{k}} \sqrt{\frac{2m\omega\left( k \right)}{V}} g_k q_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}, \qquad (4.5)$$

where  $\mathbf{x}$  represents the coordinate of an electron. This form of Lagrangian will be used in the path integral formulation in the next section.

Now the plasmon coordinates  $q_{\mathbf{k}}$  can be eliminated by defining the transformation function for the electron and the plasmons, from an initial point at time  $\tau = 0$  to a final point at time  $\tau = t$ , as

$$\langle \mathbf{x}_{2}, q_{1}, ..., q_{N}, t; \mathbf{x}_{1}, q_{1}, ..., q_{N}, 0 \rangle$$

$$= \int_{\mathbf{x}(0)=\mathbf{x}_{1}}^{\mathbf{x}(t)=\mathbf{x}_{2}} D\mathbf{x}(\tau) \int_{q_{1}(0)=q_{1}}^{q_{1}(t)=q_{1}} Dq_{1}(\tau) ... \int_{q_{N}(0)=q_{N}}^{q_{N}(t)=q_{N}} Dq_{N}(\tau) \exp\left(\frac{i}{\hbar}S\right)$$

$$= \int_{\mathbf{x}_{1}}^{\mathbf{x}_{2}} D\mathbf{x}(\tau) \prod_{\mathbf{k}} \int_{q_{\mathbf{k}}}^{q_{\mathbf{k}}} Dq_{\mathbf{k}}(\tau) \exp\left(\frac{i}{\hbar}S\right)$$

$$= \int_{\mathbf{x}_{1}}^{\mathbf{x}_{2}} D\mathbf{x}(\tau) \exp\left(\frac{i}{\hbar} \int_{o}^{t} d\tau \frac{m}{2} \dot{\mathbf{x}}^{2}(\tau)\right) \prod_{\mathbf{k}} \int_{q_{\mathbf{k}}}^{q_{\mathbf{k}}} Dq_{\mathbf{k}}(\tau) \exp\left(\frac{i}{\hbar} S\left[q_{\mathbf{k}}\right]\right) (4.6)$$

where

$$S = \int_{0}^{t} d\tau \left[\frac{m}{2}\dot{\mathbf{x}}^{2}(\tau) + \sum_{\mathbf{k}}\frac{m}{2}\left(\dot{q}_{\mathbf{k}}^{2}(\tau) - \omega^{2}\left(k\right)q_{\mathbf{k}}^{2}(\tau)\right)\right]$$
$$-\sum_{\mathbf{k}}\sqrt{\frac{2m\omega\left(k\right)}{V}}g_{k}q_{\mathbf{k}}\left(\tau\right)e^{i\mathbf{k}\cdot\mathbf{x}(\tau)}$$
$$S\left[q_{\mathbf{k}}\right] = \int_{0}^{t} d\tau \left[\frac{m}{2}\left(\dot{q}_{\mathbf{k}}^{2}(\tau) - \omega^{2}\left(k\right)q_{\mathbf{k}}^{2}(\tau)\right) - \sqrt{\frac{2m\omega\left(k\right)}{V}}g_{k}q_{\mathbf{k}}\left(\tau\right)e^{i\mathbf{k}\cdot\mathbf{x}(\tau)}\right]$$
(4.7)

The path integrals over the plasmon coordinates q's can be performed using the well-known result [7] for the forced harmonic oscillator which has the Lagrangian equal to  $\frac{1}{2} \left( \dot{q}^2 \left( \tau \right) - \omega^2 q^2 \left( \tau \right) \right) + f \left( \tau \right) q \left( \tau \right)$  where  $f \left( \tau \right)$  is the time dependent force, in this case  $f \left( \tau \right) = -\sqrt{\frac{2m\omega(k)}{V}}g_k e^{i\mathbf{k}\cdot\mathbf{x}(\tau)}$ .

After integrating over all the plasmon coordinates, from Eq. (4.6) the transformation function becomes

$$\langle \mathbf{x}_{2}, t; \mathbf{x}_{1}, 0 \rangle = \int_{-\infty}^{\infty} \langle \mathbf{x}_{2}, q_{1}, ..., q_{N}, t; \mathbf{x}_{1}, q_{1}, ..., q_{N}, 0 \rangle dq_{1} dq_{2} ... dq_{N}$$

$$= \prod_{\mathbf{k}} \left( 2i \sin\left(\frac{\omega\left(k\right)}{2}t\right) \right)^{-1} \int_{\mathbf{x}_{1}}^{\mathbf{x}_{2}} D\mathbf{x}\left(\tau\right) \exp\left[\frac{i}{\hbar} \int_{0}^{t} d\tau \frac{m}{2} \dot{\mathbf{x}}^{2}\left(\tau\right) \right]$$

$$+ \frac{i}{\hbar} \sum_{\mathbf{k}} \frac{g'_{k}}{4m\omega\left(k\right)} \int_{0}^{t} \int_{0}^{t} d\tau d\sigma \left\{ \frac{\cos\left(\omega\left(k\right)\left(t/2 - |\tau - \sigma|\right)\right)}{\sin\left(\omega\left(k\right)t/2\right)} \right\}$$

$$\times \exp\left\{i\mathbf{k}\cdot\left(\mathbf{x}\left(\tau\right) - \mathbf{x}\left(\sigma\right)\right)\right\},$$

$$(4.8)$$

where  $g'_k = \frac{2m\omega(k)}{V}g_k^2$ .

It is assumed that k is a continuous variable so the summation  $\sum\limits_k$  can be changed into the integration written as

$$\sum_{\mathbf{k}} \longrightarrow \frac{V}{\left(2\pi\right)^3} \int d\mathbf{k}.$$

This gives

$$\langle \mathbf{x}_{2}, t; \mathbf{x}_{1}, 0 \rangle = \prod_{\mathbf{k}} \left( 2i \sin\left(\frac{\omega\left(k\right)}{2}t\right) \right)^{-1} \int_{\mathbf{x}_{1}}^{\mathbf{x}_{2}} D\mathbf{x}\left(\tau\right) \exp\left[\frac{i}{\hbar} \int_{0}^{t} d\tau \frac{m}{2} \dot{\mathbf{x}}^{2}\left(\tau\right) + \frac{i}{\hbar} \frac{e^{2} \omega_{p}^{2}}{2\pi} \int \frac{d\mathbf{k}}{4\pi k^{2} \omega\left(k\right)} \int_{0}^{t} \int_{0}^{t} d\tau d\sigma \frac{\cos\left(\omega\left(k\right)\left(t/2 - |\tau - \sigma|\right)\right)}{\sin\left(\omega\left(k\right)t/2\right)} \\ \times \exp\left\{i\mathbf{k}\cdot\left(\mathbf{x}\left(\tau\right) - \mathbf{x}\left(\sigma\right)\right)\right\}\right].$$

$$(4.9)$$

Since we are interested in the effect of the coupling between an electron and plasmons, we can ignore the prefactor in Eq. (4.9) which is the partition function for the plasmons (see appendix A). Therefore we will call, from now on, the transformation function in Eq. (4.9) without the prefactor the **plasmaron propagator**  $G(\mathbf{x}_2, \mathbf{x}_1; t)$  given explicitly as

$$G\left(\mathbf{x}_{2}, \mathbf{x}_{1}; t\right) = \int_{\mathbf{x}_{1}}^{\mathbf{x}_{2}} D\mathbf{x}\left(\tau\right) \exp\left(\frac{i}{\hbar}S_{p}\right), \qquad (4.10)$$

where  $S_p$  is the plasmaron action defined by the exponent in Eq. (4.9) without the  $i/\hbar$  factor

$$S_{p} = \int_{0}^{t} d\tau \frac{m}{2} \dot{\mathbf{x}}^{2}(\tau) + \frac{e^{2} \omega_{p}^{2}}{2\pi} \int_{0}^{t} \int_{0}^{t} d\tau d\sigma \int \frac{d\mathbf{k}}{4\pi k^{2} \omega(k)} \frac{\cos\left(\omega(k)\left(t/2 - |\tau - \sigma|\right)\right)}{\sin\left(\omega(k)t/2\right)} \times \exp\left\{i\mathbf{k}\cdot\left(\mathbf{x}\left(\tau\right) - \mathbf{x}\left(\sigma\right)\right)\right\}.$$
(4.11)

### 4.2 The trial action

From the plasmaron action of Eq. (4.11) it can be seen obviously that  $S_p$  is not a quadratic action, so the plasmaron propagator cannot be evaluated exactly. To carry out the path integral for the propagator  $G(\mathbf{x}_2, \mathbf{x}_1; t)$ , Feynman's method is applied by introducing a trial action  $S_0$ . Then the plasmaron propagator can be rewritten as

$$G\left(\mathbf{x}_{2}, \mathbf{x}_{1}; t\right) = G_{0}\left(\mathbf{x}_{2}, \mathbf{x}_{1}; t\right) \left\langle \exp\left\{\frac{i}{\hbar}\left(S_{p} - S_{0}\right)\right\} \right\rangle_{S_{0}}, \qquad (4.12)$$

where

$$G_0\left(\mathbf{x}_2, \mathbf{x}_1; t\right) = \int_{\mathbf{x}_1}^{\mathbf{x}_2} D\mathbf{x}\left(\tau\right) \exp\left(\frac{i}{\hbar}S_0\right)$$
(4.13)

and the average over  $S_0$ ,  $\langle O \rangle_{S_0}$ , is defined as

$$\langle O \rangle_{S_0} = \frac{\int_{\mathbf{x}_1}^{\mathbf{x}_2} D\mathbf{x}(\tau) O \exp\left(\frac{i}{\hbar}S_0\right)}{\int_{\mathbf{x}_1}^{\mathbf{x}_2} D\mathbf{x}(\tau) \exp\left(\frac{i}{\hbar}S_0\right)}.$$
(4.14)

By approximation  $G(\mathbf{x}_2, \mathbf{x}_1; t)$  to the first cumulant, the approximate propagator  $G_1(\mathbf{x}_2, \mathbf{x}_1; t)$  can be obtained as

$$G\left(\mathbf{x}_{2},\mathbf{x}_{1};t\right)\approx G_{1}\left(\mathbf{x}_{2},\mathbf{x}_{1};t\right)=G_{0}\left(\mathbf{x}_{2},\mathbf{x}_{1};t\right)\exp\left\{\frac{i}{\hbar}\left\langle S_{p}-S_{0}\right\rangle_{S_{0}}\right\}.$$
(4.15)

The trial action  $S_0(\kappa, \Omega)$  developed by Samathiyakanit [8] is introduced as a trial action  $S_0$  in this problem

$$S_0(\kappa,\Omega) = \int_0^t d\tau \left[ \frac{m}{2} \dot{\mathbf{x}}^2(\tau) - \frac{1}{8} \kappa \Omega \int_0^t d\sigma \, |\mathbf{x}(\tau) - \mathbf{x}(\sigma)|^2 \, \frac{\cos\left(\Omega\left(t/2 - |\tau - \sigma|\right)\right)}{\sin\left(\frac{\Omega t}{2}\right)} \right],\tag{4.16}$$

where  $\kappa$  and  $\Omega$  are variational parameters.

The physical meaning of this action is that of a two-particle model system in which an electron is coupled to a second fictitious particle where the position of the fictitious particle has been eliminated.

