disturbance created by the particle still has impact on the particle's motion at later time. This particle is no longer the original electron but rather a dressed particle.

The corresponding propagator of the action in Eq. (10) is

$$G(r(t),r(0);t)=\int_{r(0)}^{r(t)}\mathrm{D}[r(\tau)]e^{iS}, \tag{11}$$

(do not confuse the propagator $G(r,r;t)$ with the dummy function $G(x)$ in Eq. (5)). However, the action in Eq. (10) is exceedingly complicated and very difficult to be solved. Thus we resort to an approximate action which has similar property but is easier to handle. In a previous work [2], a polaron-like action was chosen, which is

$$S_0=\frac{m}{2}\int_0^t \mathrm{d}\tau\,\dot{r}^2(\tau)-\frac{\kappa\Omega}{8}\int_0^t\int_0^t \mathrm{d}\tau\,\mathrm{d}\sigma\,\frac{\cos\left(\Omega t/2-|\tau-\sigma|\right)}{\sin\left(\Omega t/2\right)}|r(\tau)-r(\sigma)|^2. \tag{12}$$

This action is a harmonic trial action which composes of two variational parameters, i.e. κ and Ω. κ can be interpreted as an effective coupling strength between the particle and an external harmonic force with an effective harmonic frequency of Ω. These parameters are linked to Feynman parameters C and w by $\kappa=\dfrac{4C}{w}$ and $\Omega=w$. The action in Eq. (12) is supposed to be a good approximation to the action in Eq. (10) when $|r(\tau)-r(\sigma)|$ is not very large or there is only a short limited time available to the interaction among the particles, as discussed by Feynman [5, 6].

The approximate propagator to the first cumulant is

$$G(r(t),r(0);t)\approx G_0(r(t),r(0);t)e^{i\langle S-S_0\rangle_{S_0}}, \tag{13}$$

where

$$G_0(r(t),r(0);t)=\int_{r(0)}^{r(t)}\mathrm{D}[r(\tau)]e^{iS_0}, \tag{14}$$

and $\langle\ldots\rangle_{S_0}$ denotes an average with respect to S_0. Now if we transform $t\to -iT$ and let $T\to\infty$, the ground state energy E_0 and the effective mass m^* can be extracted from

$$G(0,0;T\to\infty)\simeq\varphi_0^*(0)\varphi_0(0)e^{-E_0T}=\left(\frac{m^*}{2\pi T}\right)^{3/2}e^{-E_0T}. \tag{15}$$

In the quantum's point of view, the physical interpretation of this propagator is as follows; firstly, the electron and the plasmons are initially in their ground states, then they are virtually excited and interact with each other, and eventually, after some time T later, they go back to their ground states. Consequently, the dressed particle is in its ground state and has zero momentum.

The explicit form of the ground state energy in Rydberg unit is written as[1]

$$E_0=\frac{3}{4}\nu(1-\rho)^2-\frac{1}{2\pi^2\nu}\int_0^\infty \mathrm{d}q\,q^2g^2(q)\,e^{-\beta}\int_0^\infty \mathrm{d}x\exp\left(\beta e^{-x}-\mu x\right), \tag{16}$$

where $\nu^2=\Omega^2+\kappa$, $\rho=\dfrac{\Omega}{\nu}$, $\beta=\dfrac{q^2(1-\rho^2)}{\nu}$ and $\mu=\dfrac{\omega_{\mathrm{p}}(q)+q^2\rho^2}{\nu}$. The variational parameters κ and Ω are now absorbed into another set of adjustable parameters ν and ρ. We concern now with the

[1] The mathematical detail in derivation of this result is quite lengthy. We suggest the reader to consult Ref. [2]. Even though the process of derivation was correct, the final expression of E_0 was not. The correction has done in this paper. There are some notes on the notations in Ref. [2], i.e. E_0 was scaled by E_{F}, so as the adjustable parameters, the frequency spectrum and the magnitude of the wave vector, and they had been renamed accordingly. Nevertheless, after adopting the same unit, the corrected results must be the same as ours.

physical meanings of E_0. It is of course the energy where the dressed particle has zero momentum but its position is not fixed. According to the classical picture, the particle is slowly moving stochastically in response to the changes of the potential field created by the particle itself and then goes back to its initial position after T. For $T \to \infty$, the particle momentum is zero on the average. Hence, E_0 can be compared with the energy of quasielectrons in a compatible physical system at $k = 0$ or at Γ point where the quasielectrons have slowest dynamics and highest symmetry.

Next, if we expand the propagator Eq. (15) in a series of $\frac{1}{T}$ where $\frac{1}{T} \to 0$, we get the effective mass which is

$$\frac{m^*}{m} = \frac{1}{\rho^2} \exp\left[\rho^2 - 1 + \frac{\rho^2}{3\pi^2\nu^3} \int_0^\infty dq\, q^4 g^2(q)\, e^{-\beta} \int_0^\infty dx\, x^2 \exp(\beta e^{-x} - \mu x)\right]. \tag{17}$$

In the next section, we will solve for ν and ρ which yield the minimum E_0. Then we get the corresponding m^*/m. We are interested in how E_0 and m^*/m behave as a function of r_s.

4 Calculation results and discussions The main purpose of this Section is to evaluate the ground state energy and the effective mass. We enter the plasmon spectra and the dielectric function from both Lundqvist's and Overhauser's models into the calculation of the ground state energy in Eq. (16) and the effective mass in Eq. (17). It is worth mentioning here that the integrals in these equations cannot be evaluated analytically. Thus we resort to a standard numerical integration and a numerical minimization [8]. The numerical minimization is adapted from the simulated annealing method which has a potential to find the global minimum in multidimensional problems. Some selected results are shown in Tables 1 and 2.

According to Table 1, we can see firstly, that ν is large at small r_s and becomes finite but irrelevant at very small r_s. It tends to zero very quickly as r_s increases. Secondly, $\rho \approx 1$ at small r_s and it is getting gradually smaller as r_s increases. Thirdly, E_0 is very large at small r_s and very small at large r_s. Lastly, $m^*/m \approx 1$ at small r_s and it is sharply increasing at very large r_s.

According to Table 2, we can see that E_0 from the two dielectric models behaves similarly, although E_0 from Overhauser's dielectric model is a little higher. This is because the local field and the vertex corrections slightly alter the dynamics of the electron gas and also affect the coupling strength of the electron–plasmon interaction.

Table 1 ν, ρ, E_0 and m^*/m are shown as a function of r_s. The plasmon spectrum and the corresponding coupling function are taken from Lundqvist's dielectric model.

r_s	ν	ρ	E_0 (Ry)	m^*/m
0.00001	finite	1	−489.77	1
0.0001	finite	1	−152.57	1
0.001	finite	1	−46.49	1
0.01	finite	1	−13.49	1
0.1	236.46	0.999	−3.56	1.002
1	7.03	0.989	-8.21×10^{-1}	1.024
2	2.46	0.979	-5.14×10^{-1}	1.046
5	6.09×10^{-1}	0.952	-2.72×10^{-1}	1.108
10	2.22×10^{-1}	0.916	-1.67×10^{-1}	1.203
100	9.59×10^{-3}	0.600	-3.23×10^{-2}	2.897
1000	7.24×10^{-4}	0.245	-6.37×10^{-3}	18.592
10000	6.06×10^{-5}	0.101	-1.22×10^{-3}	119.877
100000	4.96×10^{-6}	0.044	-2.26×10^{-4}	727.316

Table 2 E_0 shown from the different dielectric models. For comparison, the Coulomb-hole self-energy from Eq. (48) in Ref. [4] and the ground state energy of the plasmaron from Eq. (26) in Ref. [3] are also given.

r_s	Lundqvist	Overhauser	Coulomb-hole ($k = 0$) [4]	Plasmaron ($k = 0$) [3]
0.1	-3.56	-3.55	-3.55	5.20
1	-8.21×10^{-1}	-7.96×10^{-1}	-7.95×10^{-1}	1.09
2	-5.14×10^{-1}	-4.93×10^{-1}	-4.87×10^{-1}	5.94×10^{-1}
5	-2.72×10^{-1}	-2.48×10^{-1}	-2.47×10^{-1}	2.47×10^{-1}
10	-1.67×10^{-1}	-1.46×10^{-1}	-1.45×10^{-1}	1.23×10^{-1}
100	-3.23×10^{-2}	-2.29×10^{-2}	-2.22×10^{-2}	1.19×10^{-2}

As mentioned earlier, the Lagrangian and hence the Hamiltonain of the physical system we have discussed here can be related to the Coulomb-hole self-energy. Therefore, the results of the Coulomb-hole self-energy at $k = 0$ from Overhauser's work [4] using his own dielectric model are shown in Table 2. Even though, Overhauser's theory and ours originate from different approaches and have very different mathematical structures, it can be readily seen that with the same dielectric model, E_0 from our theory is in a very good agreement with Overhauser's Coulomb-hole self-energy at $k = 0$. The ground state of the plasmaron at $k = 0$ [3] are also given in the table for comparison. A more careful observation confirms that E_0 in this work is not the ground state energy of the plasmaron.

