Strongly coupled ripplonic polarons in a magnetic field

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By means of a variational scheme of the Pekar type, a system of strongly coupled ripplonic polarons on the outer surface of liquid-helium film under the influence of a magnetic field of arbitrary strength is studied. Analytical expressions for the ground-state energy, the effective mass, the average number of virtual ripplons around an electron, and the spatial extension of the electron are obtained as functions of the magnetic-field strength and the electron-ripplon coupling constant and compared with previous work.

I. INTRODUCTION

In a recent paper¹ (hereafter referred as I), we employed Larsen's method of the harmonic-oscillator algebra to treat, for weak coupling, a two-dimensional (2D) ripplonic polaron on a liquid-helium surface when a magnetic field of arbitrary strength is applied normally to the surface. The ground-state energy of the 2D polaron in the presence of a magnetic field of arbitrary strength and the polaron effective mass for the cases of a strong field and a weak field were obtained.

It is well known that the coupling strength of the electron-ripplon system can be changed by adjusting the thickness of the film or by changing the substrate. On the basis of I, the treatment is now extended to the case in which the strength of the 2D electron-ripplon coupling is strong. This problem has been treated by Jackson and Peeters² with the Feynman path-integral formalism extended by Peeters and Devreese.³ Their conclusion is that for a certain magnetic field the strongly coupled polaron undergoes a transition from a self-trapped state to a free Landau-type electron state, in which the Feynman model mass becomes a bare electron mass. Recently, the same problem was studied by Kato and Tokuda⁴ with an extended variational scheme of the Lee-Low-Pines theory. Their conclusions for a strong-coupling range are that in the weak-magnetic-field limit the polaron is in a self-trapped state and in the strong-magnetic-field limit the polaron is in a magnetically trapped state. But in their paper, there is no range over the phase-transitionlike behavior. Some authors have pointed out that the Feynman-Jensen inequality is not valid for the electron action in a magnetic field.^{4,5} A recent paper by Devreese and Brosens⁶ provides the successful extension of the Feynman-Jensen inequality to a polaron in a magnetic field.

Among the investigations of a strongly coupled electron-phonon system in a magnetic field, the variational method of Pekar's product ansatz for the state vector is one of the most effective. Porsch⁷ calculated the selfenergies and effective masses of strongly coupled optical and piezoelectric polarons at arbitrary field strengths within the Pekar ansatz. Evrard, Kartheuser, and Devreese⁸ also investigated the strongly coupled electronphonon system in a weak magnetic field by the Landau-Pekar-type method. Later, Tokuda and Katos⁹ studied the problem of strongly coupled polarons in a magnetic field within a variational scheme of the Pekar type.

In this paper, we will discuss the strongly coupled electron-ripplon system under the influence of a magnetic field by using a variational scheme of the Pekar type.⁷⁻⁹ Analytical expressions of the ground-state energy, the effective mass of the strongly coupled polaron as well as the average number of virtual ripplons around the electron, and the spatial extension of the electron are obtained as functions of the magnetic-field strength and the electron-ripplon coupling constant. The results show that these quantities change continuously versus the magnetic-field strength. Similar to the weakly coupled case in I, there is no indication of phase-transition behavior,² as expected, in our work.

II. FORMULATION

We consider a liquid-helium film of thickness d. Its free surface is taken to be the xy plane so that the half space is a vacuum when z > 0 and the half space is the substrate with dielectric constant ϵ when z < -d. The system is under the influence of an external magnetic field B along the positive z direction. For an electron interacting with the ripplon on the free surface, the Hamiltonian of the coupled system is given by^{1,2}

$$\mathcal{H} = \frac{1}{2m} \left[p_x - \frac{1}{4} \beta^2 y \right]^2 + \frac{1}{2m} \left[p_y + \frac{1}{4} \beta^2 x \right]^2 + \sum_{\mathbf{k}} \hbar \omega_k a_{\mathbf{k}}^+ a_{\mathbf{k}} + \sum_{\mathbf{k}} \left(V_k^* a_{\mathbf{k}}^+ e^{-i\mathbf{k}\cdot\mathbf{r}} + \mathbf{H.c.} \right), \quad (1)$$

