Three states of a polaron on the surface of a liquid-helium film in a uniform magnetic field

H. Kato^{*} and N. Tokuda

Department of Engineering Science, Faculty of Engineering, Hokkaido University, Sapporo, Japan

(Received 24 July 1986)

An electron on the surface of a liquid-helium film in a uniform magnetic field is studied as a polaron problem by an extended variational scheme of the Lee-Low-Pines theory. To describe the electron motion we employ a model, used in the path-integral formalism, in which an electron is coupled to a fictitious particle by a spring. The ground-state energy is obtained for the limiting values of the magnetic field strength and the electron-surface (ripplon) coupling constant. We find that the polaron can assume three kinds of states for the limiting cases: a free state, a self-trapped state, and a magnetically trapped state.

I. INTRODUCTION

Recently an electron on the surface of a liquid-helium film has attracted attention as a two-dimensional (2D) polaron system.¹⁻¹¹ In this system the electron is coupled to an excitation of the surface of the liquid-helium film called a ripplon. The strength of this coupling is varied by changing the film thickness and the strength of an electric field applied perpendicular to the surface. It is known that in this system the polaron is in a free state or a self-trapped state according to the strength of the electron-ripplon coupling. Phase-transition-like behavior from a free to a self-trapped state is obtained by two different methods of the polaron theory.^{2,5-7} Some evidence of this transition was experimentally observed by Andrei.¹¹

In this paper we study how the polaron state changes under the influence of a uniform magnetic field applied perpendicular to the surface. This problem was discussed by Jackson and Peeters⁴ with the Feynman path-integral formalism extended by Peeters and Devreese.12 Their conclusion is that at a certain magnetic field the strongly coupled polaron undergoes a transition from a selftrapped state to a quasifree state, in which the Feynman mass becomes the bare electron mass. On the other hand Larsen pointed out that the energy obtained by the pathintegral formalism is not always an upper bound for the true ground-state energy.¹³ This is a result of the fact that the Feynman-Jensen inequality is not valid for the electron action in a magnetic field because it becomes a complex number. We consider the problem by another method.

The method we employ is an extended variational scheme of the Lee-Low-Pines theory. To describe the electron motion we employ a model in which an electron is coupled to a fictitious particle by a spring. The ripplon cloud is centered on the center of a cyclotron orbit of these coupled particles. We calculate the ground-state energy, the polaron radius and the cyclotron radius of the polaron. The explicit expressions for these quantities for the limiting values of the magnetic field strength and the electron-ripplon coupling constant are derived analytically. From these expressions we construct a physical image of the states of the polaron in a magnetic field. When the electron-ripplon coupling and the magnetic field are weak, the polaron is in a free state in which an electron interacting with virtual ripplons is on a free Landau orbit. When the coupling is strong while the magnetic field is weak, the polaron is in a self-trapped state in which an electron is trapped in a ripplon cloud and is in diamagnetic motion within a potential well due to the ripplon cloud. When the magnetic field is strong, the electron is on a free Landau orbit and the ripplon cloud surrounds the orbit. We call this state a magnetically trapped state.

In Sec. II we give the formalism of the problem with a diagonalization of the coupled particles. In Sec. III the analytic expressions of the ground-state energy are discussed for the limiting values of the electron-ripplon coupling constant and the magnetic field strength. Analyzing these expressions we construct a physical image of the polaron state. Section IV is devoted to the result and discussion. In Appendix A a proof of a certain formula used in the present paper is given and in Appendix B an improved argument for the weak-coupling regime is presented and compared with the result of second-order perturbation theory.

II. FORMULATION

The 2D electron-ripplon system in a uniform magnetic field B applied perpendicular to the surface is described by the Hamiltonian:⁴

$$H = \frac{1}{2m} \left[\mathbf{p} + \frac{e}{c} \mathbf{A} \right]^2 + \sum_{\mathbf{k}} \hbar \omega_k a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + H_{\text{int}}$$
(1a)

with

$$H_{\rm int} = \sum_{\mathbf{k}} V_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} (a_{\mathbf{k}} + a_{-\mathbf{k}}^{\dagger}) , \qquad (1b)$$

where **r** and **p** are the electron position and momentum operators, *m* the electron mass, -e the electron charge, *c* the light velocity, a_k and a_k^{\dagger} the annihilation and creation operators for a ripplon with wave number **k** and frequency ω_k . The vector potential we choose is in a symmetric Coulomb gauge