Since both dielectric models have been shown to give the similar results. Thus we have chosen Lundqvist's model for further investigation because it is simpler and easier to handle. By adopting Lundqvist's dielectric function, E_0 can be written explicitly as

$$E_0 = \frac{3}{4}\nu(1-\rho^2) - \frac{2\omega_p^2}{\pi\nu}\int_0^\infty dq \frac{e^{-\beta}}{\omega_p(q)} \int_0^\infty dx \exp(\beta e^{-x} - \mu x) . \tag{18}$$

In the next two subsections, we will study this E_0 in some asymptotic limits, such as in a very high electron density, i.e. r_s is vanishingly small, and in a very low density, i.e. r_s is very large. In these limits, we find that Eq. (18) can be evaluated analytically.

4.1 High density limit In this limit, $r_s \to 0$, we find from the numerical results that ν is large and finite and $\rho = 1$ so that the first term in Eq. (18) vanishes, $\beta = 0$ and

$$\int_0^\infty dx \exp(\beta e^{-x} - \mu x) = \frac{1}{\mu} . \tag{19}$$

Moreover, ω_p and k_F become very large so that q^4 has less significant contribution to $\omega_p(q)$ and

$$\mu\nu \approx \omega_p(q) \approx \sqrt{\omega_p^2 + \tfrac{4}{3}k_F^2 q^2} . \tag{20}$$

Consequently,

$$E_0 \approx -\frac{2\omega_p^2}{\pi\nu}\int_0^\infty dq \frac{1}{\omega_p(q)\mu} \approx -\frac{2\omega_p^2}{\pi}\int_0^\infty dq \frac{1}{\omega_p^2 + \frac{4}{3}k_F^2 q^2} . \tag{21}$$

It is straightforward to perform the definite integral and writing E_0 as a function of r_s. Then we get

$$E_0 \approx -\frac{1.56}{\sqrt{r_s}} , \tag{22}$$

Table 3 E_0 shown in the high density limit, Eq. (22) and in the low density limit, Eq. (26), compared with the numerical results of Eq. (18). The relative error is also given.

r_s	numerical	high density limit	low density limit	error (%)
0.00001	−489.77	−493.32	–	0.72
0.0001	−152.57	−156.00	–	2.25
0.001	−46.49	−49.33	–	6.11
1000	-6.37×10^{-3}	–	-7.42×10^{-3}	16.53
10000	-1.22×10^{-3}	–	-1.32×10^{-3}	8.20
100000	-2.26×10^{-4}	–	-2.35×10^{-4}	3.86

which yields less than 1% error compared with the numerical value at $r_s = 10^{-5}$, see Table 3. We expect that the error would reduce as r_s is getting closer to 0. Most of all, we see that E_0 is not a constant as $r_s \to 0$ but rather diverges as $\frac{1}{\sqrt{r_s}}$.

4.2 Low density limit In this limit, $r_s \to \infty$, $\nu \to 0$ and $\rho \to 0$ so that $\beta = \frac{q^2}{\nu}$, $\mu = \frac{\omega_p(q)}{\nu}$ and the first term in Eq. (18) can be neglected. In a closer examination, we find that

$$\exp(\beta e^{-x} - \mu x) \leq \exp(\beta - \mu x) \tag{23}$$

for all x. Thus

$$E_0 \leq -\frac{2\omega_p^2}{\pi\nu}\int_0^\infty dq \frac{1}{\omega_p(q)\mu} = -\frac{2\omega_p^2}{\pi}\int_0^\infty dq \frac{1}{\omega_p^2(q)} . \tag{24}$$

We also notice that the term which contains q^2 has a smaller contribution to $\omega_p(q)$ than the q^4 term. Thus, we have

$$E_0 \approx -\frac{2\omega_p^2}{\pi}\int_0^\infty dq \frac{1}{\omega_p^2 + q^4} , \tag{25}$$

which can be readily integrated out and written in term of r_s as

$$E_0 \approx -\frac{1.32}{r_s^{3/4}} , \tag{26}$$

which yields less than 4% error compared with the numerical value at $r_s = 10^5$, see Table 3.

We have some comments on the behavior of m^*/m in the present work as it would reflect a phase transition of the dressed particle from one physical regime to another between very different scales of r_s. We can see from table 1 that in the high density limit (small r_s) the dressed particle is mobile, i.e. m^*/m is close to unity, whereas in the low density limit (large r_s) it becomes self-trapped, i.e. m^*/m is exceedingly large. In addition, we have shown that E_0 behaves differently between these two extreme limits. One possible realization of our findings is the fact that in a degenerate electron gas, the total energy can be decomposed into the kinetic, the screened exchange and the Coulomb-hole parts. Furthermore, at very high density, the dynamics of electrons are dominated by the kinetic energy while at very low density, the electrons are localized. This is just coinciding with the behavior of m^*/m in our results. We believe that these findings might be an indication of Wigner crystallization.

In this work, we have shown that Feynman path integral can be applied to a system of an electron or a hole interacting with plasmons in a Fermi gas. By choosing an appropriate dielectric model, the ground state energy and the effective mass can be calculated. Some physical systems can be studied by choosing an appropriate integral limits for the plasmon modes. In this paper, we choose to study the Coulomb-hole self-energy. Our results are in good agreement with the Coulomb-hole self energy

at $k = 0$ from Overhauser's work [4]. The theory predicts a phase transition, i.e. the dressed particle is mobile in the high density limit but it exhibits a self-trapping behavior in the low density limit. This should be an indication, or at least a precursor, of Wigner crystallization. The extension of our theory to the plasmaron should be straightforward. The plasmaron theory is important because it supports some experimental findings in metals [9] and in magneto-optical properties of semiconductors [10]. Our theory is proposed in general and can be readily extend to lower dimensionality [11]. Some studies show that the electron–plasmon interaction is more significant in 2D systems [12], such as in a quantum well [13], than in 3D system. Furthermore, it has been suggested that the electron–plasmon interaction might assist Cooper pairing in superconductors [14]. We believe that our theory would suggest a general tool for study those frontier physics involving the electron–plasmon or the hole-plasmon interaction.

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Effect of charge-plasmon interaction to the effective mass of a charge particle in solids

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We use Feynman variational path integral method to study the effective mass of a charge particle in solids in which plasmons are an elementary excitation. This approach has an advantage as the ground state energy and the effective mass can be expressed analytically. We examine a particular case, i.e. the motion of a slow positron in metals. We find that the effective mass increases with r_s. The results are compared with those of a similar approach and of experiments. Nevertheless, the effect of the charge-plasmon interaction cannot fully account for the large positron effective mass in metals. The discrepancies are discussed.

Keywords: Feynman variational path integration, charge-plasmon interaction, effective mass

1. Introduction

Plasmons are an elementary excitation in an electron gas. A charge particle interacting with plasmons is a many-body problem[1]. It has a number of applications. The exchange-correlation energy of the electron gas can be approximated by regarding a single electron as the charge particle moving in the vicinity of the plasmons. It gives fair results in metals[2,3], semiconductors and low-dimension objects[4,5]. The next example would be charge particles, such as ions or muons, in solids which have been investigated both theoretically[6,7] and experimentally[8]. These studies suggested that those charge particles excite some plasmons, called wake field, which in return affect the motion of the charge particles at later time. A slow positron in solids, i.e. metals or semiconductors, is an important example. This is because the interaction between a positron and a solid can be decomposed into, for example, positron-plasmon[9,10] and positron-phonon[11] interactions. It was pointed out that the positron-plasmon interaction is dominant in semiconductors[12]. Positrons are quite technologically important. A number of theoretical works have been devoted for the calculations of

the positron's ground state energy[13], band structures[12,14,15], effective mass[9,10,16,17], diffusion coefficient and mobility[18] in condensed matter. These calculations are very useful for the interpretation of positron annihilation measurements. These measurements are of great interests as they can reveal density and types of defects in some solids[19,20], and they are normally non-destructive and hence favorable.