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with

$$\beta^2 = \frac{2eB}{c} , \qquad (2a)$$

$$\omega_k = \left[\left[g'k + \frac{\sigma}{\rho} k^3 \right] \tanh(kd) \right]^{1/2}, \qquad (2b)$$

$$V_k = [2\pi\alpha\hbar^3 g' k \tanh(kd) / Sm\omega_k]^{1/2}, \qquad (2c)$$

$$\alpha = \frac{(e\xi)^2}{8\pi\sigma} \frac{2m}{\hbar^2 k_c^2} , \qquad (2d)$$

$$e\xi = eE^{\text{ext}} + \frac{e^2(\varepsilon - 1)}{4d^2(\varepsilon + 1)} , \qquad (2e)$$

$$k_c = (\rho g' / \sigma)^{1/2}$$
 (2f)

All the notations are the same as given in I.

Like the electron-phonon system in a magnetic field,⁹ the Hamiltonian (1) can be rewritten as

$$\mathcal{H} = \frac{p^2}{2m} + \frac{m}{8}\omega_c^2(x^2 + y^2) + \frac{1}{2}\omega_c(p_x y - p_y x) + \sum_{\mathbf{k}} \hbar \omega_k a_{\mathbf{k}}^+ a_{\mathbf{k}} + \sum_{\mathbf{k}} (V_k^* a_{\mathbf{k}}^+ e^{-i\mathbf{k}\cdot\mathbf{r}} + \mathbf{H.c.}), \quad (3)$$

where

$$\omega_c = \frac{\beta^2}{2m} = \frac{eB}{mc} \tag{4}$$

is the cyclotron frequency of the electron.

Similar to the case of the electron-phonon strongly coupled system in a magnetic field,⁹ the wave function $|\Psi\rangle$ of the Hamiltonian (3) can be written as the variational wave function of the Pekar type:

$$|\Psi\rangle = \chi(\mathbf{r})\varphi_{\rm ri} , \qquad (5)$$

where $\chi(\mathbf{r})$ depends only on the electron and φ_{ri} describes the state of the ripplon field of the liquid-helium surface:

$$\chi(\mathbf{r}) = \left[\frac{\mu}{\pi}\right]^{1/2} \exp\left[-\frac{\mu}{2}r^2 + \frac{i}{\hbar}(p_{0x}x + p_{0y}y)\right], \quad (6)$$

$$\varphi_{\rm ri} = U|0\rangle \ . \tag{7}$$

Here μ and \mathbf{p}_0 are variational parameters, $|0\rangle$ represents the state with no ripplons, i.e., the vacuum state with $a_k |0\rangle = 0$, and $U|0\rangle$ is the coherent state.

$$U = \exp\left(\sum_{\mathbf{k}} f_k a_{\mathbf{k}}^+ - f_k^* a_{\mathbf{k}}\right), \qquad (8)$$

where f_k is to be determined variationally.

In order to obtain the effective mass with the groundstate energy of the ripplonic polaron, we minimize the expectation value of the $[\mathcal{H}-\mathbf{u}\cdot(\mathbf{P}-\mathbf{P}_0)]$ for the state vector $|\Psi\rangle$,

$$\delta[\langle \Psi | \mathcal{H} - \mathbf{u} \cdot (\mathbf{P} - \mathbf{P}_0) | \Psi \rangle] = 0 , \qquad (9)$$

where **u** is the Lagrange multiplier which will be identified as the polaron velocity, as we shall see. P_0 is the expectation value vector of the total momentum operator for the state vector $|\Psi\rangle$. The total momentum operator of the system may be written as

$$\mathbf{P} = \mathbf{p} + \frac{e}{c} \mathbf{A} + \sum_{\mathbf{k}} \hbar \mathbf{k} a_{\mathbf{k}}^{+} a_{\mathbf{k}} , \qquad (10a)$$

$$\mathbf{A} = \left(-\frac{1}{2}By, \frac{1}{2}Bx\right) \,. \tag{10b}$$

The unitary operator U transforms a_k^+ and a_k into the following:

$$U^+a^+_k U = a^+_k + f^*_k$$
, (11a)

$$U^+a_k U = a_k + f_k . (11b)$$

Now we can obtain the expectation value of $[\mathcal{H}-\mathbf{u}\cdot(\mathbf{P}-\mathbf{P}_0)]$ for the wave function $|\Psi\rangle$,

$$\langle \Psi | \mathcal{H} - \mathbf{u} \cdot (\mathbf{P} - \mathbf{P}_0) | \Psi \rangle = \frac{\hbar^2 \mu}{2m} + \frac{P_0^2}{2m} + \frac{m}{8\mu} \omega_c^2$$

$$+ \sum_{\mathbf{k}} \hbar (\omega_k - \mathbf{u} \cdot \mathbf{k}) |f_k|^2$$

$$+ \sum_{\mathbf{k}} V_k (f_k + f_k^*) e^{-k^2/(4\mu)}$$

$$- \mathbf{u} \cdot \mathbf{p}_0 + \mathbf{u} \cdot \mathbf{P}_0 .$$
(12)