The above two-particle model system is well described by the Lagrangian

$$L_0(\kappa, M) = \frac{m}{2} \dot{\mathbf{x}}^2(\tau) + \frac{M}{2} \dot{\mathbf{y}}^2(\tau) - \frac{\kappa}{2} |\mathbf{x}(\tau) - \mathbf{y}(\tau)|^2, \qquad (4.17)$$

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

$$K_{2}(\mathbf{x}_{2}, \mathbf{y}_{2}, \mathbf{x}_{1}, \mathbf{y}_{1}; t) = \int D\mathbf{x}(\tau) D\mathbf{y}(\tau) \exp\left[\frac{i}{\hbar} \int_{0}^{t} d\tau \frac{1}{2} \left(m\dot{\mathbf{x}}^{2}(\tau) - \kappa \mathbf{x}^{2}(\tau)\right) + \frac{i}{\hbar} \int_{0}^{t} d\tau \frac{1}{2} \left(M\dot{\mathbf{y}}^{2}(\tau) - \kappa \mathbf{y}^{2}(\tau) + 2\kappa \mathbf{x}(\tau) \mathbf{y}(\tau)\right)\right].$$
(4.18)

Performing the path integration with respect to the second fictitious particle,

then

$$K_{2}(\mathbf{x}_{2}, \mathbf{y}_{2}, \mathbf{x}_{1}, \mathbf{y}_{1}; t) = \left(\frac{M\Omega}{2\pi i\hbar \sin\left(\Omega t\right)}\right)^{3} \int D\mathbf{x}(\tau) \exp\left[\frac{i}{\hbar} \int_{0}^{t} d\tau \frac{1}{2} \left(m\dot{\mathbf{x}}^{2}(\tau) - \kappa \mathbf{x}^{2}(\tau)\right) + \frac{i}{\hbar} S_{cl}(\mathbf{y}_{2}, \mathbf{y}_{1}; \kappa, \Omega)\right],$$

$$(4.19)$$

where

$$S_{cl}(\mathbf{y}_{2}, \mathbf{y}_{1}; \kappa, \Omega) = \frac{M\Omega}{2\sin(\Omega t)} [(\mathbf{y}_{2}^{2} + \mathbf{y}_{1}^{2})\cos(\Omega t) - 2\mathbf{y}_{2} \cdot \mathbf{y}_{1} + \frac{2\mathbf{y}_{2}}{M\Omega} \cdot \int_{0}^{t} d\tau \kappa \mathbf{x}(\tau)\sin(\Omega \tau) + \frac{2\mathbf{y}_{1}}{M\Omega} \cdot \int_{0}^{t} d\tau \kappa \mathbf{x}(\tau)\sin(\Omega(t-\tau)) - \frac{2}{M^{2}\Omega^{2}} \int_{0}^{t} \int_{0}^{t} d\tau d\sigma \kappa^{2} \mathbf{x}(\tau) \cdot \mathbf{x}(\sigma)\sin(\Omega(t-\tau))\sin(\Omega\sigma)]$$

$$(4.20)$$

with  $\Omega = \sqrt{\kappa/M}$ . The coordinate **y** can now be eliminated by first setting  $\mathbf{y}_2 = \mathbf{y}_1$  and then integrating Eq. (4.19) with respect to the variable  $\mathbf{y}_2$ . As a result, this can be written in the form

$$K_{1}(\mathbf{x}_{2}, \mathbf{x}_{1}; t) = \int d\mathbf{y}_{2} d\mathbf{y}_{1} \delta\left(\mathbf{y}_{2} - \mathbf{y}_{1}\right) K_{2}\left(\mathbf{x}_{2}, \mathbf{y}_{2}, \mathbf{x}_{1}, \mathbf{y}_{1}; t\right)$$

$$= \left(2i \sin\left(\frac{\Omega t}{2}\right)\right)^{-3} \int D\mathbf{x}\left(\tau\right) \exp\left[\frac{i}{\hbar} \int_{0}^{t} \frac{1}{2} \left(m\dot{\mathbf{x}}^{2}\left(\tau\right) - \kappa \mathbf{x}^{2}\left(\tau\right)\right)\right)$$

$$+ \frac{i}{\hbar} \frac{\kappa^{2}}{2M\Omega} \int_{0}^{t} \int_{0}^{\tau} d\tau d\sigma \mathbf{x}\left(\tau\right) \cdot \mathbf{x}\left(\sigma\right) \frac{\cos\left(\Omega\left(t/2 - |\tau - \sigma|\right)\right)}{\sin\left(\frac{\Omega t}{2}\right)} \left[.$$

$$(4.21)$$

Rearranging terms in the exponent of Eq. (4.21), it becomes

$$K_{1}(\mathbf{x}_{2}, \mathbf{x}_{1}; t) = \left(2i \sin\left(\frac{\Omega t}{2}\right)\right)^{-3} \int D\mathbf{x}(\tau) \exp\left[\frac{i}{\hbar} \int_{o}^{t} d\tau \left(\frac{m}{2} \dot{\mathbf{x}}^{2}(\tau)\right) - \frac{\kappa \Omega}{8} \int_{0}^{t} d\sigma |\mathbf{x}(\tau) - \mathbf{x}(\sigma)|^{2} \frac{\cos\left(t/2 - |\tau - \sigma|\right)}{\sin\left(\frac{\Omega t}{2}\right)}\right]$$
(4.22)

The expression in the exponent of the above equation is simply the trial action  $S_0(\kappa, \Omega)$  that has been introduced in Eq. (4.16).

#### 4.3 The approximate plasmaron propagator

As we can see from Eq. (4.15) of the previous section that the propagator can be obtained if one can calculate  $G_0$  and  $\langle S_p - S_0 \rangle_{S_0}$ .

First of all, consider  $\langle S_p - S_0 \rangle_{S_0}$  which can be rewritten as

$$\left\langle S_p - S_0 \right\rangle_{S_0} = \left\langle S_p - \int_0^t d\tau \frac{m}{2} \dot{\mathbf{x}}^2(\tau) \right\rangle_{S_0} - \left\langle S_0 - \int_0^t d\tau \frac{m}{2} \dot{\mathbf{x}}^2(\tau) \right\rangle_{S_0}.$$
 (4.23)

Substitute the first and second terms on the right-hand side with Eq. (4.11) and Eq. (4.16) respectively, we arrive at the expression

$$\langle S_p - S_0 \rangle_{S_0} = \frac{e^2 \omega_p^2}{2\pi} \int_0^t \int_0^t d\tau d\sigma \int_{-\infty}^\infty \frac{d\mathbf{k}}{4\pi k^2 \omega \left(k\right)} \frac{\cos\left(\omega\left(k\right)\left(t/2 - |\tau - \sigma|\right)\right)}{\sin\left(\frac{\omega\left(k\right)t}{2}\right)} \\ \times \langle \exp\left\{i\mathbf{k}\cdot\left(\mathbf{x}\left(\tau\right) - \mathbf{x}\left(\sigma\right)\right)\right\} \rangle_{S_0} \\ + \frac{\kappa\Omega}{8} \int_0^t \int_0^t d\tau d\sigma \frac{\cos\left(\Omega\left(t/2 - |\tau - \sigma|\right)\right)}{\sin\left(\frac{\Omega t}{2}\right)} \left\langle |\mathbf{x}\left(\tau\right) - \mathbf{x}\left(\sigma\right)|^2 \right\rangle_{S_0.}$$

$$(4.24)$$

Therefore the main task now is to calculate  $\langle \exp \{i\mathbf{k} \cdot (\mathbf{x}(\tau) - \mathbf{x}(\sigma))\} \rangle_{S_0}$  and  $\langle |\mathbf{x}(\tau) - \mathbf{x}(\sigma)|^2 \rangle_{S_0}$ .

The first quantity of Eq. (4.24) can be achieved using the generating

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functional derived by Samathiyakanit [8] as shown below

$$\left\langle \exp\left\{\frac{i}{\hbar} \int_{0}^{t} d\tau \mathbf{f}\left(\tau\right) \cdot \mathbf{x}\left(\tau\right)\right\} \right\rangle_{S_{0}}$$

$$= \exp\left\{\frac{i}{\hbar} \left[\mathbf{x}_{2} \cdot \int_{0}^{t} d\tau \mathbf{f}\left(\tau\right) \left\{\frac{\mu}{m} \left(\frac{\sin\left(\nu\tau\right)}{\sin\left(\nu\tau\right)} - \frac{\sin\left(\frac{\nu}{2}\left(t-\tau\right)\right)\sin\left(\frac{\nu}{2}\tau\right)}{\cos\left(\frac{\nu}{2}t\right)}\right) + \frac{\mu\tau}{Mt}\right\} \right.$$

$$\left. + \mathbf{x}_{1} \cdot \int_{0}^{t} d\tau \mathbf{f}\left(\tau\right) \left\{\frac{\mu}{m} \left(\frac{\sin\left(\nu\left(t-\tau\right)\right)}{\sin\left(\nu\tau\right)} - \frac{\sin\left(\frac{\nu}{2}\left(t-\tau\right)\right)\sin\left(\frac{\nu}{2}\tau\right)}{\cos\left(\frac{\nu}{2}\tau\right)}\right) + \frac{\mu}{Mt}\left(t-\tau\right)\right\} \right.$$

$$\left. - \int_{0}^{t} \int_{0}^{t} d\tau d\sigma \mathbf{f}\left(\tau\right) \cdot \mathbf{f}\left(\sigma\right) \left\{\frac{\mu}{m^{2}\nu\sin\left(\nu\tau\right)} \left(\sin\left(\nu\left(t-\tau\right)\right)\sin\left(\nu\sigma\right)\right) - 4\sin\left(\frac{\nu}{2}\left(t-\tau\right)\right)\sin\left(\frac{\nu}{2}\tau\right)\sin\left(\frac{\nu}{2}\left(t-\sigma\right)\right)\sin\left(\frac{\nu}{2}\sigma\right)\right) + \frac{\mu}{mM}\left(t-\tau\right)\frac{\sigma}{t}\right\}\right]\right\},$$

$$\left. (4.25\right)$$

where  $\mu = \frac{mM}{m+M}$ ,  $\nu = \sqrt{\kappa/\mu}$  and  $\nu^2 = \Omega^2 + \kappa/m$ .

We can express  $\langle \exp \{ i \mathbf{k} \cdot (\mathbf{x} (\tau) - \mathbf{x} (\sigma)) \} \rangle_{S_0}$  to be in the same form as the generating functional as

$$\langle \exp \left\{ i \mathbf{k} \cdot (\mathbf{x} (\tau) - \mathbf{x} (\sigma)) \right\} \rangle_{S_0} = \left\langle \exp \left\{ \frac{i}{\hbar} \int_0^t d\tau' \hbar \mathbf{k} \left[ \delta (\tau' - \tau) - \delta (\tau' - \sigma) \right] \cdot \mathbf{x} (\tau') \right\} \right\rangle_{S_0} = \left\langle \exp \left\{ \frac{i}{\hbar} \int_0^t d\tau' \mathbf{f}_\delta (\tau') \cdot \mathbf{x} (\tau') \right\} \right\rangle_{S_0},$$
(4.26)

where  $\mathbf{f}_{\delta}\left( au^{\prime}
ight)$  is the delta force defined by

$$\mathbf{f}_{\delta}\left(\tau'\right) = \hbar \mathbf{k} \cdot \left[\delta\left(\tau' - \tau\right) - \delta\left(\tau' - \sigma\right)\right]. \tag{4.27}$$

Then replace  $\mathbf{f}(\tau)$  and  $\mathbf{f}(\sigma)$  in Eq. (4.25) with the delta force, after a tedious calculation we get

$$\langle \exp\left\{i\mathbf{k}\cdot\left(\mathbf{x}\left(\tau\right)-\mathbf{x}\left(\sigma\right)\right)\right\}\rangle_{S_{0}} = \exp\left\{i\mathbf{k}\cdot\left(\mathbf{x}_{2}-\mathbf{x}_{1}\right)\mu\left[\frac{\sin\left(\frac{\nu}{2}\left(\tau-\sigma\right)\right)\cos\left(\frac{\nu}{2}\left(t-\tau-\sigma\right)\right)}{m\sin\left(\frac{\nu}{2}t\right)}+\frac{1}{Mt}\left(\tau-\sigma\right)\right] - \frac{i\hbar\mu k^{2}}{2m\nu^{2}}\left[\frac{2\nu\sin\left(\frac{\nu}{2}\left(\tau-\sigma\right)\right)\sin\left(\frac{\nu}{2}\left(t-|\tau-\sigma|\right)\right)}{m\sin\left(\frac{\nu}{2}t\right)}+\frac{\nu^{2}}{Mt}\left|\tau-\sigma\right|\left(t-|\tau-\sigma|\right)\right]\right\}.$$

$$(4.28)$$

The next step is to find  $\left\langle \left| \mathbf{x} \left( \tau \right) - \mathbf{x} \left( \sigma \right) \right|^2 \right\rangle_{S_0}$ .