Because of the many-body nature of the problem, a charge particle interacting with plasmons cannot be solved accurately by an ordinary quantum theory. In this work, we propose that a charge particle interacting with plasmons can be modeled by Fröhlich-type Lagrangian. This Lagrangian was employed to study the system of an electron interacting with plasmons[21,22]. It has been shown that this kind of Lagrangian can be solved analytically by using Feynman variational path integral. Also, a similar approach has been used for examining the polaron problem. It gives the best analytical results in the polaron case[1]. From the path integral method, we obtain the corresponding propagator and, then the ground state energy and the effective mass. To verify our theory, we compare our results with a special case-the effective mass of a slow positron in metals. The effective mass is important as it can be related to the mobility and the diffusion coefficient of the positron[18]. In addition, the results from theoretical approaches[9,10,16,17] and experimental determination[23,24] are not in a good agreement. Some possible discrepancies will be discussed.

This paper is organized as follows. The interaction model is discussed in section 2. The effective mass from variational path integral method is in section 3. Results and discussions are in section 4. Conclusions are laid in section 5.

2. Interaction Model

The interaction between a charge particle and plasmon field can be modeled by a Fröhlich-type Lagrangian[2,21] as

$$L = \frac{1}{2}m_c\dot{r}^2 + \sum_{\mathbf{q}}\frac{1}{2}m_e\left(\dot{Q}_{\mathbf{q}}^2 - \omega_q^2 Q_{\mathbf{q}}^2\right) - \sum_{\mathbf{q}}\sqrt{\frac{2m_e\omega_q}{V}}g_q Q_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{r}}, \qquad (1)$$

where m_c is the charge mass, $\mathbf{r}$ is the position vector of the charge particle, m_e is the bare electron mass as electrons are the bases of the plasmons, $\mathbf{Q_q}$ are the plasmon generalized coordinates and $\dot{\mathbf{Q}}_\mathbf{q}$ are their conjugate momenta, $\mathbf{q}$ denote the plasmon wavevectors, ω_q is the plasmon spectrum, V is the volume of the system. The system is assumed isotropic so that the dispersion of the plasmons is directionally independent. The first term in Eq. (1) describes the kinetic energy of the charge particle. The second term is the harmonic representation of the plasmon modes. The third term is the interaction between the charge particle and the plasmons. The strength of the interaction is enclosed in a coupling function g_q. The remaining task is to select a suitable ω_q and g_q.

In the present work, we intend to use a simplified picture for the many-body interaction. Thus, the plasmon spectrum ω_q and the coupling function g_q are taken from the so-called plasmon-pole approximation. In this approximation, the electron-

hole excitations are absorbed into the effective plasmon excitations. The f sum rules are imposed as a particle conservation rule. There are several plasmon-pole models for metals[2,3], semiconductors[5,25] and liquids[26]. For the purpose of illustration, we choose a simple model introduced by Lundqvist[2]. He proposed that an electron gas can be described by a simplified dielectric function,

$$\varepsilon(q,\omega) = \frac{\omega_q^2 - \omega^2}{\omega_q^2 - \omega_p^2 - \omega^2}. \tag{2}$$

This dielectric function is not a full extension of the celebrated random phase approximation (RPA) but rather an approximation, and it was chosen to satisfy the f sum rules[2]. The plasmon spectrum is

$$\omega_q^2 = \omega_p^2 + \frac{4}{3}k_F^2 q^2 + q^4. \tag{3}$$

The coupling function can be written as

$$g_q^2 = \frac{8\pi}{q^2}\left(\frac{\partial\varepsilon(q,\omega)}{\partial\omega}\right)^{-1}_{\omega=\omega_p} = \frac{4\pi\omega_p^2}{q^2\omega_q}. \tag{4}$$

This model is simple and yet allow us to find some useful analytic solutions. It also gives reasonable ground state energy and correlation energy of the electron gas in the metallic densities[2].

Throughout this work, we adopt the Bohr radius as the unit of length and Rydbergs (Ry) as the unit of energy. In these units, the long wavelength plasmon frequency $\omega_p = \frac{3.4641}{r_s^{3/2}}$ and the magnitude of Fermi wave vector $k_F = \frac{1.9192}{r_s}$, where r_s is a parameter defined from the electron gas density $n = (\frac{4}{3}\pi r_s^3)^{-1}$. The charge particle states will be labeled by k and the plasmon states will be labeled by q.

It is worthy of note that the Lagrangian for a positive or negative charge particle is the same as in Eq. (1). Only appropriate dielectric response must be selected accordingly. To a crude approximation, the dielectric response for an electron in the electron gas should be the same as that for a positron in the electron gas. Some refinement to the interaction model has been suggested, i.e. for a positron in an electron gas, the coupling function must be multiplied by some enhancement factor and the plasmon dispersion relation must be modified accordingly[3,27,28]. This refinement will be taken into account in our subsequent works.

3. Effective Mass from Variational Path Integral Method

The main objective of this work is to calculate the effective mass of a charge particle interacting with plasmons. In this section, we give a brief description of Feynman variational path integration. The mathematical details have been presented elsewhere[21,29,30,31,32,33,34]. We discuss here only the physical aspects of the method and how it can be compared with experiments and other approaches.

By using path integration technique[29,30], Sa-yakanit *et.al.*[21] showed that the corresponding action of Eq. (1), after integrating out the plasmon coordinates, can be written as

$$S = \frac{1}{2}m_c\int_0^t d\tau\dot{r}^2(\tau) + \frac{1}{16\pi^3}\int dq g_q^2\int_0^t\int_0^t d\tau d\sigma\frac{\cos[\omega_q(t/2-u)]}{\sin[\omega_q t/2]}e^{iq\cdot(r(\tau)-r(\sigma))}, \quad (5)$$

where $u = |\tau - \sigma|$. This action describes a system of a particle moving in a non-local potential field. This potential field reflects the disturbance caused by the presence of the particle and affecting the particle's motion at later time.

However, the action in Eq. (5) is too complicated to be solved. By using variational principle, we have freedom to choose a simpler action and use variational technique to obtain some useful information. In a previous work[21], a polaron-like action was chosen, which is

$$S_0 = \frac{1}{2}m_c\int_0^t d\tau\dot{r}^2(\tau) - \frac{\kappa\Omega}{8}\int_0^t\int_0^t d\tau d\sigma\frac{\cos[\Omega t/2-u]}{\sin[\Omega t/2]}|r(\tau)-r(\sigma)|^2. \quad (6)$$

This action is quadratic and composes of two variational parameters, i.e. κ and Ω which are related to Feynman parameters C and w by $\kappa = \frac{4C}{w}$ and $\Omega = w$. The first term in Eq. (6) is the kinetic energy of the particle. The second term is a non-local harmonic potential in which κ is an effective coupling strength between the particle and an external harmonic force with an effective harmonic frequency of Ω. This trial action is a good approximation to the action in Eq. (5) when $|r(\tau) - r(\sigma)|$ is fairly small or there is only a short interaction time available, as discussed by Feynman[29,30]. From this action, Feynman stated that it leads to the construction of a approximate propagator[29,30]. Furthermore, the propagator already contains all the information of the system, such as the ground state energy and the effective mass. Thus knowing the propagator is equivalent to solving the problem. The full treatment of the polaron and polaron-like problems using variational path integrals has been given several times in the literature[21,29,30,31,32,33,34]. We summarize only some essential expressions in appendix A.

From the approximate propagator in Eqs. (A.12) and (A.14), the ground state energy is written as[21,22]

$$E_0 = \frac{3}{4}\nu(1-\rho)^2 - \frac{1}{2\pi^2\nu}\int dq q^2 g_q^2 e^{-\beta}\int_0^\infty dx\exp(\beta e^{-x} - \mu x), \quad (7)$$

where $\nu^2 = \Omega^2 + \frac{\kappa}{m_c}$, $\rho = \frac{\Omega}{\nu}$, $\beta = \frac{q^2(1-\rho^2)}{2m_c\nu}$ and $\mu = \frac{\omega_q}{\nu} + \frac{q^2\rho^2}{2m_c\nu}$. The variational parameters κ and Ω are now absorbed into another set of adjustable parameters ν and ρ. The system is assumed spherical symmetry. Thus we can replace $\int dq$ by $\int 4\pi^2 q^2 dq$. According to the propagator $G(0,0;T)$, E_0 can be interpreted as the energy of the particle which is moving stochastically in response to the changes in the potential field created by the motion of the particle itself and then goes back to its initial position after a duration T. For $T \to \infty$, the particle has an average zero momentum. Hence, E_0 can be compared with the energy of a particle in a compatible physical system at $k = 0$ or at Γ point where the particle has slowest

dynamics and its wavefunction has highest symmetry. It is readily to see that this method is quite suitable for the problem of a thermalized positron in solids because the positron is slowing moving and it occupies the Γ state[12,15].