Minimizing (12) with respect to \mathbf{p}_0 and f_k^* leads to

$$f_k = -\frac{V_k \exp[-k^2/(4\mu)]}{\hbar(\omega_k - \mathbf{u} \cdot \mathbf{k})} , \qquad (13)$$

and

$$\mathbf{p}_0 = m \mathbf{u} \ . \tag{14}$$

In the low-temperature limit $T \rightarrow 0$ K, we have neglected the recoil of ripplon in Eq. (13).

Because of the complicated dispersion relation (2b) and the electron-ripplon-interaction amplitude (2c), an analytical expression for the ground-state energy can only be obtained in an approximation. Following Jackson and Peeters,² we assume $\tanh(kd) \simeq kd$ and consider a linearized cut-off ripplon spectrum; that is, $\omega_k = sk$ with the cut-off ripplon wave number $k = k_c$, where $s = (g'd)^{1/2}$ for $k < k_c$. This has been shown^{1,2,4} to be a good approximation for d < 100 Å. Using the parameters f_k and \mathbf{p}_0 in (13) and (14), we discover the expectation value of the energy up to the second order in **u** is

$$\langle \Psi | \mathcal{H} | \Psi \rangle = E + \frac{1}{2}m^* u^2 , \qquad (15)$$

and for the momentum we obtain

$$\langle \Psi | \mathbf{P} | \Psi \rangle = \mathbf{P}_0 = m^* \mathbf{u} , \qquad (16)$$

where E and m^* , respectively, are the ground-state energy and the effective mass of the polaron in a magnetic field. They are given by

$$E = \frac{\hbar^2 \mu}{2m} + \frac{m}{8\mu} \omega_c^2 - \frac{\alpha \hbar^2 \mu}{m} [1 - \exp(-k_c^2/2\mu)], \quad (17)$$

$$m^* = m \left\{ 1 + \frac{\alpha \hbar^2 \mu}{m^2 s^2} [1 - \exp(-k_c^2/2\mu)] \right\}.$$
 (18)

Thus, we can say that the Lagrange multiplier u is the

polaron velocity from (15)-(18). Here the definition of the effective mass is the same as Ref. 9 but different from the effective cyclotron mass, which is defined by using the cyclotron resonance frequency.¹⁰

The variational parameter μ is determined by minimizing E. Thus, from the equation

$$\frac{\hbar^2}{2m} - \frac{\lambda^2 \hbar^2 k_c^2}{32m\mu^2} - \frac{\alpha \hbar^2}{m} [1 - \exp(-k_c^2/2\mu)] + \frac{\alpha \hbar^2 k_c^2}{2m\mu} \exp(-k_c^2/2\mu) = 0, \quad (19)$$

with

$$\lambda^2 = \frac{\omega_c}{\omega_0}, \quad \omega_0 = \frac{\hbar k_c^2}{2m} , \qquad (20)$$

if we take the exponential function e^{-x} in (19) up to second order in x, we find the parameter is

$$\mu = [k_c^2 (\lambda^4 + 4\alpha)^{1/2}]/4 , \qquad (21)$$

from which we finally obtain the ground-state energy,

$$E = \frac{1}{2}\hbar\omega_c + \Delta E \quad , \tag{22}$$

with

$$\Delta E = -\alpha \hbar \omega_0 \left\{ \frac{\lambda^2 (\lambda^4 + 4\alpha)^{1/2} - (\lambda^4 + 2\alpha)}{2\alpha (\lambda^4 + 4\alpha)^{1/2}} + \frac{(\lambda^4 + 4\alpha)^{1/2}}{2} [1 - e^{-2/(\lambda^4 + 4\alpha)^{1/2}}] \right\},$$
(23)

and the effective mass is

$$m^{*} = m \left\{ 1 + \frac{\alpha}{\eta^{2}} (\lambda^{4} + 4\alpha)^{1/2} [1 - e^{-2} / (\lambda^{4} + 4\alpha)^{1/2}] \right\}.$$
(24)

The first term in (22) is the Landau-level energy of the free electron in a magnetic field. The last term, ΔE , is the energy shift due to the interaction among the electron, magnetic field, and ripplon field. In (24), the parameter η has been defined as $\eta = sk_c / \omega_0$.