The left-hand side of Eq. (4.28) can be expanded in cumulants [22], and because  $S_0(\kappa, \Omega)$  is quadratic, the expansion can be written as (see appendix B)

$$\langle \exp \{ i \mathbf{k} \cdot (\mathbf{x} (\tau) - \mathbf{x} (\sigma)) \} \rangle_{S_0}$$
  
=  $\exp \{ i \mathbf{k} \cdot \langle (\mathbf{x} (\tau) - \mathbf{x} (\sigma)) \rangle_{S_0}$   
 $+ \frac{1}{2} \sum_{i=1}^{3} k_i^2 \left( \langle (\mathbf{x}_i (\tau) - \mathbf{x}_i (\sigma)) \rangle_{S_0}^2 - \langle (\mathbf{x}_i (\tau) - \mathbf{x}_i (\sigma))^2 \rangle_{S_0} \right) \}.$  (4.29)

When comparing with the result from Eq. (4.28), we obtain

$$\langle (\mathbf{x} (\tau) - \mathbf{x} (\sigma)) \rangle_{S_0} = \mu \left[ \frac{\sin \left( \frac{\nu}{2} (\tau - \sigma) \right) \cos \left( \frac{\nu}{2} (t - \tau - \sigma) \right)}{m \sin \left( \frac{\nu}{2} t \right)} + \frac{1}{Mt} (\tau - \sigma) \right] (\mathbf{x}_2 - \mathbf{x}_1) (4.30)$$

and

$$\left\langle \left| \mathbf{x} \left( \tau \right) - \mathbf{x} \left( \sigma \right) \right|^{2} \right\rangle_{S_{0}}$$

$$= \frac{3i\hbar\mu}{m\nu^{2}} \left[ \frac{2\nu\sin\left(\frac{\nu}{2}\left( \tau - \sigma \right) \right)\sin\left(\frac{\nu}{2}\left( t - \left| \tau - \sigma \right| \right) \right)}{m\sin\left(\frac{\nu}{2}t\right)} + \frac{\nu^{2}}{Mt} \left| \tau - \sigma \right| \left( t - \left| \tau - \sigma \right| \right) \right]$$

$$+ \mu^{2} \left[ \frac{\sin\left(\frac{\nu}{2}\left( \tau - \sigma \right) \right)\cos\left(\frac{\nu}{2}\left( t - \tau - \sigma \right) \right)}{m\sin\left(\frac{\nu}{2}t\right)} + \frac{1}{Mt} \left( \tau - \sigma \right) \right]^{2} \left| \mathbf{x}_{2} - \mathbf{x}_{1} \right|^{2}. (4.31)$$

We are now ready to get the quantity of our interest by substituting Eq. (4.28)

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and Eq. (4.31) into Eq. (4.24), then the result is

$$\begin{aligned} &\langle S_p - S_0 \rangle_{S_0} \\ &= \frac{e^2 \omega_p^2}{2\pi} \int_0^t \int_0^t d\tau d\sigma \int \frac{d\mathbf{k}}{4\pi k^2 \omega(k)} \frac{\cos\left(\omega\left(k\right)\left(t/2 - |\tau - \sigma|\right)\right)}{\sin\left(\frac{\omega(k)}{2}t\right)} \\ &\times \exp\{i\mathbf{k} \cdot (\mathbf{x}_2 - \mathbf{x}_1) \,\mu[\frac{\sin\left(\frac{\nu}{2}\left(\tau - \sigma\right)\right)\cos\left(\frac{\nu}{2}\left(t - \tau - \sigma\right)\right)}{m\sin\left(\frac{\nu}{2}t\right)} + \frac{1}{Mt}\left(\tau - \sigma\right)] \\ &- \frac{i\hbar\mu k^2}{2m\nu^2} [\frac{2\nu\sin\left(\frac{\nu}{2}\left(\tau - \sigma\right)\right)\sin\left(\frac{\nu}{2}\left(t - |\tau - \sigma|\right)\right)}{m\sin\left(\frac{\nu}{2}t\right)} + \frac{\nu^2}{Mt} \left|\tau - \sigma\right|\left(t - |\tau - \sigma|\right)]\} \\ &+ \frac{\kappa\Omega}{8} \int_0^t \int_0^t d\tau d\sigma \frac{\cos\left(\Omega\left(t/2 - |\tau - \sigma|\right)\right)}{\sin\left(\frac{\Omega}{2}t\right)} \\ &\times \frac{3i\hbar\mu}{m\nu^2} [\frac{2\nu\sin\left(\frac{\nu}{2}\left(\tau - \sigma\right)\right)\sin\left(\frac{\nu}{2}\left(t - |\tau - \sigma|\right)\right)}{m\sin\left(\frac{\nu}{2}t\right)} + \frac{\nu^2}{Mt} \left|\tau - \sigma\right|\left(t - |\tau - \sigma|\right)] \\ &+ \frac{\kappa\Omega}{8} \int_0^t \int_0^t d\tau d\sigma \frac{\cos\left(\Omega\left(t/2 - |\tau - \sigma|\right)\right)}{\sin\left(\frac{\Omega}{2}t\right)} \\ &\times \mu^2 [\frac{\sin\left(\frac{\nu}{2}\left(\tau - \sigma\right)\right)\cos\left(\frac{\nu}{2}\left(t - \tau - \sigma\right)\right)}{m\sin\left(\frac{\nu}{2}t\right)} + \frac{1}{Mt} \left(\tau - \sigma\right)]^2 \left|\mathbf{x}_2 - \mathbf{x}_1\right|^2. \end{aligned} \tag{4.32}$$

The propagator  $G_0$  has already been derived by Samathiyakanit [8]. It is written as

$$G_0\left(\mathbf{x}_2, \mathbf{x}_1; t\right) = \left(\frac{m}{2\pi i\hbar t}\right)^{\frac{3}{2}} \left(\frac{\nu\sin\left(\frac{\Omega}{2}t\right)}{\Omega\sin\left(\frac{\nu}{2}t\right)}\right)^3 \exp\left[\frac{i}{\hbar}\left(\frac{\mu\nu}{4}\cot\left(\frac{\nu}{2}t\right) + \frac{m\mu}{2Mt}\right) |\mathbf{x}_2 - \mathbf{x}_1|^2\right].$$
(4.33)

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Therefore, the approximate propagator becomes

$$G_{1}\left(\mathbf{x}_{2},\mathbf{x}_{1};t\right) = \left(\frac{m}{2\pi i \hbar t}\right)^{\frac{3}{2}} \left(\frac{\nu \sin\left(\frac{\Omega}{2}t\right)}{\Omega \sin\left(\frac{\nu}{2}t\right)}\right)^{3} \exp\left\{\frac{i}{\hbar}\left(\frac{\mu\nu}{4}\cot\left(\frac{\nu}{2}t\right) + \frac{m\mu}{2Mt}\right)|\mathbf{x}_{2} - \mathbf{x}_{1}|^{2} + \frac{i}{\hbar}\frac{e^{2}\omega_{p}^{2}}{2\pi}\int_{0}^{t}\int_{0}^{t}d\tau d\sigma \int \frac{d\mathbf{k}}{4\pi k^{2}\omega\left(k\right)}\frac{\cos\left(\omega\left(k\right)\left(t/2 - |\tau - \sigma|\right)\right)}{\sin\left(\frac{\omega\left(k\right)}{2}t\right)} \\ \times \exp\left\{i\mathbf{k}\cdot\left(\mathbf{x}_{2} - \mathbf{x}_{1}\right)\mu\right|\frac{\sin\left(\frac{\nu}{2}\left(\tau - \sigma\right)\right)\cos\left(\frac{\nu}{2}\left(t - \tau - \sigma\right)\right)}{m\sin\left(\frac{\nu}{2}t\right)} + \frac{1}{Mt}\left(\tau - \sigma\right)\right] \\ -\frac{i\hbar\mu k^{2}}{2m\nu^{2}}\left[\frac{2\nu\sin\left(\frac{\nu}{2}\left(\tau - \sigma\right)\right)\sin\left(\frac{\nu}{2}\left(t - |\tau - \sigma|\right)\right)}{m\sin\left(\frac{\nu}{2}t\right)} + \frac{\nu^{2}}{Mt}\left|\tau - \sigma\left(t - |\tau - \sigma|\right)\right]\right\} \\ -\frac{\kappa\Omega}{8}\frac{3\mu}{m\nu^{2}}\int_{0}^{t}\int_{0}^{t}d\tau d\sigma\frac{\cos\left(\Omega\left(t/2 - |\tau - \sigma|\right)\right)}{\sin\left(\frac{\Omega}{2}t\right)} \\ \times\left[\frac{2\nu\sin\left(\frac{\nu}{2}\left(\tau - \sigma\right)\right)\sin\left(\frac{\nu}{2}\left(t - |\tau - \sigma|\right)\right)}{m\sin\left(\frac{\nu}{2}t\right)} + \frac{\nu^{2}}{Mt}\left|\tau - \sigma\left(t - |\tau - \sigma|\right)\right] \\ + \frac{i}{\hbar}\frac{\kappa\Omega}{8}\int_{0}^{t}\int_{0}^{t}d\tau d\sigma\frac{\cos\left(\Omega\left(t/2 - |\tau - \sigma|\right)\right)}{\sin\left(\frac{\Omega}{2}t\right)} \\ \times\mu^{2}\left[\frac{\sin\left(\frac{\nu}{2}\left(\tau - \sigma\right)\right)\cos\left(\frac{\nu}{2}\left(t - \tau - \sigma\right)\right)}{m\sin\left(\frac{\nu}{2}t\right)} + \frac{1}{Mt}\left(\tau - \sigma\right)\right]^{2}\left|\mathbf{x}_{2} - \mathbf{x}_{1}\right|^{2}\right\}.$$
(4.34)

Before we go on to find the ground state energy or any interesting quantities, the propagator has to be transformed into the density matrix by just replacing t,  $\tau$ ,  $\sigma$  as followed

$$\begin{array}{cccc} t & \longrightarrow & -i\beta\hbar \\ \tau & \longrightarrow & -i\tau \\ \sigma & \longrightarrow & -i\sigma \end{array}$$

After doing this, the density matrix will be expressed in the form

$$\begin{aligned} \rho_{1}\left(\mathbf{x}_{2},\mathbf{x}_{1};\beta\right) &= \left(\frac{m}{2\pi\hbar^{2}\beta}\right)^{\frac{3}{2}} \left(\frac{\nu\sinh\left(\frac{\Omega}{2}\beta\hbar\right)}{\Omega\sinh\left(\frac{\nu}{2}\beta\hbar\right)}\right)^{3} \\ &\times\exp\{-\frac{1}{\hbar}\left(\frac{\mu\nu}{4}\coth\left(\frac{\nu}{2}\beta\hbar\right) + \frac{m\mu}{2M\beta\hbar}\right)|\mathbf{x}_{2} - \mathbf{x}_{1}|^{2} \\ &+ \frac{e^{2}\omega_{p}^{2}}{2\pi\hbar}\int_{0}^{\beta\hbar}\int_{0}^{\beta\hbar}d\tau d\sigma\int\frac{d\mathbf{k}}{4\pi k^{2}\omega\left(k\right)}\frac{\cosh\left(\omega\left(k\right)\left(\beta\hbar/2 - |\tau - \sigma|\right)\right)}{\sinh\left(\frac{\omega\left(k\right)}{2}\beta\hbar\right)} \\ &\times\exp\{i\mathbf{k}\cdot\left(\mathbf{x}_{2} - \mathbf{x}_{1}\right)\mu\left[\frac{\sinh\left(\frac{\nu}{2}\left(\tau - \sigma\right)\right)\cosh\left(\frac{\nu}{2}\left(\beta\hbar - \tau - \sigma\right)\right)}{m\sinh\left(\frac{\nu}{2}\beta\hbar\right)} \\ &+ \frac{1}{M\beta\hbar}\left(\tau - \sigma\right)\right] - \frac{\hbar k^{2}}{2m\nu^{2}}f\left(|\tau - \sigma|,\beta\right)\} \\ &+ \frac{3}{2}\left(1 - \frac{\Omega^{2}}{\nu^{2}}\right)\left[\frac{\nu}{2}\beta\hbar\coth\left(\frac{\nu}{2}\beta\hbar\right) - 1\right] \\ &+ \frac{\kappa\Omega}{8}\int_{0}^{\beta\hbar}\int_{0}^{\beta\hbar}d\tau d\sigma\frac{\cosh\left(\Omega\left(\beta\hbar/2 - |\tau - \sigma|\right)\right)}{\sinh\left(\frac{\Omega}{2}\beta\hbar\right)} \\ &\times\mu^{2}\left[\frac{\sinh\left(\frac{\nu}{2}\left(\tau - \sigma\right)\right)\cosh\left(\frac{\nu}{2}\left(\beta\hbar - \tau - \sigma\right)\right)}{m\sinh\left(\frac{\nu}{2}\beta\hbar\right)} + \frac{1}{M\beta\hbar}\left(\tau - \sigma\right)\right]^{2}|\mathbf{x}_{2} - \mathbf{x}_{1}|^{2}\}, \end{aligned}$$

$$(4.35)$$

where

$$f(|\tau - \sigma|, \beta) = \mu \left[ \frac{2\nu \sinh\left(\frac{\nu}{2}(\tau - \sigma)\right) \sinh\left(\frac{\nu}{2}(\beta\hbar - |\tau - \sigma|)\right)}{m \sinh\left(\frac{\nu}{2}\beta\hbar\right)} + \frac{\nu^2}{M\beta\hbar} |\tau - \sigma|(\beta\hbar - |\tau - \sigma|)\right]$$
(4.36)