The limits of $\int dq$ in Eq. (7) are worth discussing. Overhauser[3] show that if the charge particle is an electron and we perform $\int_0^{k_F} dq$, E_0 is a major contribution to the correlation energy of the electron gas at $k = 0$. If we perform $\int_0^{\infty} dq$, E_0 is the Coulomb-hole self-energy of the electron gas at $k = 0$[3,22]. For a positron, we have no prior reasons to exclude short wavelength plasmons. Thus we simply perform $\int_0^{\infty} dq$. Then E_0 should be the lowest possible ground state energy for the positron-plasmon interaction in our model. The reason is as follows. Firstly, it is readily seen that the first term, the second term and its integrand in Eq. (7) are always positive. Owing to the minus sign in front of the second term, for a given set of variational parameters, the lowest E_0 is where the second term is largest. Performing $\int_0^{\infty} dq$ with appropriate variational parameters will give the largest possible value of the second term and hence the lowest possible E_0.

Next, the effective mass can also be extracted from Eqs. (A.12) and (A.14). Sa-yakanit[33] showed that if we expand the propagator Eq. (A.14) in a series of $\frac{1}{T}$ where $\frac{1}{T} \to 0$, we get the low energy limit effective mass which is[22]

$$\frac{m_c^*}{m_c} = \frac{1}{\rho^2} \exp\left[\rho^2 - 1 + \frac{\rho^2}{3\pi^2\nu^3} \int dq q^4 g_q^2 e^{-\beta} \int_0^{\infty} dx x^2 \exp(\beta e^{-x} - \mu x)\right]. \quad (8)$$

The expressions (7) and (8) differ from those of a previous work[22]. This is because we do not assume here that $m_c = m_e$. Therefore, we can implicitly take the effects of a periodic potential or a phonon interaction into the account. This is the major improvement in our theory.

4. Results and Discussions

In this section, we show that the interaction model and Feynman variational path integration can be applied for the calculation of the effective mass of a slow positron in metals. The metallic densities of the electron gas are a density in which r_s is between 2.0-6.0. According to the variational principle, in order to obtain the ground state properties of a slow positron in metals, we insert ω_q from Eq. (3) and g_q from Eq. (4) into Eq. (7), and solve for ν and ρ which yield the lowest E_0. Then we insert these ν and ρ into Eq. (8) to get the corresponding m_c^*/m_c. The expressions (7) and (8) cannot be evaluated analytically. Thus, we resort to a standard numerical integration and a simulated annealing minimization[35].

Apart from ω_q and g_q, another input parameter in this theory is the ratio m_c/m_e. It has been shown that m_c/m_e differs from unity because it depends on band structures[12,14,15] or phonon effects[11]. For illustration, we explore three different values of m_c/m_e, i.e. 0.8, 1.0 and 1.2. The results are shown in Table 1-3. It can be readily seen that the ground state energy decreases as r_s increases and it increases a little as m_c/m_e increases. The effective mass, m_c^*/m_c increases as r_s increases

Table 1. Shows ν, ρ, E_0, m_c^*/m_c and m_c^*/m_e as a function of r_s. The plasmon spectrum and the coupling function are taken from Lundqvist's model. We set $m_c/m_e = 0.8$.

r_s	ν	ρ	E_0 (Ry)	m_c^*/m_c	m_c^*/m_e
1	7.05	0.988	-0.791	1.020	0.816
2	2.55	0.978	-0.494	1.039	0.831
3	1.37	0.968	-0.373	1.057	0.846
4	8.90×10^{-1}	0.959	-0.305	1.074	0.859
5	6.33×10^{-1}	0.950	-0.261	1.091	0.873
6	6.15×10^{-1}	0.931	-0.232	1.110	0.888
10	2.27×10^{-1}	0.911	-0.160	1.173	0.938

and as m_c/m_e increases. Moreover, at fixed r_s, ν and ρ are different for a different m_c/m_e. Evidently, this shows the internal effects of m_c/m_e to the ground state properties.

Table 2. Same as table 1 but with $m_c/m_e = 1.0$.

r_s	ν	ρ	E_0 (Ry)	m_c^*/m_c	m_c^*/m_e
1	7.03	0.989	-0.821	1.024	1.024
2	2.46	0.979	-0.514	1.046	1.046
3	1.31	0.969	-0.388	1.067	1.067
4	8.65×10^{-1}	0.961	-0.318	1.088	1.088
5	6.09×10^{-1}	0.952	-0.272	1.108	1.108
6	4.74×10^{-1}	0.945	-0.239	1.127	1.127
10	2.22×10^{-1}	0.916	-0.167	1.203	1.203

A similar approach to our theory was introduced by Hamann[17]. By using the many-body techniques and Feynman diagrams, he evaluated m_c^*/m_c of a positron in metals. Some selected values of m_c^*/m_c from Hamann's work are shown in Table 4. We find that those m_c^*/m_c in his calculations are 3-8% higher than ours. This is because he used a slightly different dielectric function. However, the trend is quite the same.

Table 3. Same as table 1 but with $m_c/m_e = 1.2$.

r_s	ν	ρ	E_0 (Ry)	m_c^*/m_c	m_c^*/m_e
1	7.13	0.990	-0.843	1.027	1.232
2	2.38	0.980	-0.528	1.052	1.262
3	1.29	0.971	-0.400	1.076	1.291
4	8.43×10^{-1}	0.963	-0.328	1.099	1.319
5	6.02×10^{-1}	0.955	-0.280	1.122	1.346
6	4.64×10^{-1}	0.948	-0.247	1.144	1.373
10	2.16×10^{-1}	0.920	-0.172	1.229	1.475

There were a number of experiments which aimed to determine m_c^*/m_c of a thermalized positron in metals[23,24]. Some selected values of m_c^*/m_c from the experiments are also shown in Table 4. We find that those m_c^*/m_c from the experiments are quite large, i.e. almost twice larger than those from our calculations. It should be pointed out that m_c^*/m_c from the experiments should include all the interactions in metals. The large m_c^*/m_c could result from other effects, such as positron-phonon or positron-defect interaction. An experiment showed that the positron-polaron also has a large effective mass[36]. Other experiments suggested that positrons are easily trapped in the vicinity of defects[19,20]. A path integral theory showed that interacting with defects can modify the effective mass[31,32]. Moreover, the effective mass determination experiments were carried out over a range of high temperature. They cannot be done at very low temperature because a positron annihilates with an electron before thermalization. At the present, our theory does not include temperature effects. However, the extension of our theory to include the temperature effects should be straightforward. This was done in the case of polaron by modifying the approximate propagator to account for the effects of some thermally excited states[37,38]. It was suggested that the plasmon spectrum can be modified to include the effect of temperature as well[39]. All these thermal modifications will be considered in our future works.

Table 4. Some selected values of m_c^*/m_c from Hamann's work and from the experiments compared with our results where $m_e/m_e = 1.0$.

r_s	m_c^*/m_c (Ours)	m_c^*/m_c (Hamann[17])	r_s	m_c^*/m_c (Experiments[23,24])
2	1.05	1.08	3.25	1.8
3	1.07	1.12	3.93	1.8
4	1.09	1.15	4.86	2.1
5	1.11	1.19	5.20	2.3
6	1.13	1.22	5.63	2.5

5. Conclusions

We propose a general theory for studying a charge particle moving in the vicinity of plasmons using Fröhlich Lagrangian and Feynman variational path integration. The motion of a slow positron in metals is extensively investigated. We find that the effective mass increases with r_s and it is in an agreement with the results from Hamann's work. However, the experiments showed a large effective mass. The discrepancies should be that in our work the effects of phonon and defects are not fully accounted for and the temperature effects are absent. We believe that our theory could be applied for other physical systems, such as electron-plasmon interaction, wake interaction and so on.

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Appendix A. Feynman Variational Path Integral Method for the Charge-plasmon System

In this appendix, we outline some crucial results from Feynman variational path integral method. The main aim is to find the propagator $G(\mathbf{r}_2, \mathbf{r}_1, t)$ from which some useful information, i.e. E_0 and m_c^*/m_c, can be extracted.