<u>35</u> 7879

$$\mathbf{A} = (-By/2, Bx/2) = -\frac{B}{2} \vec{\sigma} \cdot \mathbf{r}$$
⁽²⁾

with a dyadic $\vec{\sigma}$ defined by $\vec{\sigma} = \hat{\mathbf{x}}\hat{\mathbf{y}} - \hat{\mathbf{y}}\hat{\mathbf{x}}$, which is equivalent to the matrix:

$$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \tag{3}$$

and satisfies the equation $\dot{\sigma}^2 = -1$. Following Jackson and Peeters,⁴ we use the capillary wave number k_c as a cutoff for the ripplon wave number, and take

$$\omega_k = sk \quad , \tag{4}$$

$$V_{\mathbf{k}} = \left[\frac{2\pi\alpha\hbar^3 sk}{\Omega m}\right]^{1/2},\tag{5}$$

with $k = |\mathbf{k}|$. Here Ω is the area of the system, s is the velocity of the third sound in a helium film, defined by $s = (g'd)^{1/2}$ with d the film thickness and g' the acceleration due to the van der Waals coupling of the helium to the substrate. The constant g' is defined by $g' = (3\alpha_v / \rho d^{4})^{1/2}$ with α_v the coefficient of the van der Waals potential¹⁴ and ρ the helium mass density. The capillary wave number is defined by $k_c = (g'\rho/\tau)^{1/2}$ with τ the helium surface tension. The dimensionless constant α is the electron-ripplon coupling constant, which is varied by changing the electric field pressing the electron against the surface.^{1,2}

A. Electron coupled to a fictitious particle

To describe the motion of the electron coupled to the ripplon we employ a model where an electron is coupled to a fictitious particle by a spring. This model is equivalent to one used in the Feynman path-integral formalism.^{12,15} The Hamiltonian for the model is

$$H_m = \frac{1}{2m} \left[\mathbf{p} + \frac{e}{c} \mathbf{A} \right]^2 + \frac{1}{2m'} \mathbf{p}'^2 + \frac{K}{2} |\mathbf{r} - \mathbf{r}'|^2, \quad (6)$$

where m', $\mathbf{r'}$, and $\mathbf{p'}$ are the mass, position, and momentum of the fictitious particle and K is the spring constant.

The diagonalization of H_m is equivalent to the diagonalization of a symmetric 8×8 matrix. We performed this diagonalization following a method suggested by Peeters and Devreese¹² and obtained the four normal coordinates. In the Heisenberg picture the time evolution of the position and momentum of the electron is given by

$$\mathbf{r}(t) = \mathbf{R}_0 + \sum_{j=1}^3 \overleftrightarrow{\Omega}_j(t) \cdot \mathbf{R}_j , \qquad (7a)$$

$$\left[\mathbf{p} + \frac{e}{c} \mathbf{A}\right](t) = \sum_{j=1}^{3} (-1)^{j} m s_{j} \vec{\Omega}_{j}(t) \cdot \vec{\sigma} \cdot \mathbf{R}_{j} , \qquad (7b)$$

and the position of the fictitious particle is

$$\mathbf{r}'(t) = \mathbf{R}_0 + \sum_{j=1}^3 \kappa_j \vec{\Omega}_j(t) \cdot \mathbf{R}_j , \qquad (8)$$

where

$$\Omega_{j}(t) = \exp[(-1)^{j} \overrightarrow{\sigma} \overrightarrow{s}_{j} t]$$

$$= \begin{bmatrix} \cos(s_{j}t) & (-1)^{j} \sin(s_{j}t) \\ -(-1)^{j} \sin(s_{j}t) & \cos(s_{j}t) \end{bmatrix}, \quad (9)$$

and

$$\kappa_j = w^2 / (w^2 - s_j^2), \quad j = 1, 2, 3$$
 (10)

Here the frequencies $s_1 \leq s_2 \leq s_3$ are given by the positive roots of the equation:

$$s^{2}(s^{2}-v^{2})^{2}-\omega_{c}^{2}(s^{2}-w^{2})^{2}=0, \qquad (11)$$

with

$$v^2 = K(1/m + 1/m')$$
, (12a)

$$w^2 = K/m' , \qquad (12b)$$

$$\omega_c = eB/cm \quad . \tag{13}$$

The vectors \mathbf{R}_j (j=0,1,2,3) are the normal coordinates of the model. The coordinates \mathbf{R}_0 and \mathbf{R}_1 are interpreted as the center and radius of the cyclotron orbit for the coupled particles, respectively. \mathbf{R}_2 and \mathbf{R}_3 are the coordinates describing the relative motion of the particles. A sketch for the coordinates is given in Fig. 1. We denote the x and y component of \mathbf{R}_j by X_j and Y_j , respectively. Then these operators satisfy the following commutation relations:

$$[X_j, Y_{j'}] = \delta_{jj'}(-1)^j 2id_j^2 , \qquad (14a)$$

$$[X_j, X_{j'}] = [Y_j, Y_{j'}] = 0, \ j, j' = 0, 1, 2, 3$$
(14b)

with

٢

$$d_{j}^{2} = \begin{cases} \frac{\hbar}{2m\omega_{c}}, & j = 0, \\ \frac{\hbar}{2ms_{j}} \frac{s_{j}^{2} - w^{2}}{3s_{j}^{2} + 2(-1)^{j}s_{j}\omega_{c} - v^{2}}, & j = 1, 2, 3. \end{cases}$$
(15)