Note that the term  $\frac{3}{2}\left(1-\frac{\Omega^2}{\nu^2}\right)\left[\frac{\nu}{2}\beta\hbar\coth\left(\frac{\nu}{2}\beta\hbar\right)-1\right]$  on the seventh line has been derived from the expression

$$\frac{\kappa\Omega}{8} \frac{3\mu}{m\nu^2} \int_0^{\beta\hbar} \int_0^{\beta\hbar} d\tau d\sigma \frac{\cosh\left(\Omega\left(\beta\hbar/2 - |\tau - \sigma|\right)\right)}{\sinh\left(\frac{\Omega}{2}\beta\hbar\right)} \times \left[\frac{2\nu\sinh\left(\frac{\nu}{2}\left(\tau - \sigma\right)\right)\sinh\left(\frac{\nu}{2}\left(\beta\hbar - |\tau - \sigma|\right)\right)}{m\sinh\left(\frac{\nu}{2}\beta\hbar\right)} + \frac{\nu^2}{M\beta\hbar} \left|\tau - \sigma\right|\left(\beta\hbar - |\tau - \sigma|\right)\right].$$

By setting  $|\tau - \sigma| = u$  and using the relation

$$\int_{0}^{\beta} \int_{0}^{\beta} d\tau d\sigma g\left(\left|\tau - \sigma\right|\right) = 2 \int_{0}^{\beta} du \left(\beta - u\right) g\left(u\right), \qquad (4.37)$$

we obtain the result as mentioned above.



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### Chapter 5 The ground state of the plasmaron

In this chapter the plasmaron ground state energy and its effective mass will be derived from the density matrix obtained in the previous chapter. First of all, we would like to discuss the effective mass defined by the off-diagonal part, called **Feynman mass**, and the diagonal part, called **Krivoglaz-Pekar mass**, of the density matrix as mentioned in the polaron problem, then the relation between the two effective masses is revealed.

### 5.1 The path integral definition of the effective mass

Consider an electron moving in an interacting electron gas. If we neglect the electron-electron interaction, only electron-plasmon interaction is taken into account. It is possible to replace the system of an electron interacting with its surrounding (in this case, a set of plasmons) by regarding this system as a free particle with finite ground state energy. Owing to collecting every effect of plasmons on an electron, these will appear in the form of an inertia which gives an additional value to the electron mass. A new value of this quasi-particle mass is called an **effective mass** denoted by  $m^*$ .

The definition of an effective mass can be determined by various ways. The most common approach is to first looking at the following equation,

$$E = E_0 + \frac{\mathbf{p}^2}{2m^*},\tag{5.1}$$

where  $E_0$  is the ground state energy or self-energy of the quasi-particle,

 $m^\ast$  is an effective mass of the equivalent system.

In this thesis, we will focus on the path integral definition. Assuming that the velocity of the quasi-particle is small, so it can be written as

$$\mathbf{U} = \frac{\mathbf{R}_2 - \mathbf{R}_1}{t},\tag{5.2}$$

where t is the time interval between two points  $\mathbf{R}_1$  and  $\mathbf{R}_2$ ,

U is a mean group velocity.

According to Feynman [6, 23], the effective mass can be determined by the off-diagonal part of the density matrix which can be expressed in an approximate form of a free particle as

$$\rho \xrightarrow{\beta \longrightarrow \infty} \exp\left(-m_F \frac{|\mathbf{R}_2 - \mathbf{R}_1|^2}{2\beta\hbar^2}\right).$$
(5.3)

We will call the effective mass obtained by this method the **Feynman mass**,  $m_F$ .

There is another way to treat this problem. That is, the effective mass may be defined using the diagonal part of the density matrix (setting  $\mathbf{R}_2 = \mathbf{R}_1$ ), introduced by Krivoglaz and Pekar [24]. For this method the density matrix can be written in an approximate form as

$$\rho \stackrel{\beta \longrightarrow \infty}{\sim} \left( \frac{m_{KP}}{2\pi\beta\hbar^2} \right)^{\frac{3}{2}} \exp\left(-E_0\beta\right).$$
(5.4)

The effective mass will be called the **Krivoglaz-Pekar mass**,  $m_{KP}$ , following the name used in the polaron problem.

We are now in a position to study the ground state energy and the effective mass of the plasmaron from the last two equations mentioned above.

## 5.2 The ground state energy and the effective mass of the plasmaron

To obtain the quantities of interest, it is very important to note that from the two-particle model system in previous chapter, instead of considering the electron coordinates, it is more convenient to transform these coordinates into the center of mass coordinates in which

$$\mathbf{R} = \frac{m\mathbf{x} + M\mathbf{y}}{m+M},\tag{5.5}$$

where  $\mathbf{R}$  is the center of mass coordinate between the electron and the fictitious particle,

 $\mathbf{x}$  is the electron coordinate of mass m,

 $\mathbf{y}$  is the fictitious particle coordinate of mass M.

Hence the center of mass coordinates can be transformed into

$$\mathbf{R}_2 - \mathbf{R}_1 = \frac{m}{m_0} \left( \mathbf{x}_2 - \mathbf{x}_1 \right), \tag{5.6}$$

where  $m_0 = m + M$ .

After the electron coordinates have been transformed, the full form of density

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matrix can be written as

$$\rho_{1}(\mathbf{R}_{2},\mathbf{R}_{1};\beta) = \left(\frac{m}{2\pi\hbar^{2}\beta}\right)^{\frac{3}{2}} \left(\frac{\nu\sinh\left(\frac{\Omega}{2}\beta\hbar\right)}{\Omega\sinh\left(\frac{\nu}{2}\beta\hbar\right)}\right)^{3} \\ \times \exp\left\{-\frac{1}{\hbar}\left(\frac{\mu\nu}{4}\coth\left(\frac{\nu}{2}\beta\hbar\right) + \frac{m\mu}{2M\beta\hbar}\right)\left(\frac{m_{0}}{m}\right)^{2}|\mathbf{R}_{2} - \mathbf{R}_{1}|^{2} \\ + \frac{e^{2}\omega_{p}^{2}}{2\pi\hbar}\int_{0}^{\beta\hbar}\int_{0}^{\beta\hbar}d\tau d\sigma \int \frac{d\mathbf{k}}{4\pi k^{2}\omega\left(k\right)}\frac{\cosh\left(\omega\left(k\right)\left(\beta\hbar/2 - |\tau - \sigma|\right)\right)}{\sinh\left(\frac{\omega\left(k\right)}{2}\beta\hbar\right)} \\ \times \exp\left\{i\mathbf{k}\cdot\left(\mathbf{R}_{2} - \mathbf{R}_{1}\right)\frac{m_{0}}{m}\mu\left[\frac{\sinh\left(\frac{\nu}{2}\left(\tau - \sigma\right)\right)\cosh\left(\frac{\nu}{2}\left(\beta\hbar - \tau - \sigma\right)\right)\right)}{m\sinh\left(\frac{\nu}{2}\beta\hbar\right)} \\ + \frac{1}{M\beta\hbar}\left(\tau - \sigma\right)\right] - \frac{\hbar k^{2}}{2m\nu^{2}}f\left(|\tau - \sigma|,\beta\right)\right\} \\ + \frac{3}{2}\left(1 - \frac{\Omega^{2}}{\nu^{2}}\right)\left[\frac{\nu}{2}\beta\hbar\coth\left(\frac{\nu}{2}\beta\hbar\right) - 1\right] \\ + \frac{\kappa\Omega}{8}\int_{0}^{\beta\hbar}\int_{0}^{\beta\hbar}d\tau d\sigma\frac{\cosh\left(\Omega\left(\beta\hbar/2 - |\tau - \sigma|\right)\right)}{\sinh\left(\frac{\Omega}{2}\beta\hbar\right)}\mu^{2}\left[\frac{1}{M\beta\hbar}\left(\tau - \sigma\right) \\ + \frac{\sinh\left(\frac{\nu}{2}\left(\tau - \sigma\right)\right)\cosh\left(\frac{\nu}{2}\left(\beta\hbar - \tau - \sigma\right)\right)}{m\sinh\left(\frac{\nu}{2}\beta\hbar\right)}\right]^{2}\left(\frac{m_{0}}{m}\right)^{2}|\mathbf{R}_{2} - \mathbf{R}_{1}|^{2}\right).$$
(5.7)

Let us firstly consider the off-diagonal part of the density matrix. As  $\mathbf{R}_2 - \mathbf{R}_1 \longrightarrow 0$ , the exponent on the fifth and sixth lines of Eq. (5.7) can be expanded in power series of  $(\mathbf{R}_2 - \mathbf{R}_1)$ . By keeping terms inside the curly bracket up to

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second order  $(\mathbf{R}_2 - \mathbf{R}_1)^2$ , we can write

$$\frac{e^{2}\omega_{p}^{2}}{2\pi\hbar}\int_{0}^{\beta\hbar}\int_{0}^{\beta\hbar}d\tau d\sigma\int_{0}^{\infty}\frac{dk}{\omega(k)}\frac{\cosh\left(\omega(k)\left(\beta\hbar/2-|\tau-\sigma|\right)\right)}{\sinh\left(\frac{\omega(k)}{2}\beta\hbar\right)}$$

$$\times\exp\left(-\frac{\hbar k^{2}}{2m\nu^{2}}f\left(|\tau-\sigma|,\beta\right)\right)$$

$$-\frac{e^{2}\omega_{p}^{2}}{12\pi\hbar}\int_{0}^{\beta\hbar}\int_{0}^{\beta\hbar}d\tau d\sigma\int\frac{dk}{\omega(k)}k^{2}\mu^{2}\frac{\cosh\left(\omega(k)\left(\beta\hbar/2-|\tau-\sigma|\right)\right)}{\sinh\left(\frac{\omega(k)}{2}\beta\hbar\right)}$$

$$\times\left[\frac{\sinh\left(\frac{\nu}{2}\left(\tau-\sigma\right)\right)\cosh\left(\frac{\nu}{2}\left(\beta\hbar-\tau-\sigma\right)\right)}{m\sinh\left(\frac{\nu}{2}\beta\hbar\right)}$$

$$+\frac{1}{M\beta\hbar}\left(\tau-\sigma\right)\right]^{2}\exp\left(-\frac{\hbar k^{2}}{2m\nu^{2}}f\left(|\tau-\sigma|,\beta\right)\right)\left(\frac{m_{0}}{m}\right)^{2}|\mathbf{R}_{2}-\mathbf{R}_{1}|^{2}.$$
 (5.8)

At low temperature and small velocity, we take  $\beta \longrightarrow \infty$ ,  $\mathbf{R}_2 - \mathbf{R}_1 \longrightarrow 0$ . One can show that

$$= \frac{\frac{\cosh\left(\omega\left(k\right)\left(\beta\hbar/2 - |\tau - \sigma|\right)\right)}{\sinh\left(\frac{\omega(k)}{2}\beta\hbar\right)}}{\exp\left(\omega\left(k\right)\left(\beta\hbar/2 - |\tau - \sigma|\right)\right) + \exp\left(-\omega\left(k\right)\left(\beta\hbar/2 - |\tau - \sigma|\right)\right)}}{\exp\left(\omega\left(k\right)\beta\hbar/2\right) - \exp\left(-\omega\left(k\right)\beta\hbar/2\right)}$$

$$\stackrel{\beta \longrightarrow \infty}{\longrightarrow} \exp\left(-\omega\left(k\right)|\tau - \sigma|\right),$$

similarly

$$\frac{\cosh\left(\Omega\left(\beta\hbar/2-|\tau-\sigma|\right)\right)}{\sinh\left(\frac{\Omega}{2}\beta\hbar\right)} \stackrel{\beta\longrightarrow\infty}{\longrightarrow} \exp\left(-\Omega\left|\tau-\sigma\right|\right)$$

and the term

$$\frac{\sinh\left(\frac{\nu}{2}\left(\tau-\sigma\right)\right)\cosh\left(\frac{\nu}{2}\left(\beta\hbar-\tau-\sigma\right)\right)}{\sinh\left(\frac{\nu}{2}\beta\hbar\right)} = \frac{\exp\left(-\nu\sigma\right)-\exp\left(-\nu\tau\right)}{2} \stackrel{\beta\longrightarrow\infty}{\longrightarrow} 0.$$

The last expression goes to zero under the integration of the imaginary time from zero to infinity.