From the action in Eq. (5), the corresponding propagator is

$$G(\mathbf{r}_2, \mathbf{r}_1; t) = \int_{\mathbf{r}_1}^{\mathbf{r}_2} D\left[\mathbf{r}(t)\right] e^{iS}. \tag{A.1}$$

This propagator is complicated and we cannot find its solutions directly. Thus we impose the variational principle and choose a polaron-like action as in Eq. (6). Its corresponding propagator is

$$G_0(\mathbf{r}_2, \mathbf{r}_1; t) = \int_{\mathbf{r}_1}^{\mathbf{r}_2} D\left[\mathbf{r}(t)\right] e^{iS_0}. \tag{A.2}$$

The chosen trial action is in a quadratic form so that it can be solved analytically. From the cumulant expansion, we find that the true propagator can be approximated in term of the trial action as

$$G(\mathbf{r}_2, \mathbf{r}_1; t) \approx G_0(\mathbf{r}_2, \mathbf{r}_1; t) e^{i\langle S - S_0 \rangle_{S_0}}, \tag{A.3}$$

where $\langle ... \rangle_{S_0}$ denotes an average with respect to S_0. Eq. (A.3) can be solved in term of $\mathbf{r}_1$, $\mathbf{r}_2$ and the variational parameters. Here we simply quote the solutions which are[21,31,32,33,34]

$$\begin{aligned} G_0(\mathbf{r}_2, \mathbf{r}_1; t) = & \left(\tfrac{m_c}{2\pi i t}\right)^{3/2} \left(\tfrac{\nu \sin[\Omega t/2]}{\Omega \sin[\nu t/2]}\right)^3 \\ & \times \exp\left\{-\tfrac{i m_c}{2t}\left(\tfrac{(1-\rho^2)\nu t}{2}\cot\left[\tfrac{\nu t}{2}\right] + \rho^2\right)|\mathbf{r}_2 - \mathbf{r}_1|^2\right\}. \end{aligned} \tag{A.4}$$

The average of S and S_0 can be decomposed as

$$< S - S_0 >_{S_0} = < S >_{S_0} - < S_0 >_{S_0}, \tag{A.5}$$

and

$$< S >_{S_0} = \frac{1}{16\pi^3} \int dq q_q^2 \int_0^t \int_0^t d\tau d\sigma \frac{\cos[\omega_q(t/2 - u)]}{\sin[\omega_q t/2]} e^{-\frac{1}{2}iq^2 A + iq\cdot(\mathbf{r}_2 - \mathbf{r}_1)B}, \tag{A.6}$$

and

$$\begin{aligned} < S_0 >_{S_0} = & \tfrac{3i(1-\rho^2)}{2}\left(\tfrac{\nu t}{2}\cot[\tfrac{\nu t}{2}] - 1\right) \\ & - \tfrac{\kappa\Omega}{8}\int_0^t \int_0^t d\tau d\sigma \tfrac{\cos[\Omega t/2 - u]}{\sin[\Omega t/2]}(\mathbf{r}_2 - \mathbf{r}_1)^2 B^2, \end{aligned} \tag{A.7}$$

where

$$A = \frac{(1-\rho^2)}{m_c}\left\{\frac{2\sin[\nu u/2]\sin[\nu(t-u)/2]}{\nu\sin[\nu t/2]} + \frac{\Omega^2}{\nu^2-\Omega^2}\frac{u(t-u)}{t}\right\}, \tag{A.8}$$

and

$$B = (1-\rho^2)\left\{\frac{\sin[\nu u/2]\cos[\nu(t-(\tau+\sigma))/2]}{\sin[\nu t/2]} + \frac{\Omega^2}{\nu^2-\Omega^2}\frac{u}{t}\right\}. \tag{A.9}$$

The diagonal part of $G(\mathrm{r}_2,\mathrm{r}_1;t)$ can be explicitly written as

$$\begin{aligned} G(\mathrm{r},\mathrm{r};t) = &\left(\tfrac{m_c}{2\pi i t}\right)^{3/2}\left(\tfrac{\nu\sin[\Omega t/2]}{\Omega\sin[\nu t/2]}\right)^3 \exp\left\{\tfrac{3(1-\rho^2)}{2}\left(\tfrac{\nu t}{2}\cot[\tfrac{\nu t}{2}]-1\right)\right\} \\ &\times\exp\left\{\tfrac{i}{16\pi^3}\int dq g_q^2\int_0^t\int_0^t d\tau d\sigma\tfrac{\cos[\omega_q(t/2-u)]}{\sin[\omega_q t/2]}e^{-\frac{1}{2}iq^2A}\right\}. \end{aligned} \tag{A.10}$$

Our system is isotropic and thus translational invariant. Therefore $G(\mathrm{r},\mathrm{r};t) \equiv G(0,0;t)$. By using the identity

$$\int_0^t\int_0^t d\tau d\sigma f(u) = 2\int_0^t dz(t-z)f(z), \tag{A.11}$$

we get

$$\begin{aligned} G(0,0;t) = &\left(\tfrac{m_c}{2\pi i t}\right)^{3/2}\left(\tfrac{\nu\sin[\Omega t/2]}{\Omega\sin[\nu t/2]}\right)^3 \exp\left\{\tfrac{3(1-\rho^2)}{2}\left(\tfrac{\nu t}{2}\cot[\tfrac{\nu t}{2}]-1\right)\right\} \\ &\times\exp\left\{\tfrac{i}{8\pi^3}\int dq g_q^2\int_0^t dz(t-z)\tfrac{\cos[\omega_q(t/2-z)]}{\sin[\omega_q t/2]}e^{-\frac{1}{2}iq^2C}\right\}, \end{aligned} \tag{A.12}$$

where

$$C = \frac{(1-\rho^2)}{m_c}\left\{\frac{2\sin[\nu z/2]\sin[\nu(t-z)/2]}{\nu\sin[\nu t/2]} + \frac{\Omega^2}{\nu^2-\Omega^2}\frac{z(t-z)}{t}\right\}. \tag{A.13}$$

To avoid dealing with some oscillating behavior in the solutions, we transform $t \to -iT$. This transformation is valid as long as spin is not explicitly taken into account, as discussed by Feynman[29]. In order to find some ground state properties, we let $T \to \infty$, the ground state energy E_0 and the effective mass m_c^*/m_c can be extracted from

$$G(0,0;T\to\infty) \simeq \varphi_0^*(0)\varphi_0(0)e^{-E_0T} = \left(\frac{m_c^*}{2\pi T}\right)^{3/2}e^{-E_0T}. \tag{A.14}$$

This propagator describes the charge particle and the plasmons which are initially in their ground states, then they are virtually excited and interact with each other, and eventually, after some time T later, they go back to their ground states. This picture is analogous to the self-energy scheme in quantum many-body theory[1]. The explicit expressions for E_0 and m_c^*/m_c are shown in Eqs. (7) and (8) respectively.

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Application of Feynman path integration to the electron-plasmon interaction

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Abstract

We use Feynman path integral to calculate some physical properties, *i.e.* the ground state energy and the effective mass of the electron-plasmon system. The Lagrangian and then the action which describe the motion of a particle, called the plasmaron, are derived. We have studied two models of the dielectric media proposed by Lundqvist and Overhauser. By using numerical integration and minimization, we evaluate the ground state energy and the effective mass as a function of r_s. We found that both models give similar ground state energy. There is a possibility that the theory would predict a phase transition in the plasmaron system. The analytic expansion of the ground state energy in some extreme limits are discussed. We also found that in low electron density the ground state energy is proportional to $\frac{1}{r_s}$ which is in a good agreement with Wigner's prediction.

I. Introduction

In this work, the interaction between an electron and plasmons is investigated. This electron, together with the plasmons and their interactions, is called a plasmaron. The plasmons are the quantized harmonic oscillations having electrons as oscillators. They exist naturally in real metals and any electron gas. The interaction is described by FrÖhlich Hamiltonian and can be solved by using Feynman path integral method[1]. This problem is analogous to the polaron problem which can be solved successfully by Feynman path integrals[2]. The polaron problem is a simplest way to show how a particle interacts with a field. However, the polaron problem concerns only two parameters: one constant phonon frequency and one constant coupling parameter. In the present work, it concerns a dispersion of plasmon frequencies and leads to a momentum-dependence coupling function[3]. Thus the plasmaron is much more complicated than the polaron problem.

The interaction among electrons is extremely important because the world is made of the Pauli exclusion principle of electrons. Without electrons, life cannot exist. There were many theoretical approaches attempt to explain the electron-electron interaction[4]. However, all of them are of perturbation methods in which mathematics becomes more invincible as higher-order terms are added. Furthermore, one needs different approaches for different regimes and hence most of the approaches lose their transferability. This work on the plasmaron problem is an alternative

method for studying the electron-electron interaction. We uses Feynman method which is non-perturbative and non-local in time. The non-local term means that the motion of the electron creates a distorted environment at a point of time. This distorted environment will decay with a finite lifetime. As long as it exists, this environment will affect the motion of the electron at later time. The non-perturbative term implies that this method has a potential to give a more accurate calculation value. Feynman had shown that this method can accurately describe the properties of the polaron for the whole range of its coupling constants[5]. Sa-yakanit had also shown that the same method was successfully applied to study a number of frontier physics problems such as disordered systems, heavily doped semiconductors, anharmonic crystals and *etc.*[6].