Besides the ground-state energy and the effective mass, we can also calculate the spatial extension of the electron as follows:

$$R = (\langle \Psi | x^2 + y^2 | \Psi \rangle)^{1/2} = (1/\mu)^{1/2} = \frac{2}{k_c (\lambda^4 + 4\alpha)^{1/4}} ,$$
(25)

and the average number of virtual ripplons around the electron as

$$N = \langle \Psi | \sum_{\mathbf{k}} a_{\mathbf{k}}^{+} a_{\mathbf{k}} | \Psi \rangle$$

= $\frac{\sqrt{2\pi\alpha}}{2\eta (1 - u^{2}/s^{2})^{3/2}} (\lambda^{4} + 4\alpha)^{1/4} \Phi \left[\frac{\sqrt{2}}{(\lambda^{4} + 4\alpha)^{1/4}} \right],$
(26)

where the function $\Phi(t)$ is the probability integral defined as

$$\Phi(t)=\frac{2}{\sqrt{\pi}}\int_0^t e^{-x^2}dx \; \; .$$

III. RESULTS AND DISCUSSION

We have investigated the ground-state properties of the 2D strongly coupled polarons on the outer surface of the liquid-helium film in a magnetic field within a variational scheme of the Pekar type. Not only the analytical expressions of the ground-state energy and the effective mass of the polaron, but also the spatial extension of the electron and the mean number of ripplons in the cloud around the electron are obtained as functions of the strength of the magnetic field λ^2 and the electron-ripplon coupling constant α .

In the weak-field limit, $\lambda^2 \rightarrow 0$, if we expand the terms to second order in $\omega_c(\lambda^2)$, Eqs. (22)–(26) become

$$E = -\alpha \hbar \omega_0 + \sqrt{\alpha} \hbar \omega_0 + \frac{\lambda^4}{8\sqrt{\alpha}} \hbar \omega_0 , \qquad (27)$$

$$m^*/m = 1 + \frac{2\alpha}{\eta^2} - \frac{\sqrt{\alpha}}{\eta^2} + \frac{\lambda^4}{8\sqrt{\alpha}\eta^2} , \qquad (28)$$

$$R = \frac{\sqrt{2}}{k_c \alpha^{1/4}} \left[1 - \frac{\lambda^4}{16\alpha} \right] , \qquad (29)$$

$$N = \frac{2\alpha}{\eta} \left[1 - \frac{1}{3\sqrt{\alpha}} + \frac{\lambda^4}{24\alpha^{3/2}} \right].$$
(30)

The first two terms in (27) give the ground-state energy of the strongly coupled electron-rippion system without a magnetic field and the last term is due to the diamagnetic motion of the electron in a potential well of the rippion cloud surrounding it.⁴ When $\lambda^2=0$, the results of Eqs. (27)-(30), as expected, agree with the results of our recent work which studied the ground-state properties of the strongly coupled polaron on the liquid-helium film in the absence of magnetic field.¹¹

On the other hand, in the strong magnetic-field limit, that is, $\lambda^2 \rightarrow \infty$, we can find from Eqs. (22)–(24),

$$E = \frac{1}{2}\hbar\omega_c - \alpha\hbar\omega_0 , \qquad (31)$$

and

$$m^*/m = 1 + \frac{2\alpha}{\eta^2} . \tag{32}$$

The first term in (31) is the Landau-level energy of the electron in a magnetic field, while the last term is the ground-state-energy shift due to the electron-ripplon interaction and it shows that the ground-state-energy shift approaches the limit $-\alpha\hbar\omega_0$ in the strong-magnetic-field limit. The effective mass is proportional to the electron-ripplon coupling constant but has nothing to do with the field.