By using again the relation

$$\int_{0}^{\beta} \int_{0}^{\beta} d\tau d\sigma g \left( |\tau - \sigma| \right) = 2 \int_{0}^{\beta} dx \left( \beta - x \right) g \left( x \right)$$
$$\stackrel{\beta \longrightarrow \infty}{\simeq} 2\beta \int_{0}^{\infty} dx g \left( x \right)$$

The expression of the second term of Eq. (5.8) becomes

$$-\frac{e^2\omega_p^2}{6\pi\hbar}\beta \int_0^\infty \frac{dk}{\omega(k)}k^2 \int_0^\infty du\mu^2 \left(\frac{u}{M\beta}\right)^2 \times \exp\left(-\frac{\hbar k^2}{2m\nu^2}f(u,\beta\longrightarrow\infty) - \omega(k)u\right) \left(\frac{m_0}{m}\right)^2 |\mathbf{R}_2 - \mathbf{R}_1|^2, \quad (5.9)$$

where

$$f(u,\beta \longrightarrow \infty) = \mu \left[\frac{\nu}{m} \left(1 - e^{-\nu u}\right) + \frac{\nu^2}{M}u\right]$$
(5.10)

and that of the eighth and ninth lines of Eq. (5.7) is

$$\frac{\kappa\Omega}{4\hbar}\beta\int_0^\infty du\mu^2 \left(\frac{u}{M\beta}\right)^2 \exp\left(-\Omega u\right) \left(\frac{m_0}{m}\right)^2 |\mathbf{R}_2 - \mathbf{R}_1|^2.$$
(5.11)

Collecting Eq. (5.9), Eq. (5.11) and substitute into Eq. (5.7), the off-diagonal part of the density matrix at zero temperature will be expressed in the form as

$$\rho_{1} \left(\mathbf{R}_{2}, \mathbf{R}_{1}; \beta \longrightarrow \infty\right) \sim \exp\{-\left[m_{0} + \frac{e^{2}\omega_{p}^{2}}{3\pi} \int_{0}^{\infty} \frac{dk}{\omega\left(k\right)} k^{2} \int_{0}^{\infty} du u^{2} \\ \times \exp\left(-\frac{\hbar k^{2}}{2m\nu^{2}} f\left(u, \beta \longrightarrow \infty\right) - \omega\left(k\right) u\right) \\ -\frac{\kappa\Omega}{2} \int_{0}^{\infty} du u^{2} \exp\left(-\Omega u\right) \left[\frac{\left|\mathbf{R}_{2} - \mathbf{R}_{1}\right|^{2}}{2\beta\hbar^{2}}\right\}.$$
(5.12)

Comparing this form with Eq. (5.3), we get

$$m_F = m_0 + \frac{e^2 \omega_p^2}{3\pi} \int_0^\infty \frac{dk}{\omega(k)} k^2 \int_0^\infty du u^2 \exp\left(-\frac{\hbar k^2}{2m\nu^2} f\left(u, \beta \longrightarrow \infty\right) - \omega(k) u\right) - \frac{\kappa\Omega}{2} \int_0^\infty du u^2 \exp\left(-\Omega u\right).$$
(5.13)

The last term can be integrated to give  $\kappa \Omega \int_{-\infty}^{\infty} dx^{2} dx = 0$ 

$$\frac{\kappa\Omega}{2}\int_0^\infty du u^2 \exp\left(-\Omega u\right) = M.$$

This M together with  $m_0$  will give m, the mass of an electron. So we arrive at the Feynman effective mass of the plasmaron

$$m_F = m + \frac{e^2 \omega_p^2}{3\pi} \int_0^\infty \frac{dk}{\omega(k)} k^2 \int_0^\infty du u^2 \exp\left(-\frac{\hbar k^2}{2m\nu^2} f\left(u,\beta \longrightarrow \infty\right) - \omega(k) u\right).$$
(5.14)

Now we turn to the other part of the plasmaron density matrix, the diagonal part. From Eq. (5.7), Eq. (5.8) and Eq.(4.37), only parts which is independent of the plasmaron coordinates will be taken into account. So we can write

$$\rho_{1}(0,0;\beta) = \left(\frac{m}{2\pi\hbar^{2}\beta}\right)^{\frac{3}{2}} \left(\frac{\nu\sinh\left(\frac{\Omega}{2}\beta\hbar\right)}{\Omega\sinh\left(\frac{\nu}{2}\beta\hbar\right)}\right)^{3} \exp\left\{\frac{3}{2}\left(1-\frac{\Omega^{2}}{\nu^{2}}\right) \left[\frac{\nu}{2}\beta\hbar\coth\left(\frac{\nu}{2}\beta\hbar\right)-1\right] + \frac{e^{2}\omega_{p}^{2}}{\pi\hbar}\int_{0}^{\infty}\frac{dk}{\omega\left(k\right)}\int_{0}^{\beta\hbar}du\left(\beta\hbar-u\right)\exp\left(-\frac{\hbar k^{2}}{2m\nu^{2}}f\left(u,\beta\right)\right) \times \frac{\cosh\left(\omega\left(k\right)\left(\beta\hbar/2-|\tau-\sigma|\right)\right)}{\sinh\left(\frac{\omega\left(k\right)}{2}\beta\hbar\right)}\right\}.$$
(5.15)

As taking  $\beta \longrightarrow \infty$ , in this case, we will also keep the term including  $1/\beta$  in the function  $f(u, \beta \longrightarrow \infty)$  and will denote this new function  $F(u, \beta \longrightarrow \infty)$  which can be written as

$$F(u,\beta \longrightarrow \infty) = \mu \left[\frac{\nu}{m} \left(1 - e^{-\nu u}\right) + \frac{\nu^2}{M}u + \frac{\nu^2 u^2}{M\hbar}\frac{1}{\beta}\right] .$$
 (5.16)

Then expand the function  $\exp\left(-\frac{\hbar k^2}{2m\nu^2}F\left(u,\beta\longrightarrow\infty\right)\right)$  with respect to  $1/\beta$  about  $1/\beta = 0$  up to first order

$$\exp\left(-\frac{\hbar k^2}{2m\nu^2}F\left(u,\beta\longrightarrow\infty\right)\right)$$

$$= \exp\left(-\frac{\hbar k^2}{2m\nu^2}F\left(u,\beta\longrightarrow\infty\right)\right)_{1/\beta=0}$$

$$+\frac{\partial}{\partial\frac{1}{\beta}}\left[\exp\left(-\frac{\hbar k^2}{2m\nu^2}F\left(u,\beta\longrightarrow\infty\right)\right)\right]_{1/\beta=0}\frac{1}{\beta}+\dots$$

$$= \exp\left(-\frac{\hbar k^2}{2m\nu^2}f\left(u,\beta\longrightarrow\infty\right)\right)$$

$$+\frac{\hbar\mu k^2 u^2}{2mM}\exp\left(-\frac{\hbar k^2}{2m\nu^2}f\left(u,\beta\longrightarrow\infty\right)\right)\frac{1}{\beta}+\dots$$
(5.17)

Substituting back into the density matrix in Eq. (5.15), we obtain

$$\rho_{1}\left(0,0;\beta\longrightarrow\infty\right)$$

$$= \left[\frac{m}{2\pi\beta\hbar^{2}}\left(\frac{\nu}{\Omega}\right)^{2}\exp\left\{\left(\frac{\Omega^{2}}{\nu^{2}}-1\right)+\frac{\Omega^{2}}{\nu^{2}}\frac{e^{2}\omega_{p}^{2}}{3\pi m}\int_{0}^{\infty}\frac{dk}{\omega\left(k\right)}k^{2}\int_{0}^{\infty}duu^{2}\right.$$

$$\times\exp\left(-\frac{\hbar k^{2}}{2m\nu^{2}}f\left(u,\beta\longrightarrow\infty\right)-\omega\left(k\right)u\right)\right]^{\frac{3}{2}}\exp\left\{-\left[\frac{3}{4}\nu\left(1-\frac{\Omega}{\nu}\right)^{2}\hbar\right]^{\frac{3}{2}}\left.\left.\left(\frac{e^{2}\omega_{p}^{2}}{\pi}\int_{0}^{\infty}\frac{dk}{\omega\left(k\right)}\int_{0}^{\infty}du\exp\left(-\frac{\hbar k^{2}}{2m\nu^{2}}f\left(u,\beta\longrightarrow\infty\right)-\omega\left(k\right)u\right)\right]\beta\right\},$$

$$\left.\left(5.18\right)\right\}$$

where  $f(u, \beta \longrightarrow \infty)$  can be expressed in terms of only parameter  $\Omega$  and  $\nu$  as

$$f(u,\beta \longrightarrow \infty) = \nu \left(1 - \frac{\Omega^2}{\nu^2}\right) \left(1 - e^{-\nu u}\right) + \Omega^2 u.$$
 (5.19)

Compare the density matrix of Eq. (5.18) with Eq. (5.4), we can obviously conclude that

$$m_{KP} = m \left(\frac{\nu}{\Omega}\right)^2 \exp\{\frac{\Omega^2}{\nu^2} - 1 + \frac{\Omega^2}{\nu^2} \frac{e^2 \omega_p^2}{3\pi m} \int_0^\infty \frac{dk}{\omega(k)} k^2 \int_0^\infty du u^2 \\ \times \exp\left(-\frac{\hbar k^2}{2m\nu^2} f(u,\beta \longrightarrow \infty) - \omega(k) u\right)\}$$
(5.20)

and the ground state energy

$$E_{0} = \frac{3}{4}\nu\left(1-\frac{\Omega}{\nu}\right)^{2}\hbar - \frac{e^{2}\omega_{p}^{2}}{\pi}\int_{0}^{\infty}\frac{dk}{\omega\left(k\right)}\int_{0}^{\infty}du$$
$$\times \exp\left(-\frac{\hbar k^{2}}{2m\nu^{2}}f\left(u,\beta\longrightarrow\infty\right) - \omega\left(k\right)u\right), \qquad (5.21)$$

where  $\Omega$  and  $\nu$  are variational parameters.

It is easy to see that the Krivoglaz-Pekar effective mass is related to the Feynman mass through the equation

$$m_{KP} = m \left(\frac{\nu}{\Omega}\right)^2 \exp\left(\frac{\Omega^2}{\nu^2} \frac{m_F}{m} - 1\right).$$
(5.22)

The Feynman effective mass of Eq. (5.14), the Krivoglaz-Pekar effective mass of Eq. (5.20) and the ground state energy of Eq. (5.21) can be expressed as functions of some dimensionless variables by introducing  $u = \hbar s/E_F$  where  $E_F$  is the Fermi energy. This gives

$$\frac{m_F}{m} = 1 + \frac{2}{3} \frac{E_p^2}{\pi} \sqrt{\frac{E_H}{E_F}} \int_0^\infty \frac{dE(k)}{E_\omega(k)} \sqrt{E(k)} \int_0^\infty ds s^2 \\
\times \exp\{-E(k) \left[\frac{E_\Omega^2}{E_\nu^2} s + \frac{1}{E_\nu} \left(1 - \frac{E_\Omega^2}{E_\nu^2}\right) \left(1 - e^{-E_\nu s}\right)\right] - E_\omega(k) s\},$$
(5.23)

$$\frac{m_{KP}}{m} = \left(\frac{E\nu}{E_{\Omega}}\right)^2 \exp\left(\frac{E_{\Omega}^2}{E_{\nu}^2}\frac{m_F}{m} - 1\right)$$
(5.24)

and

$$E'_{0} = \frac{3}{4} E_{\nu} \left( 1 - \frac{E_{\Omega}}{E_{\nu}} \right)^{2} - \frac{E_{p}^{2}}{\pi} \sqrt{\frac{E_{H}}{E_{F}}} \int_{0}^{\infty} \frac{dE(k)}{E_{\omega}(k)\sqrt{E(k)}} \int_{0}^{\infty} ds \\ \times \exp\{-E(k) \left[ \frac{E_{\Omega}^{2}}{E_{\nu}^{2}} s + \frac{1}{E_{\nu}} \left( 1 - \frac{E_{\Omega}^{2}}{E_{\nu}^{2}} \right) \left( 1 - e^{-E_{\nu}s} \right) \right] - E_{\omega}(k) s\}(5.25)$$

where

$$E'_{0} = E_{0}/E_{F} \text{ is measured in the unit of Fermi energy,}$$

$$E_{\nu} = \hbar\nu/E_{F}, E_{\Omega} = \hbar\Omega/E_{F}, E_{\omega}(k) = \hbar\omega(k)/E_{F}, E_{p} = \hbar\omega_{p}/E_{F},$$

$$E(k) = \hbar^{2}k^{2}/2mE_{F}, E_{H} = me^{4}/2\hbar^{2} = 1 \text{ Ry,}$$

$$E_{\omega}(k) = \sqrt{E_{p}^{2} + \frac{4}{3}E(k) + E^{2}(k)}.$$
(5.26)