There are a number of further applications. Firstly, the 3D plasmaron can be applied for the calculations of the electron correlation energy. The electron correlation energy is very difficult to obtain an accurate value because it contains two excitation modes: plasmons and electron-hole pairs. Overhauser[3] suggested that this problem can be simplified by using modified plasmon modes which incorporate the effect of both plasmons and electron-hole pair. He successfully reproduced the electron correlation energy for the metallic density. This application will be served as a test for the present research. Secondly, the plasmaron could give a prediction of the crystallization of electrons, the so-called Wigner crystallization, as their density becomes very low. Thirdly, the 2D plasmaron is used for describing the superconductivity in a number of high-T_C superconductors, such as Y-Ba-Cu-O or Bi-Sr-Ca-Cu-O[7]. Fourthly, the quasi-1D plasmaron is used for explaining the high-frequency behavior of organic semimetals[8]. Lastly, there is a possibility that the plasmaron can give a description of the metal to insulator transition[9].

This paper is organized as follows: the models of the electron-plasmon interaction are in section II, the general Feynman path integral theory of the plasmaron is in section III and calculation results and discussions are in section IV.

II. The models of the electron-plasmon interaction

Firstly, we consider an electron moving in a dielectric medium such as a degenerate electron gas or a jellium. The electron and the dielectric medium will interact with each other. The spectrum of excitation modes will determine the strength of the interaction. However, there are two elementary excitations in dielectric media; plasmons and electron-hole pairs. Calculations involving electron-hole pairs are quite tedious[3] and we shall try to avoid. Lundqvist[10] suggested that the whole excitation spectrum can be replaced by a modified plasmon spectrum. This

modified plasmon spectrum obeys the sum rules[4]. Those sum rules limit the contributions of plasmons to the dielectric function and hence serve as a convenient interpolation scheme. This approximation is sometimes called the single-mode approximation.

The first model was introduced by Lundqvist[10]. He considered the electron gas in the random phase approximation (RPA) and proposed that the dielectric medium in this case can be described by a simplified dielectric function,

$$\varepsilon(k,\omega) = \frac{\omega_p^2(k) - \omega^2}{\omega_p^2(k) - \omega_p^2 - \omega^2}. \tag{1}$$

This dielectric function is not a full cover of RPA but rather an approximation, called one pole approximation, and it was chosen to satisfy the sum rules[10]. The plasmon spectrum is

$$\omega_p^2(k) = \omega_p^2 + \frac{4}{3}k_F^2k^2 + k^4. \tag{2}$$

The coupling function can be written as

$$g^2(k) = \frac{8\pi}{k^2}\left(\frac{1}{\partial\varepsilon(k,\omega)/\partial\omega}\right)_{\omega=\omega_p} = \frac{4\pi\omega_p^2}{k^2\omega_p(k)}. \tag{3}$$

Note that in order to compare our results with some existing data, we need to follow a natural unit widely used in the physics of atomic scale, *i.e.* $\hbar = 1$, $e^2 = 2$, $\frac{\hbar^2}{2m} = 1$. By using r_s unit, the long wavelength plasmon frequency $\omega_p = \frac{3.4641}{r_s^{3/2}}$ and the magnitude of Fermi wave vector $k_F = \frac{1.9192}{r_s}$.

The second model was suggested by Overhauser[3]. He noticed that RPA is not account for the exchange and correlation effects of the electron gas. Thus he included some correction terms into the dielectric function, which can be expressed as

$$\varepsilon(k) = 1 + \frac{P(x)}{1 - G(x)P(x)}, \tag{4}$$

where

$$x = \frac{k}{2k_F},$$

$$G(x) = \frac{1.1x^2}{\sqrt{1 + 10x^2 + 1.5x^4}},$$

$$P(x) = \frac{\Sigma(x)}{\pi k_F x^2},$$

$$\Sigma(x) = \frac{1}{2} + \left[\frac{1 - x^2}{4x}\right]\ln\left|\frac{1+x}{1-x}\right|.$$

The form of eq. (4) is similar to incorporating the local field corrections and the vertex corrections into the dielectric function[4]. This model is phenomenological because the exact corrections are not known. Nevertheless, Overhauser showed that his dielectric function reproduced correct correlation energy in the metallic density range[3]. The plasmon spectrum is then

$$\omega_p^2(k) = \frac{\omega_p^2 \varepsilon(k)}{\varepsilon(k) - 1}. \tag{5}$$

The coupling function is slightly modified as

$$g'(k) = g(k)\left[1 - G(x)\right], \tag{6}$$

where $g(k)$ is defined in eq. (3).

In the next section, we will discuss Feynman path integral method for the electron-plasmon system. The information needed in Feynman method is the plasmon spectra and the coupling functions defined in eq. (2), (3), (5) and (6).

III. Feynman path integral theory of the plasmaron

In this section, we will give a general description of the path integral theory of the electron-plasmon system. The general theory can be stated without referring to a specific interaction model. Firstly, we construct the Lagrangian of the electron-plasmon system[1] which is of FrÖhlich-type;

$$L = \frac{P^2}{2m} + \sum_{\vec{k}} \frac{m}{2}(\dot{q}_{\vec{k}}^2 - \omega_p^2(k) q_{\vec{k}}^2) - \sum_{\vec{k}} \sqrt{\frac{2m\omega_p(k)}{V}} g(k) q_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}, \tag{7}$$

where m is the electron mass and $2m = 1$ in the atomic unit, P is the electron momentum, $q_{\vec{k}}$ are the plasmons' generalized coordinates and $\dot{q}_{\vec{k}}$ are their conjugate momentum, $\vec{k}$ denote plasmons' wave vector, V is the volume of the system. This Lagrangian represents a coupled system of an electron and plasmons. The plasmons are created by the presence of the electron and in return affect the motion of the electron. The first term in the Lagrangian describes the kinetic energy of the electron. The second term is the harmonic representation of the acoustic plasmon modes. The third term is the interaction between the electron and the plasmons. The strength of the interaction is enclosed in $g(k)$. We can choose $g(k)$ and its corresponding $\omega_p(k)$ from the previous section. We will see later that both models give very similar results.

Follow Feynman's method, Sa-yakanit *et.al.*[1] showed that the corresponding action is

$$S=\frac{m}{2}\int_0^t \dot{r}^2 d\tau+\frac{1}{4\pi^2}\int_0^\infty dk k^2 g^2(k)\int_0^t\int_0^t d\tau d\sigma \frac{\cos\left[\omega_p(k)(\frac{t}{2}-|\tau-\sigma|)\right]}{\sin\left[\omega_p(k)\frac{t}{2}\right]} e^{i\bar{k}\cdot(\bar{r}(\tau)-\bar{r}(\sigma))}. \quad (8)$$

The system is assumed to have spherical symmetry. Thus we can replace $\int d\bar{k}$ by $\int 4\pi^2 k^2 dk$. This action is analogous to a system of a particle in a potential field, the second term of eq. (8), which is non-local in time. The classical picture is that the disturbance created by the particle still has impact on its motion at later time. This particle is the so-called plasmaron. The plasmaron propagator is

$$G(\bar{r},\bar{r}';t)=\int_{\bar{r}'}^{\bar{r}} D[\bar{r}(t)]e^{\frac{i}{\hbar}S}. \quad (9)$$

However, the action in eq. (8) is exceedingly complicated and very difficult to be solved. One solution is to find an approximate action which has similar property but is easy to handle. In the previous work[1], a polaron-like action was chosen, which is

$$S_0=\frac{m}{2}\int_0^t \dot{r}^2 d\tau-\frac{\kappa\Omega}{8}\int_0^t\int_0^t d\tau d\sigma\left|\bar{r}(\tau)-\bar{r}(\sigma)\right|^2\frac{\cos\Omega(\frac{t}{2}-|\tau-\sigma|)}{\sin\Omega\frac{t}{2}}. \quad (10)$$