It is noted that the limiting expressions of the groundstate energy (27) and (31) are essentially equivalent to those obtained in Refs. 2 and 4. We also find that the main term in (32), $2\alpha/\eta^2$, is just the same as the model mass of the strongly coupled electron-ripplon system in a magnetic field obtained by Jackson and Peeters.² In order to provide the figured presentation of the analytical expressions, we calculate numerically the ground-stateenergy shifts and the effective masses of the system in a wide range of the magnetic-field strength and large electron-ripplon coupling constants in the following. From Eq. (23), we have obtained the ground-state-energy shift $\Delta E = \Delta E(\alpha, \lambda)$ which is the function of the electron-ripplon coupling constant α and the strength of the magnetic field. First, we plot values of the energy shift versus the electron-ripplon coupling constant α with several different values of the magnetic field, $\lambda^2 = 0, 1, 4, 10$, as shown in Fig. 1. Then we plot the energy shift as functions of the magnetic field with several electron-ripplon coupling different constants. $\alpha = 1,5,10,20$, as shown in Fig. 2. We observe that the value of the energy shift increases continuously with the increasing value of the electron-rippling coupling constant (Fig. 1) and with the increasing value of the magnetic field (Fig. 2). The result of phase-transition behavior at a certain value of the magnetic-field strength² is not observed in our calculation. Taking $\alpha \hbar \omega_0$ as the unit of the energy shift, we also find that the larger the λ^2 , the less the dependence of the energy shift ΔE on α , and that the energy shift is almost invariable along with α in the strong-magnetic-field limit. As shown in Eq. (31), the limit of the trapping energy of the ripplonic polaron in the strong-magnetic field is $\alpha \hbar \omega_0$. This is in agreement with the results obtained by Jackson and Peeters² and







FIG. 2. The energy shift as a function of the magnetic field with several different electron-ripplon coupling constants: $\alpha = 1, 5, 10, 20.$



FIG. 1. The energy shift as a function of the electron-ripplon coupling constant for several different values of the magnetic field: $\lambda^2 = 0, 1, 4, 10$.

FIG. 3. Effective-mass ratio as a function of the electronripplon coupling constant. Two values of the magnetic field are considered: $\lambda^2 = 0.1$ and $\lambda^2 = 10$. (As in Ref. 2, $\eta \approx 2.5 \times 10^{-3}$.)

1.0

Kato and Tokuda.⁴ But in a weak field, the groundstate-energy shift (with $\alpha \hbar \omega_0$ as the unit) changes with the electron-rippion coupling constant. For example, when $\lambda^2 = 0.1$, $-\Delta E / \alpha \hbar \omega_0 \sim 0.18$ or 0.79 for $\alpha = 1$ or 20, respectively. This is different from the weak-coupling case in which the energy shift (with $\alpha \hbar \omega_0$ as the unit) does not change with the electron-rippion coupling constant.¹

In Fig. 3, we also calculate the two effective-mass ratios,¹¹ which are the ratios of the polaron effective masses to the free-electron mass and take them as functions of the electron-ripplon coupling constant when the values of the magnetic field are $\lambda^2 = 0.1$ and $\lambda^2 = 10$. We can see the effective-mass ratio increases monotonically in magnitude with the increase of the value of the electron-ripplon coupling constant within a magnetic field. We can also see from these curves that the polaron's effective mass is mainly determined by the electron-ripplon coupling constant but slightly determined by the strength of the magnetic field.

The results from Figs. 1-3 show clearly that both the ground-state-energy shift and the effective mass of the strongly coupled ripplonic polaron within a magnetic field change continuously versus the magnetic-field strength, which is similar to the weak-coupling case in I.

The phenomenon that the polaronic electron undergoes a phase transition from a self-trapped state to a quasifree state at a certain magnetic-field value² is not expected in our present model. This is the same as the result of the strongly coupled electron-LO-phonon system within a magnetic field, which was obtained by Tokuda and Kato.⁹

We hope that in the near future, experimental fact will be able to answer the question of whether there exists a phase-transition-like behavior in the strongly coupled system of electron-ripplon within a magnetic field.

Finally, we should note that the results obtained in this paper only suit the strongly coupled electron-ripplon system but do not apply to the weak-coupling $(\alpha \rightarrow 0)$ range. Those interested in weakly coupled ripplonic polarons in a magnetic field may refer to Refs. 1, 2, and 4.

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