Since

$$E_F = \left(\frac{9\pi}{4}\right)^{\frac{2}{3}} \frac{1}{r_s^2}$$
 Ry and  $E_p = \sqrt{12} \left(\frac{4}{9\pi}\right)^{\frac{2}{3}} r_s^{\frac{1}{2}}$  Ry,

where  $r_s$  is the interparticle distance in units of Bohr radius. We have

$$\frac{E_p^2}{\pi} \sqrt{\frac{E_H}{E_F}} = cr_s^2$$

with  $c = \left(\frac{12}{\pi}\right) \left(\frac{9\pi}{4}\right)^{-\frac{5}{3}}$  and by setting  $x = E_{\nu}s$ , we obtain

$$\frac{m_F}{m} = 1 + \frac{2}{3} \frac{cr_s^2}{E_\nu^3} \int_0^\infty \frac{dE(k)}{E_\omega(k)} \sqrt{E(k)} \int_0^\infty dx x^2 \\ \times \exp\{-\alpha x - \lambda \left(e^{-x} - 1\right)\},$$
(5.27)

$$\frac{m_{KP}}{m} = \frac{1}{\rho^2} \exp\left(\rho^2 \frac{m_F}{m} - 1\right) \tag{5.28}$$

and

$$E'_{0} = \frac{3}{4} E_{\nu} (1-\rho)^{2} - \frac{cr_{s}^{2}}{E_{\nu}} \int_{0}^{\infty} \frac{dE(k)}{E_{\omega}(k)\sqrt{E(k)}} \int_{0}^{\infty} dx \\ \times \exp\{-\alpha x - \lambda \left(e^{-x} - 1\right)\},$$
(5.29)

where we have used  $\rho = E_{\Omega}/E_{\nu}$ ,  $\lambda = -\frac{E(k)}{E_{\nu}}(1-\rho^2)$ ,  $\alpha = \frac{1}{E_{\nu}}(E(k)\rho^2 + E_{\omega}(k))$ .

To obtain the best approximation for the actual ground state energy  $E'_0$ , the two parameters  $\rho$  and  $E_{\nu}$  have to be varied separately to yield the minimum  $E'_0$ . This can be accomplished generally by minimizing Eq. (5.29) with respect to both  $\rho$  and  $E_{\nu}$ . Unfortunately, since these variational equations cannot be calculated in closed forms, numerical method must be employed. When we get  $\rho$ and  $E_{\nu}$  that give minimum  $E'_0$ , they can be substituted back into Eq. (5.27) and Eq. (5.28) to find the plasmaron effective mass.

#### 5.3 Numerical results and discussions

In this section, the plasmaron ground state energy and its effective mass will be evaluated numerically. We choose to adopt, for simplicity, the **MATHEMAT**-**ICA** program [25], since it provides many built-in functions and can perform a numerical integration appeared in the formulas for the ground state energy and the effective mass. FindMinimum function of the MATHEMATICA program will be applied in the minimization process (see appendix C). We can understand something about how FindMinimum works by thinking of the values of our function as defining the height of a surface. What FindMinimum does is essentially to start at the points we specify, then follow the path of steepest descent on the surface. After applying this program to Eq. (5.29), the results of the ground state energy and the two variational parameters ( $\rho$  and  $E_{\nu}$ ) plotted versus  $r_s$  are shown in Fig. (5.1), Fig. (5.2) and Fig. (5.3) respectively.



Figure 5.1: A plot of the plasmaron ground state energy at wide ranges of  $r_s$ .

As mentioned in chapter 2, there are three different regimes of densities. It is very important to connect this to the behaviour of all ranges of coupling. At very high density  $(r_s \longrightarrow 0)$ , the kinetic term dominates all terms of interaction. So it corresponds to **weak coupling.** Meanwhile, at very low density  $(r_s \longrightarrow \infty)$ , the interaction term becomes important. This is called **strong coupling** which



Figure 5.2: The parameter  $\rho$  obtained from the minimization process.

is opposite to the first case. **Intermediate coupling** goes to the region where we cannot neglect both kinetic and interaction terms such as the region of real metallic density, for example.

In Fig. (5.1), the plasmaron ground state energy is plotted in all regions of coupling. It is shown that the energy increases as going from the weak coupling to the strong coupling limit. It is interesting to compare this result with some methods for the same Fröhlich-type electron-plasmon interaction model.

When we consider characteristic of both two parameters  $\rho$  and  $E_{\nu}$ , it can readily be seen that  $\rho$ , in Fig. (5.2), varies from 1 to 0 as  $r_s$  increases. Whereas  $E_{\nu}$ , in Fig. (5.3), tends to go to infinity.

Now we would like to compare the ground state energy of our numerical result with the method called **generalized path integral method** which is introduced by Luttinger and Lu for the polaron problem [26] and taken into the calculation for our model by Sa-yakanit, Lakno and Hass [27]. The energy is



Figure 5.3: The other parameter  $E_{\nu}$  which has a characteristic different from  $\rho$ .

approximated to be

$$E_{0} = \frac{3}{2\mu}B^{2} - \frac{2}{\pi}\sqrt[4]{12}r_{s}^{-3/4}\int_{0}^{\infty}dx \frac{\exp\left(-\sqrt{3}r_{s}^{-3/2}\mu^{2}x^{2}/B^{2}\right)}{\sqrt{1 + \left(\pi^{2/3}/\sqrt[6]{3}\sqrt[3]{2}\sqrt{r_{s}}\right)x^{2} + x^{4}}}$$
$$\times \frac{1}{\sqrt{1 + \left(\pi^{2/3}/\sqrt[6]{3}\sqrt[3]{2}\sqrt{r_{s}}\right)x^{2} + x^{4}} + (1 - \mu)x^{2}} \operatorname{Ry}, \quad (5.30)$$

where B and  $\mu$  are variational parameters.

In the case of weak coupling limit, when  $\mu \longrightarrow 0$ , the energy is

$$E_0 \approx -1.0984 \frac{1}{r_s^{3/4}} \text{ Ry}$$
 (5.31)

and in the region of strong coupling, when  $\mu \longrightarrow 1$ , they get

$$E_0 \approx -0.1085 \text{ Ry} \tag{5.32}$$

Plots of the ground state energy compared with the energy obtained from the generalized path integral method in the two extreme cases are shown in Fig. (5.4) and Fig. (5.5)



Figure 5.4: Comparison of the ground state energy obtained from the generalized path integral method with our result in the weak coupling limit.

In the weak coupling limit, the energy from the generalized path integral method is much lower than that of our result but tends to converge to our approach as  $r_s$  going to 1, the difference is about 10 %. This is due to the fact that the energy in Eq. (5.31) increases more rapidly than our result. When we turn to the strong coupling limit, it behaves differently. That is, as  $r_s$  becomes greater, the ground state energies of the two methods seem to diverge from each other.

In the case of intermediate coupling, we use the energy of a few metals evaluated by generalized path integral method [28] and compare this with our result as shown in Table (5.1).

Surprisingly, although the energies are calculated by different approaches, this table demonstrates a good agreement between them.

Up to now, we have not yet discussed about the plasmaron effective mass. When we obtain the two parameters  $\rho$  and  $E_{\nu}$  from the minimization process,



Figure 5.5: Comparison of the ground state energy obtained from the generalized path integral method with our result in the strong coupling limit.

	Li	Na	Be	Mg	Al
$r_s$	3.26	4.00	1.88	2.66	2.07
$\phi_1\left(\mathrm{Ry}\right)$	-0.36	-0.32	-0.53	-0.42	-0.5
$E_0$ (Ry)	-0.37	-0.32	-0.54	-0.42	-0.5

Table 5.1: Comparison of the ground state energy of some metals from the two methods, where  $\phi_1$  denotes the energy obtained from the generalized path integral method and  $E_0$  is our result.

they can be substituted back into Eq. (5.27) and Eq. (5.28). The results of the two definitions of the plasmaron effective mass, the Feynman mass and Krivoglaz-Pekar mass, are shown in Fig. (5.6).

In Fig. (5.6), the Krivoglaz-Pekar mass is greater than the Feynman mass  $(m_{KP} > m_F)$  at all ranges of coupling. The two masses seem to coincide with each other, within a six-digit accuracy of the MATHEMATICA program, in the weak coupling limit and they begin to diverge from each other when entering into the region of strong coupling.



Figure 5.6: A plot of Feynman and Krivoglaz-Pekar effective masses at various  $r_s.$ 

It is worth studying the behaviour of the effective mass in both extreme regions of coupling. We firstly consider the effective mass derived from the generalized path integral method [28], it can be expressed as

$$\frac{m^*}{m} = 1 + \frac{2}{9} 12^{3/4} r_s^{3/4} \int_0^\infty dx x^2 \frac{\exp\left(-\sqrt{3}r_s^{-3/2}\mu^2 x^2/B^2\right)}{\sqrt{1 + \left(\pi^{2/3}/\sqrt[6]{3}\sqrt[3]{2}\sqrt{r_s}\right)x^2 + x^4}} \times \frac{1}{\left(\sqrt{1 + \left(\pi^{2/3}/\sqrt[6]{3}\sqrt[3]{2}\sqrt{r_s}\right)x^2 + x^4} + (1 - \mu)x^2\right)^3}.$$
(5.33)

In the case of weak coupling,  $\mu \longrightarrow 0$ , it gives

$$\frac{m^*}{m} \approx 1 + \frac{2}{3} r_s^{3/2}.$$
(5.34)

When comparing with our two effective masses in Fig. (5.7), it coincides with our results for small  $r_s$ , but becomes larger obviously as  $r_s$  approaches 1.



Figure 5.7: A plot of Feynman and Krivoglaz effective masses compared with the mass derived by the generalized path integral method in the weak coupling limit.

In the case of strong coupling,  $\mu \longrightarrow 1$ , the approximate form is

$$\frac{m^*}{m} \approx 1 + \frac{\pi}{2\sqrt[4]{3}} r_s^{3/4}.$$
(5.35)

When comparing with our two effective masses as in Fig. (5.8), it is about 10 times greater than our results and tends to infinity.

The behaviour of  $m^*/m$  in Fig. (5.6) is worth discussing in more detail. It shows that both  $m_F/m$  and  $m_{KP}/m$  are close to 1 in the high density limit and they become very large in the low density limit. We can interpret this characteristic in the way that the particle in the high density limit is mobile, because of its small effective mass. While the particle in the low density limit has very large effective mass, so it cannot move away from its own field. The particle in this limit becomes localized. This may reflect an interesting phenomenon called a phase transition, which occurs in an interacting system, from the weak



Figure 5.8: A plot of Feynman and Krivoglaz-Pekar effective masses compared with the mass derived by the generalized path integral method in the strong coupling limit.

coupling limit to the strong coupling limit. Comparing our result with the theory of the electron gas, we find that at very high density, the electrons are essentially mobile. While at very low density, the electrons are localized known as **Wigner crystallization**. However, our theory cannot describe at what value of  $r_s$  the phase transition will take place.

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### Chapter 6 Conclusions

In this thesis, the ground state energy and the effective mass of the plasmaron, defined as the dressing of an electron by the plasmons, have been investigated. We start at the Fröhlich-type electron-plasmon Hamiltonian, introduced by Lundqvist, which is expressed in the second-quantization form. The electronhole pair excitation is neglected in this model. It corresponds to taking the critical  $k_c$ , the maximum value of the wave number that plasmons can exist, to infinity. We chose the Feynman path integral method to study this system since it can be applied very successfully to the polaron problem in all ranges of coupling constants.