This action composes of two variational parameters, *i.e.* κ and Ω. These parameters are linked to Feynman parameters C and w by $\kappa=\frac{4C}{w}$ and $\Omega=w$. The approximate plasmaron propagator to the first cumulant is

$$G(\bar{r},\bar{r}';t)\approx G_0(\bar{r},\bar{r}';t)e^{\frac{i}{\hbar}(S-S_0)_{S_0}}, \quad (11)$$

where

$$G_0(\bar{r},\bar{r}';t)=\int_{\bar{r}'}^{\bar{r}} D[\bar{r}(t)]e^{\frac{i}{\hbar}S_0}.$$

There are a number of physical properties containing in this propagator such as the ground state energy, the effective mass and the density of states. As discussed by Feynman[2], if we transform $t\rightarrow -iT$ and let $T\rightarrow\infty$, the ground state energy and the effective mass m^* can be extracted from

$$G(0,0;T\rightarrow\infty)=\varphi_0^*(0)\varphi_0(0)e^{-E_0T}=\left(\frac{m^*}{2\pi T}\right)^{3/2}e^{-E_0T}. \quad (12)$$

The explicit form of the ground state energy is written as[11]

$$E_0 = \frac{3}{4}V(1-\rho)^2 - \frac{1}{2\pi^2 V}\int_0^\infty dk k^2 g^2(k) e^{-\beta}\int_0^\infty dx e^{\beta e^{-x}-\mu x}, \qquad (13)$$

where

$$V^2 = \Omega^2 + \kappa,$$

$$\rho = \frac{\Omega}{V},$$

$$\beta = \frac{k^2(1-\rho^2)}{V},$$

$$\mu = \frac{\omega_p(k) + k^2\rho^2}{V}.$$

According to the atomic unit, this ground state energy is expressed in Rydberg and we are interested in how it behaves as a function of density parameter r_s. Note that it is the energy where the plasmaron has zero momentum, *i.e.* it is slowly moving stochastically in the potential field in response to the changes and yet its momentum is zero on the average. If we expand the propagator eq. (12) in a series of $\beta = \frac{1}{T}$ where $\beta \to 0$, we get the effective mass[12] which is

$$m^* = \frac{1}{\rho^2}\exp\left[\rho^2 - 1 + \frac{\rho^2}{3\pi^2 V^3}\int_0^\infty dk k^4 g^2(k) e^{-\beta}\int_0^\infty dx x^2 e^{\beta e^{-x}-\mu x}\right]. \qquad (14)$$

The variation parameters κ and Ω are now absorbed into another set of adjustable parameters V and ρ. In the next section, we will solve for V and ρ which yield the minimum E_0.

IV. Calculation results and discussions

The main purpose of this section is to evaluate the ground state energy and the effective mass. We enter the plasmon spectra and the dielectric function from both Lundqvist's and Overhauser's models into the calculation of the ground state energy in eq. (13) and the effective mass in eq. (14). It is worth mentioning here that these integrals cannot be evaluated analytically. Thus we resort to a standard numerical integration and a numerical minimization[13]. The accuracy of the numerical integration is eight decimal points. All the results are compared with those obtained from Mathematica package[14]. The numerical minimization is adapted from the simulated annealing method which has a potential to find the global minimum in multidimensional problems.

We plot E_0 and m^* as a function of r_s. The results are shown below. In the E_0's graph, the minus sign is omitted. Surprisingly, E_0 from both models are quite similar even though m^* behaves differently at large r_s. The adjustable parameters are also plotted against

r_s. For clarity, we plot $E_v = \frac{V}{E_F}$ instead of V because V is very small at large r_s. It is interesting to see how ρ is changing from 1 to about 0 as r_s is increasing. The curve of ρ is similar to a mirror image of $\tanh$. There is a point where the slope almost diverges. In the polaron's problem, $\rho = 1$ in the weak coupling limit and $\rho = 0$ in the strong coupling limit. The plasmaron's problem is one of its analogy. Therefore, the behaviour of ρ in the present work would reflect a phase transition of the plasmaron from one physical regime to another between very different scales of r_s. One possible realization is the fact that at very high density, the electrons are essentially mobile while at very low density, the electrons are localized, known as Wigner crystallization.

We have shown that Lundqvist's model exhibits similar behaviour to Overhauser's. Because of its simplicity, we will use Lundqvist's dielectric function to analytically evaluate E_0, which now is

$$E_0 = \frac{3}{4}V(1-\rho)^2 - \frac{2\omega_p^2}{\pi V}\int_0^\infty dk \frac{e^{-\beta}}{\omega_\rho(k)}\int_0^\infty dx e^{\beta e^{-x}-\mu x}, \tag{15}$$

in the limit of very high electron density, *i.e.* vanishingly small r_s, and very low density, *i.e.* very large r_s.

High density limit

In this limit, $r_s \to 0$, and $\rho = 1$ so that $\beta = 0$ and $\int_0^\infty dx e^{\beta e^{-x}-\mu x} = \frac{1}{\mu}$. Moreover, ω_p and k_F become very large so that $\omega_\rho(k) \approx \mu V \approx \sqrt{\omega_p^2 + \frac{4}{3}k_F k^2}$. Consequently,

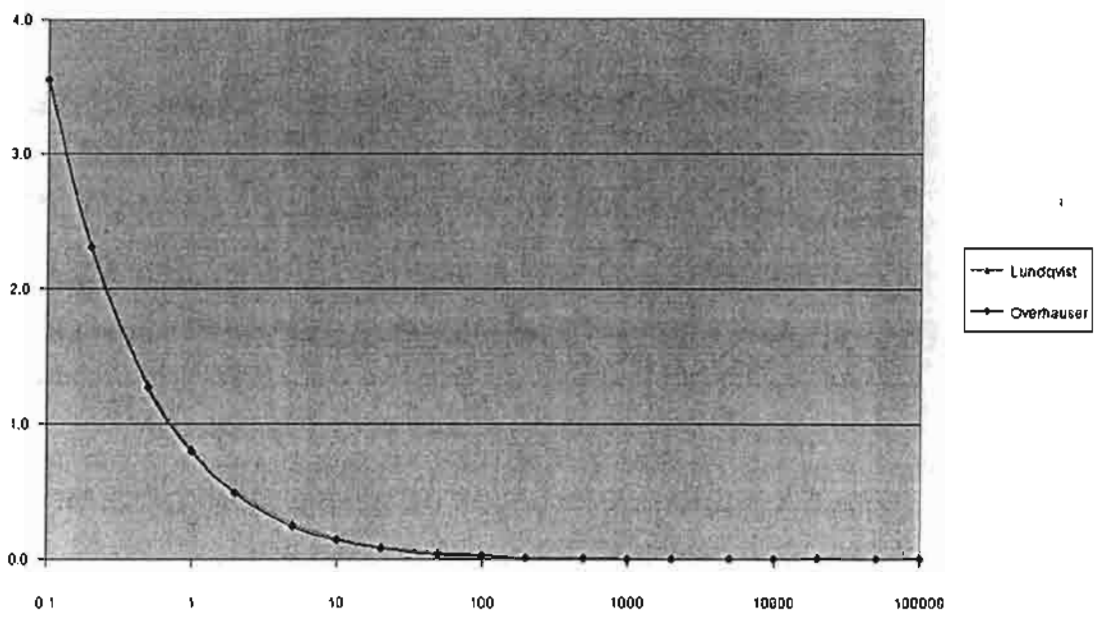
$$E_0 = -\frac{2\omega_p^2}{\pi V}\int_0^\infty dk \frac{1}{\omega_\rho(k)\mu} = -\frac{2\omega_p^2}{\pi}\int_0^\infty dk \frac{1}{\omega_p^2 + \frac{4}{3}k_F k^2}. \tag{16}$$

Performing the definite integral and writing as a function of r_s, we get

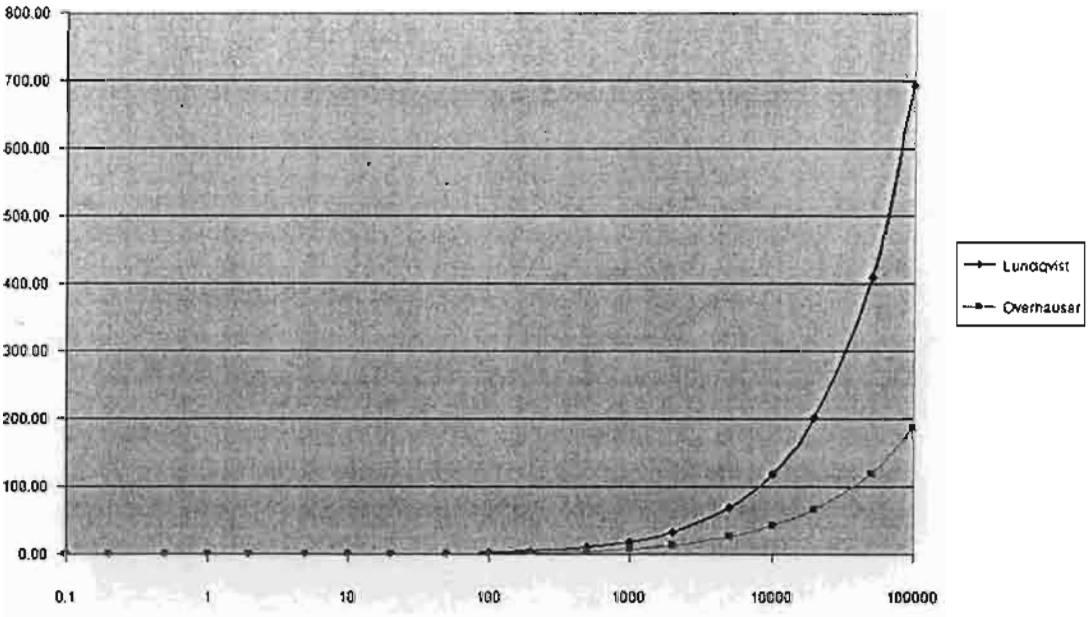
$$E_0 = -\frac{1.5633}{r_s^{1/2}}, \tag{17}$$

which yields about 16% error of E_0 compared with the numerical value at $r_s = 0.01$. We expect that the error would reduce as r_s is getting closer to 0. Most of all, we see that E_0 diverges as $r_s^{1/2}$.

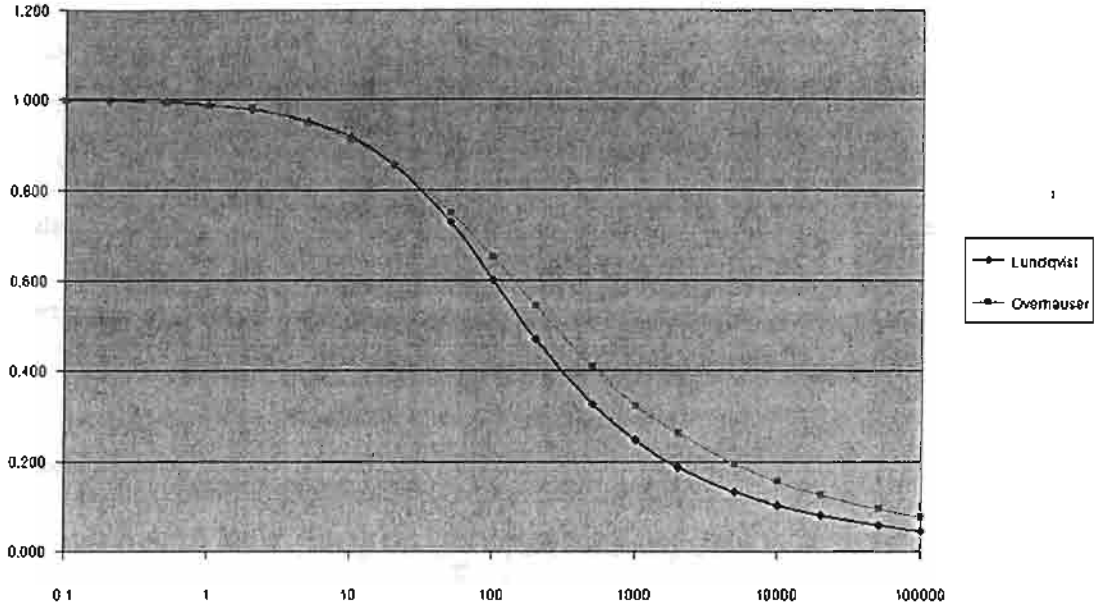
E0



Effective Mass



rho


1.200
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10000
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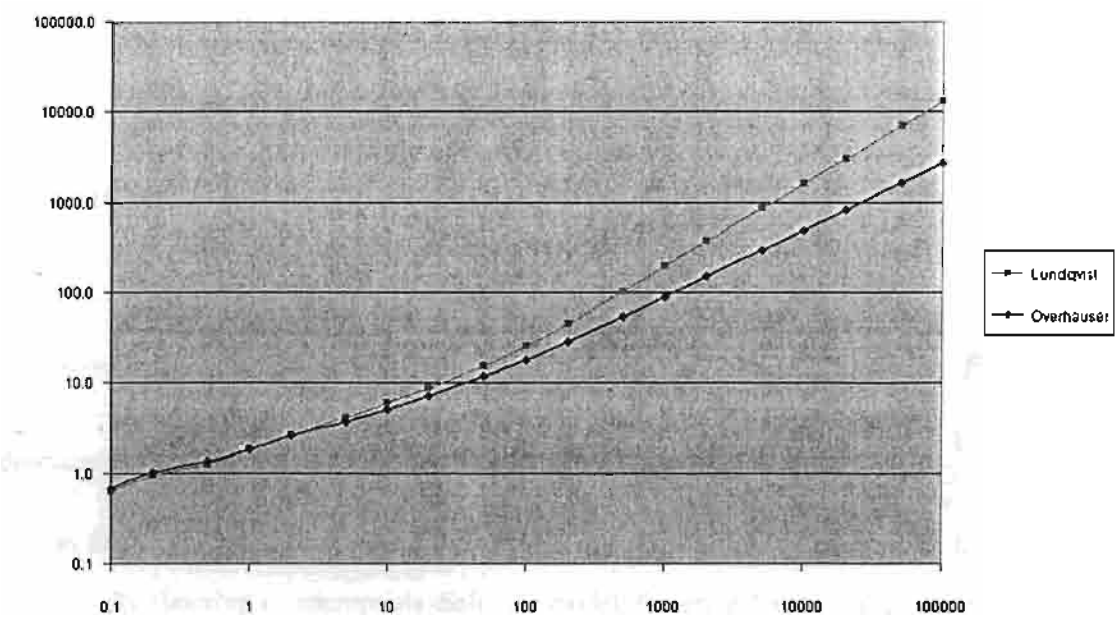
Overhauser

Ev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Lundqvist
Overhauser

Low density limit

In this limit, $r_s \to \infty$, and $\rho \to 0$ so that $\beta = \frac{k^2}{v}$ and $\mu = \frac{\omega_p(k)}{v}$. In a closer examination, we found that $e^{\beta e^{-x} - \mu x} \le e^{\beta - \mu x}$ for all x. Thus

$$E_0 \le -\frac{2\omega_p^2}{\pi v}\int_0^\infty dk \frac{1}{\omega_p(k)\mu} = -\frac{2\omega_p^2}{\pi}\int_0^\infty dk \frac{1}{\omega_p^2(k)}. \tag{18}$$

We also notice that $\frac{1}{\omega_p^2(k)}$ decays very rapidly around $k \approx 0$. If we expand it as a function of k, we get

$$\frac{1}{\omega_p^2(k)} \approx 0.0833 r_s^3 + O(k^2), \tag{19}$$

and the essence of the integral in eq. (18) is just

$$E_0 = -\frac{2\omega_p^2}{\pi}\int_0^{k_c} dk 0.0833 r_s^3, \tag{20}$$

where k_c is a small number in which eq. (19) is a good approximation. A trick is to expand $\frac{1}{\omega_p^2(k)}$ as a function of $\frac{1}{r_s}$ and we find that $\frac{1}{\omega_p^2(k)} \approx \frac{1}{k^4} - \frac{4.91}{k^6 r_s^2}$. We know that $\frac{1}{r_s} \to 0$, hence at large k, *i.e.* $k > k_c$, $\frac{4.91}{k^6 r_s^2}$ become very small comparing with $\frac{1}{k^4}$. Therefore k_c must satisfy the inequality $\frac{1}{k_c^4} >> \frac{4.91}{k_c^6 r_s^2}$,

and then

$$k_c \propto \frac{1}{r_s}. \tag{21}$$

Insert this relation into eq. (20), we get

$$E_0 \propto -\frac{1}{r_s}. \tag{22}$$

This should be compared with $E_0 = -\frac{0.88}{r_s}$ obtained by Wigner[15]. However, E_0 is solely depended on k_c. Further study[12] shows a better approximation in which $E_0 \propto -\frac{1}{r_s^{3/4}}$.

In this work, we have shown that Feynman path integral can be applied to the plasmaron problem. By choosing an appropriate dielectric model, the ground state energy and the effective mass can be calculated. The theory predicts a phase transition from the weak coupling to the strong coupling limits. The ground state energy has the same behaviour as of Wigner's prediction at very low electron density. We believe this theory is useful for the study of the plasmaron.

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