First of all, the Hamiltonian must be transformed into the first-quantization representation which is suitable for this method. Then the Lagrangian is obtained. Secondly, the transformation function which connects the initial and final states of the electron and plasmons is set up. After eliminating the plasmon coordinates, we obtain the transformation function consisting of the prefactor which is the partition function for the plasmons in the imaginary time representation and the resulting contribution due to the effect of plasmons on an electron. The later transformation function is called the plasmaron propagator. Since this propagator cannot be evaluated in an exact form, the variational method must be taken into account by introducing a trial action proposed by Sa-yakanit. If we keep the off-diagonal part, then we arrive at the fullform of the propagator and also the density matrix.

The ground state energy and the Krivoglaz-Pekar effective mass of the

plasmaron is obtained from the diagonal part of the density matrix by letting  $\beta$  go to infinity, whereas the Feynman effective mass is derived from the offdiagonal part. We can find the ground state energy and the two effective masses numerically by using the MATHEMATICA program. Our results are compared with that obtained from the generalized path integral method. In the weak coupling case, we have found that the energy of such method is much larger than our result but tends to come closer as  $r_s$  becomes greater. The energy in the high density limit has a different characteristic. The two ground state energies diverge from each other as  $r_s$  increases. Surprisingly, in the region of intermediate coupling, considering for a few metals, they both are in a good agreement. When turning to the effective mass, the Krivoglaz-Pekar mass is larger than the Feynman mass in all regions of coupling and the difference between them increases as  $r_s$  goes to infinity. We again compare our results with the generalized path integral method in the two extreme limits. In the weak coupling case, it coincides with  $m_F/m$  and  $m_{KP}/m$  for small  $r_s$ , but becomes larger than our results obviously as  $r_s$  approaches 1. In the strong coupling case, it is about 10 times greater than our effective masses. There is an interesting behaviour of the effective mass which is worth discussing. We can see that both  $m_F/m$  and  $m_{KP}/m$  are close to 1 in the high density limit. This means that the particle is mobile, because of its small effective mass, whereas they are very large in the low density limit. It can be interpreted that the particle cannot move away from its own field and becomes localized. This result may be connected to the phenomenon known as Wigner crystallization. Unfortunately, we do not know at what value of  $r_s$  the phase transition begins to occur.

It is noted that we use Lundqvist's Fröhlich-type Hamiltonian which as-

sumes the electron gas to be a continuous medium and allows RPA to be valid in all regions of coupling. But in real system, when going from the high density limit to the low density limit, the electron gas loses its homogenity and becomes a discrete structure. So it is interesting to improve our model and the method of calculation for future research.



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#### References

- Bohm, D., and Pines, D. A Collective Description of Electron Interactions: III. Coulomb Interactions in a Degenerate Electron Gas. Phys. Rev. 92 (1953): 609.
- [2] Gell-Mann, M., and Brueckner, K. A. Correlation Energy of an Electron Gas at High Density. Phys. Rev. 106 (1957): 364.
- [3] Nozieres, P., and Pines, D. Il Nuovo Cimento [x] 9 (1958): 470.
- [4] Pines, D. The Many-Body Problem. New York: W. A. Benjamin, 1962.
- [5] Lundqvist, B. I. Single-particle Spectrum of the Degenerate Electron Gas: I. The Structure of the Spectral Weight Function. Phys. Kondens. Ma terie. 6 (1967): 193.
- [6] Feynman, R. P. Slow Electron in a Polar Crystal. Phys. Rev. 97 (1955):660.
- [7] Feynman, R. P., and Hibbs, A. R. Quantum Mechanics and Path Inte grals. Taiwan: McGraw-Hill, 1965.
- [8] Samathiyakanit, V. Path-Integral theory of a model disordered system. J.
   Phys. C 7 (1974): 2849.
- [9] Bohm, D., and Pines, D. A Collective Description of Electron Interactions: II. Collective vs Individual Particle Aspects of the Interactions. Phys. Rev. 85 (1952): 338.
- [10] Sachs, M. Solid State Theory. New York: McGraw-Hill, 1963.
- [11] Medelung, O. Introduction to Solid-State Theory. New York: Springer-Verlag, 1981.

- [12] Pines, D. A Collective Description of Electron Interactions: IV. Electron Interaction in Metals. Phys. Rev. 92 (1953): 626.
- [13] Pines, D. Electrons and Plasmons. Il Nuovo Cimento [x] 7 (1958): 329.
- [14] Wigner, E. P. Trans. Faraday Soc. 34 (1938): 678.
- [15] Nozieres, P. The theory of interacting Fermi systems. New York: W. A. Benjamin, 1964.
- [16] Schrieffer, J. R. Theory of Superconductivity. New York: W. A. Ben jamin, 1964.
- [17] Engelsberg, S., and Platzman, P. M. Single-Particle Coupling to Collective Excitations; Sound in He<sup>3</sup>. Phys. Rev. 148 (1966): 103.
- [18] Kittel, C. Quantum Theory of Solids. Canada: John Wiley & Sons, 1987.
- [19] Lundqvist, B. I. Single-particle Spectrum of the Degenerate Electron Gas:
   II. Numerical results for Electrons Coupled to Plasmons. Phys. Kon dens. Materie. 6 (1967): 206.
- [20] Sa-yakanit, V. Electron density of states in a Gaussian random potential: Path-integral approach. Phys. Rev. B 19 (1979): 2266.
- [21] Sa-yakanit, V., Nithisoontorn, M., and Sritrakool, W. Path-integral Theory of the Plasmaron. Physica Scripta 32 (1985): 334.
- [22] Kubo, R. Generalized Cumulant Expansion Method. J. Phys. Soc. Jpn. 17 (1962): 1100.
- [23] Sa-yakanit, V. The Feynman effective mass of the polaron. Phys. Rev. B 19 (1979): 2377.
- [24] Krivoglaz, M. A., and Pekar, S. I. Bull. Acad. Sci. USSR 21 (1957): 13.
- [25] Wolfram, S. The Mathematica Book, 3<sup>rd</sup> Ed. New York: Cambridge

University Press, 1996.

- [26] Luttinger, J. M., and Lu, C. Y. Generalized path-integral formalism of the polaron problem and its second-order semi-invariant correction to the ground-state energy. Phys. Rev. B 21 (1980): 4251.
- [27] Sa-yakanit, V., Lakno, V. D., and Hass, K. Path-integral approach to singleparticle excitation in Coulomb systems. Phys. Rev. B 57 (1998): 5772.
- [28] Sa-yakanit, V., Lakno, V. D., and Hass, K. Path integral calculations of par ticle self-energy and effective mass in Coulomb systems. Mod. Phys. Lett. B 11 (1997): 129.



# Appendices

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### Appendix A: The plasmon partition function

Consider a set of plasmons of which the Lagrangian can be written as

$$L = \sum_{\mathbf{k}} \frac{m}{2} \left( \dot{q}_{\mathbf{k}}^2(\tau) - \omega^2(k) q_{\mathbf{k}}^2(\tau) \right).$$
(B.1)

It is similar to the Lagrangian of a set of harmonic oscillators, hence the propagator for this system can be obtained from the well-known result for the path integral of the harmonic oscillator. This gives

$$G(q_{1},...,q_{N},t;q_{1}',...,q_{N}',0) = \int_{q_{1}'}^{q_{1}} Dq_{1}(\tau)...\int_{q_{N}'}^{q_{N}} Dq_{N}(\tau) \exp\left(\frac{i}{\hbar}\sum_{\mathbf{k}}\int_{0}^{t}d\tau \frac{m}{2}\left(\dot{q}_{\mathbf{k}}^{2}(\tau)-\omega^{2}(k)q_{\mathbf{k}}^{2}(\tau)\right)\right)$$

$$=\prod_{\mathbf{k}}\int_{q_{\mathbf{k}}'}^{q_{\mathbf{k}}} Dq_{\mathbf{k}}(\tau) \exp\left(\frac{i}{\hbar}\int_{0}^{t}d\tau \frac{m}{2}\left(\dot{q}_{\mathbf{k}}^{2}(\tau)-\omega^{2}(k)q_{\mathbf{k}}^{2}(\tau)\right)\right)$$

$$=\prod_{\mathbf{k}}\left(\frac{m\omega(k)}{2\pi i\hbar\sin(\omega(k)t)}\right)^{\frac{1}{2}} \exp\left(\frac{im\omega(k)}{2\hbar\sin(\omega(k)t)}\left[\left(q_{\mathbf{k}}^{2}+q_{\mathbf{k}}'^{2}\right)\cos(\omega(k)t)-2q_{\mathbf{k}}q_{\mathbf{k}}'\right]\right).$$
(B.2)

Note that  $q_{\mathbf{k}}(0) = q'_{\mathbf{k}}$  and  $q_{\mathbf{k}}(t) = q_{\mathbf{k}}$ .

The partition function of such propagator in the real time (if we replace  $t = -i\hbar\beta$ , we call  $\beta$  the imaginary time) can be performed using the formula

$$Z = \int_{-\infty}^{\infty} dq_1 \dots dq_N \int_{-\infty}^{\infty} dq'_1 \dots dq'_N \delta(q'_1 - q_1) \dots \delta(q'_N - q_N) G$$
  

$$= \int_{-\infty}^{\infty} dq_1 \dots dq_N G(q_1, \dots, q_N, t; q_1, \dots, q_N, 0)$$
  

$$= \prod_{\mathbf{k}} \int_{-\infty}^{\infty} dq_{\mathbf{k}} \left( \frac{m\omega(k)}{2\pi i \hbar \sin(\omega(k) t)} \right)^{\frac{1}{2}} \exp\left( \frac{im\omega(k)}{2\hbar \sin(\omega(k) t)} \left[ 2q_{\mathbf{k}}^2 \cos(\omega(k) t) - 2q_{\mathbf{k}}^2 \right] \right)$$
  

$$= \prod_{\mathbf{k}} \left( \frac{m\omega(k)}{2\pi i \hbar \sin(\omega(k) t)} \right)^{\frac{1}{2}} \int_{-\infty}^{\infty} dq_{\mathbf{k}} \exp\left( -\frac{2im\omega(k)}{\hbar \sin(\omega(k) t)} \sin^2\left(\frac{\omega(k)}{2}t\right) q_{\mathbf{k}}^2 \right). (B.3)$$

This is the Gaussian integral, therefore

$$Z = \prod_{\mathbf{k}} \left( \frac{m\omega(k)}{2\pi i\hbar \sin(\omega(k)t)} \right)^{\frac{1}{2}} \left( \frac{\pi\hbar \sin(\omega(k)t)}{2im\omega(k)\sin^2\left(\frac{\omega(k)}{2}t\right)} \right)^{\frac{1}{2}}$$
$$= \prod_{\mathbf{k}} \left( 2i\sin\left(\frac{\omega(k)}{2}t\right) \right)^{-1}$$
(B.4)

which is the partition function for the plasmons.



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### Appendix B: The calculation of cumulant expansion

We would like to approximate  $\langle \exp\{i\mathbf{k}\cdot(\mathbf{x}(\tau)-\mathbf{x}(\sigma))\}\rangle_{S_0}$  by using the cumulant expansion

$$\langle \exp(a) \rangle = \exp\left[ \langle a \rangle + \frac{1}{2!} \left( \langle a^2 \rangle - \langle a \rangle^2 \right) + \dots \right],$$
 (B.1)

we use  $\langle a \rangle$  instead of  $\langle a \rangle_{S_0}$  for convenience.

By keeping the terms up to the second order and replacing *a* with  $\exp\{i\mathbf{k}\cdot(\mathbf{x}(\tau)-\mathbf{x}(\sigma))\}\)$ , we have

$$\langle \exp\{i\mathbf{k} \cdot (\mathbf{x}(\tau) - \mathbf{x}(\sigma))\} \rangle$$

$$= \exp\left(\langle i\mathbf{k} \cdot (\mathbf{x}(\tau) - \mathbf{x}(\sigma)) \rangle + \frac{1}{2} \left[ \langle (i\mathbf{k} \cdot (\mathbf{x}(\tau) - \mathbf{x}(\sigma)))^2 \rangle - \langle i\mathbf{k} \cdot (\mathbf{x}(\tau) - \mathbf{x}(\sigma)) \rangle^2 \right] \right).$$
(B.2)

First of all, consider the second term on the right-hand side

$$\left\langle \left(i\mathbf{k} \cdot \left(\mathbf{x}\left(\tau\right) - \mathbf{x}\left(\sigma\right)\right)\right)^{2} \right\rangle$$

$$= -\left\langle \left[k_{x}\left(x\left(\tau\right) - x\left(\sigma\right)\right) + k_{y}\left(y\left(\tau\right) - y\left(\sigma\right)\right) + k_{z}\left(z\left(\tau\right) - z\left(\sigma\right)\right)\right]^{2} \right\rangle\right.$$

$$= -\left\langle k_{x}^{2}\left(x\left(\tau\right) - x\left(\sigma\right)\right)^{2} \right\rangle - \left\langle k_{y}^{2}\left(y\left(\tau\right) - y\left(\sigma\right)\right)^{2} \right\rangle - \left\langle k_{z}^{2}\left(z\left(\tau\right) - z\left(\sigma\right)\right)^{2} \right\rangle\right.$$

$$\left. -2k_{x}k_{y}\left(\left(x\left(\tau\right) - x\left(\sigma\right)\right)\left(y\left(\tau\right) - y\left(\sigma\right)\right)\right)\right.$$

$$\left. -2k_{x}k_{z}\left(\left(x\left(\tau\right) - x\left(\sigma\right)\right)\left(z\left(\tau\right) - z\left(\sigma\right)\right)\right)\right).$$
(B.3)

Next turn to the third term

$$\langle i\mathbf{k} \cdot (\mathbf{x}(\tau) - \mathbf{x}(\sigma)) \rangle^{2}$$

$$= -[k_{x} \langle (x(\tau) - x(\sigma)) \rangle + k_{y} \langle (y(\tau) - y(\sigma)) \rangle + k_{z} \langle (z(\tau) - z(\sigma)) \rangle]^{2}$$

$$= -k_{x}^{2} \langle (x(\tau) - x(\sigma)) \rangle^{2} - k_{y}^{2} \langle (y(\tau) - y(\sigma)) \rangle^{2} - k_{z}^{2} \langle (z(\tau) - z(\sigma)) \rangle^{2}$$

$$-2k_{x}k_{y} \langle (x(\tau) - x(\sigma)) \rangle \langle (y(\tau) - y(\sigma)) \rangle$$

$$-2k_{y}k_{z} \langle (y(\tau) - y(\sigma)) \rangle \langle (z(\tau) - z(\sigma)) \rangle$$

$$(B.4)$$

It can be readily seen ,for only a quadratic trial action, that

$$\langle (x(\tau) - x(\sigma)) (y(\tau) - y(\sigma)) \rangle = \langle (x(\tau) - x(\sigma)) \rangle \langle (y(\tau) - y(\sigma)) \rangle, \langle (y(\tau) - y(\sigma)) (z(\tau) - z(\sigma)) \rangle = \langle (y(\tau) - y(\sigma)) \rangle \langle (z(\tau) - z(\sigma)) \rangle, \langle (x(\tau) - x(\sigma)) (z(\tau) - z(\sigma)) \rangle = \langle (x(\tau) - x(\sigma)) \rangle \langle (z(\tau) - z(\sigma)) \rangle.$$
(B.5)

Then substitute Eq.(B.3), Eq.(B.4) and apply the relation of Eq.(B.5), we get

$$\langle \exp\{i\mathbf{k} \cdot (\mathbf{x}(\tau) - \mathbf{x}(\sigma))\} \rangle$$

$$= \exp(i\mathbf{k} \cdot \langle (\mathbf{x}(\tau) - \mathbf{x}(\sigma)) \rangle + \frac{1}{2} [k_x^2 (\langle (x(\tau) - x(\sigma)) \rangle^2 - \langle (x(\tau) - x(\sigma))^2 \rangle) + k_y^2 (\langle (y(\tau) - y(\sigma)) \rangle^2 - \langle (y(\tau) - y(\sigma))^2 \rangle) + k_z^2 (\langle (z(\tau) - z(\sigma)) \rangle^2 - \langle (z(\tau) - z(\sigma))^2 \rangle)].$$
(B.6)

Compare Eq.(B.6) with Eq. (4.28 ), we obtain  $\sim$ 

$$\langle (\mathbf{x}(\tau) - \mathbf{x}(\sigma)) \rangle = A(\mathbf{x}_2 - \mathbf{x}_1),$$
 (B.7)

where

$$A = \mu \left[ \frac{\sin\left(\frac{\nu}{2}\left(\tau - \sigma\right)\right)\cos\left(\frac{\nu}{2}\left(t - \tau - \sigma\right)\right)}{m\sin\left(\frac{\nu}{2}t\right)} + \frac{1}{Mt}\left(\tau - \sigma\right) \right]$$

And

$$\langle (x(\tau) - x(\sigma)) \rangle^2 - \langle (x(\tau) - x(\sigma))^2 \rangle = B$$
(B.8)

$$\langle (y(\tau) - y(\sigma)) \rangle^2 - \langle (y(\tau) - y(\sigma))^2 \rangle = B$$
(B.9)

$$\langle (z(\tau) - z(\sigma)) \rangle^2 - \langle (z(\tau) - z(\sigma))^2 \rangle = B, \qquad (B.10)$$

where

$$B = -\frac{i\hbar\mu}{m\nu^2} \left[ \frac{2\nu\sin\left(\frac{\nu}{2}\left(\tau - \sigma\right)\right)\sin\left(\frac{\nu}{2}\left(t - |\tau - \sigma|\right)\right)}{m\sin\left(\frac{\nu}{2}t\right)} + \frac{\nu^2}{Mt} \left|\tau - \sigma\right|\left(t - |\tau - \sigma|\right)\right].$$

By taking Eq.(B.8) + Eq.(B.9) + Eq.(B.10) and using Eq.(B.7), the result is

$$\left\langle \left(\mathbf{x}\left(\tau\right) - \mathbf{x}\left(\sigma\right)\right)^{2} \right\rangle$$

$$= \frac{3i\hbar\mu}{m\nu^{2}} \left[ \frac{2\nu\sin\left(\frac{\nu}{2}\left(\tau - \sigma\right)\right)\sin\left(\frac{\nu}{2}\left(t - |\tau - \sigma|\right)\right)}{m\sin\left(\frac{\nu}{2}t\right)} + \frac{\nu^{2}}{Mt}\left|\tau - \sigma\right|\left(t - |\tau - \sigma|\right)\right]$$

$$+ \mu^{2} \left[ \frac{\sin\left(\frac{\nu}{2}\left(\tau - \sigma\right)\right)\cos\left(\frac{\nu}{2}\left(t - \tau - \sigma\right)\right)}{m\sin\left(\frac{\nu}{2}t\right)} + \frac{1}{Mt}\left(\tau - \sigma\right) \right]^{2} |\mathbf{x}_{2} - \mathbf{x}_{1}|^{2} \cdot (B.11)$$



### Appendix C: The numerical calculation

Here is the MATHEMATICA program used in this work to minimize the ground state energy:

Clear[r,c,p,x,Ep,EF,Ev,Ek] r = 1.88; c =  $(12/Pi) (4/(9 Pi))^{(5/3)};$ Ep =  $(4/(9 Pi))^{(2/3)} (12 r)^{0.5};$ EF =  $((9 Pi)/4)^{(2/3)}/(r^2);$ FindMinimum[ EF  $((3/4) \text{ Ev } (1-p)^2 - c (r^2)/\text{Ev NIntegrate}[1/(Ep^2 Ek+(4/3) Ek^2+Ek^3)^{0.5}]$ NIntegrate[Exp[- x (Ek p^2+(Ep^2+(4/3) Ek+Ek^2)^{0.5})/Ev+Ek  $(1-p^2)/\text{Ev } (\text{Exp}[-x]-1)], \{x, 0, \text{Infinity}\}], \{Ek, 0, \text{Infinity}\}], \{p, 2\}, \{Ev, 1\}]$ 

When we get  $\rho$  and  $E\nu$ , we can evaluate Feynman and Krivoglaz-Pekar effective mass by the following program:

Clear[r,c,p,x,mF,mKP,Ep,Ev,Ek] r = 1.88;  $c = (12/Pi) (4/(9 Pi))^(5/3);$   $Ep = (4/(9 Pi))^(2/3) (12 r)^0.5;$  p = 0.979968; Ev = 2.56577; $mF = 1+(2/3) c (r^2)/(Ev^3) NIntegrate[(Ek)^0.5]$ 

$$\label{eq:linear} \begin{split} /(Ep^2+(4/3)Ek+Ek^2)^{\circ}0.5 \\ & \mbox{NIntegrate}[(x^2)\ Exp[-x\ (Ek\ p^2+(Ep^2+(4/3)\ Ek+Ek^2)^{\circ}0.5)/Ev+Ek\ (1-p^2)/Ev\ (Exp[-x]-1)],\ \{x,0,Infinity\}],\ \{Ek,0,Infinity\}]; \\ & \mbox{mKP}\ =\ 1/(p^2)\ Exp[(p^2)\ mF-1]; \\ & \mbox{Print}["mF/m = ",\ mF\ ,\ " ","mKP/m = ",\ mKP] \end{split}$$

The results are shown in table (C.1)

We also plot the graphs between the ground state energy and the variational parameters at  $r_s = 1.88$  in different cases as shown in Fig. (C.1), when the two parameters  $\rho$  and  $E_{\nu}$  are both varied, Fig. (C.2), when setting  $E_{\nu} = 2.56577$ , and Fig. (C.3), setting  $\rho = 0.979968$ .



$r_s$	ρ	$E_{\nu}$	$E_0$ (Ry)	$m_F/m$	$m_{KP}/m$
0.1	0.998895	0.499572	-3.5627	1.00206	1.00206
0.2	0.997931	0.790546	-2.32549	1.00449	1.00449
0.4	0.995159	1.05166	-1.49785	1.00941	1.00941
0.6	0.993355	1.47742	-1.15094	1.01427	1.01427
0.8	0.99105	1.69202	-0.952173	1.01903	1.01903
1.88(Be)	0.979968	2.56577	-0.535701	1.04349	1.04349
2.07(Al)	0.97806	2.68379	-0.501558	1.04762	1.04762
2.66(Mg)	0.972551	3.03965	-0.422117	1.0602	1.0602
3.26(Li)	0.967118	3.35984	-0.366692	1.07269	1.07269
4(Na)	0.960677	3.71846	-0.318049	1.08775	1.08776
6	0.944484	4.58411	-0.2394	1.12717	1.12718
8	0.929551	5.3289	-0.19543	1.16534	1.16537
10	0.91557	6.0029	-0.166859	1.20275	1.20279
20	0.855564	8.84784	-0.101863	1.38522	1.38536
40	0.764542	13.5546	-0.0620851	1.75008	1.75053
60	0.696294	17.8349	-0.0464928	2.12436	2.12529
80	0.642807	21.9661	-0.0378873	2.50691	2.50848
100	0.59963	26.0258	-0.0323373	2.89482	2.89718
200	0.467285	45.9268	-0.0198105	4.84637	4.85429
400	0.35441	84.777	-0.0121577	8.58202	8.60685
800	0.267687	159.869	$-7.45648 \times 10^{-3}$	15.3547	15.4272
1000	0.248225	170.135	$-6.36347 \times 10^{-3}$	18.1577	18.2768
2000	0.186212	373.511	$-3.89106 \times 10^{-3}$	32.6952	32.9648
4000	0.142615	709.237	$-2.36891 \times 10^{-3}$	57.1365	57.8188
8000	0.109881	1343.8	$-1.43676 \times 10^{-3}$	98.8757	100.537
10000	0.0972196	1567.07	$-1.22213 \times 10^{-3}$	$1\overline{17.592}$	$1\overline{18.274}$
20000	0.0782011	3111.56	$-7.37908 \times 10^{-4}$	201.868	206.737
40000	0.0606485	5852.1	$-4.44215 \times 10^{-4}$	344.269	354.826
100000	0.0434786	13432.9	$-2.26266 \times 10^{-4}$	693.361	721.762
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Table C.1: The table shows the numerical values of the two variational parameters, the ground state energy and the two effective masses at some selected  $r_s$ .



Figure C.1: A plot of the ground state energy versus the two variational parameters  $\rho$  and  $E_{\nu}$  at  $r_s = 1.88$ .





Figure C.2: A plot of the ground state energy versus the variational parameter  $\rho$  keeping  $E_{\nu} = 2.56577$  at  $r_s = 1.88$ .



Figure C.3: A plot of the ground state energy versus the variational parameter  $E_{\nu}$  keeping  $\rho = 0.979968$  at  $r_s = 1.88$ .

#### Vitae

Mr. Alongkorn Khudwilat was born in January 5, 1977. He received the Bachelor degree of Science in Physics from Chiangmai university in 1999. He was supported financially by the Development and Promotion of Science and Technology talents project of Thailand (DPST) during his study.



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