Based on these commutation relations we introduce the creation and annihilation operators C_j^{\dagger} and C_j (j=0,1,2,3,)

$$X_j = d_j (C_j^\dagger + C_j) , \qquad (16a)$$

$$Y_j = (-1)^j i d_j (C_j^{\dagger} - C_j), \quad j = 0, 1, 2, 3 ,$$
 (16b)

where C_j^{\dagger} and C_j satisfy $[C_j, C_{j'}^{\dagger}] = \delta_{jj'}$. The Hamiltonian H_m is then described with these operators as

$$H_m = \sum_{j=1}^{3} \hbar s_j (C_j^{\dagger} C_j + \frac{1}{2}) .$$
(17)

7880

B. Trial state and expression for the ground-state energy

Substitution of (7a) and (7b) into (1) yields

$$H = \frac{m}{2} \sum_{j,j'=1}^{3} (-1)^{j+j'} s_j s_{j'} \mathbf{R}_j \cdot \mathbf{R}_{j'} + \sum_{\mathbf{k}} \hbar \omega_k a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \sum_{\mathbf{k}} V_{\mathbf{k}} \exp[i\mathbf{k} \cdot (\mathbf{R}_0 + \mathbf{R}_1 + \mathbf{R}_2 + \mathbf{R}_3)] (a_{-\mathbf{k}}^{\dagger} + a_{\mathbf{k}}) .$$
(18)

We determine the ground state of (18) within a variational procedure. The trial state we choose is

$$|\Psi\rangle = U_1 U_2 |0\rangle , \qquad (19)$$

with

$$U_1 = \exp\left[-i(\mathbf{R}_0 + \mathbf{R}_1) \cdot \sum_{\mathbf{k}} \mathbf{k} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}\right], \qquad (20)$$

$$U_2 = \exp\left[\sum_{\mathbf{k}} (f_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} - f_{\mathbf{k}}^* a_{\mathbf{k}})\right], \qquad (21)$$

$$|0\rangle = \prod_{\mathbf{k}} |\mathbf{r}_{\mathbf{k}}\rangle \prod_{j} |\mathbf{e}_{j}\rangle , \qquad (22)$$

where $|r_{\mathbf{k}}\rangle$ and $|e_{j}\rangle$ are, respectively, the vacuums for $a_{\mathbf{k}}$ and C_{j} , satisfying $\langle r_{\mathbf{k}} | r_{\mathbf{k}} \rangle = 1$ and $\langle e_{j} | e_{j} \rangle = 1$. The variational parameters are $f_{\mathbf{k}_{1}}$ in (21), v in (12a), and w in (12b) which determine \mathbf{R}_{j} , C_{j}^{\dagger} , C_{j} and $|e_{j}\rangle$. When v = w and $\omega_{c} < v$, $\mathbf{R}_{0} + \mathbf{R}_{1}$ becomes \mathbf{r} . In this case the unitary

operator U_1 reduces to the Lee-Low-Pines transformation.¹⁶ When v = w and $\omega_c > v$, $\mathbf{R}_0 + \mathbf{R}_1$ reduces to $\mathbf{r}/2 - \vec{\sigma} \cdot \mathbf{p}/m\omega_c$ which is the center of the cyclotron orbit for a free electron. In this case the state (19) is essentially equivalent to one given by Whitfield, Parker, and Rona.¹⁷ The trial state (19) is composed of the ground state of H_m and the coherent state of ripplon centered on the position $\mathbf{R}_0 + \mathbf{R}_1$. The unitary operator U_1 transforms \mathbf{R}_i (j = 0, 1, 2, 3) and a_k as in the following:

$$U_{1}^{\dagger}\mathbf{R}_{j}U_{1} = \mathbf{R}_{j} + (\delta_{j0} + \delta_{j1})(-1)^{j2}d_{j}^{2}\vec{\sigma} \cdot \sum_{\mathbf{k}} \mathbf{k}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}} ,$$

$$j = 0, 1, 2, 3 , \quad (23)$$

$$U_{1}^{\dagger}a_{\mathbf{k}}U_{1} = \exp\left[-i\mathbf{k} \cdot (\mathbf{R}_{0} + \mathbf{R}_{1}) - \sum_{\mathbf{k}'} 2i\Delta(\mathbf{k}, \mathbf{k}')a_{\mathbf{k}'}^{\dagger}a_{\mathbf{k}'}\right]a_{\mathbf{k}} , \quad (24)$$

with

$$\Delta(\mathbf{k},\mathbf{k}') = (d_0^2 - d_1^2)\mathbf{k} \cdot \vec{\sigma} \cdot \mathbf{k}'/2 . \qquad (25)$$

The unitary operator U_2 transforms a_k as

$$U_{2}^{\dagger}a_{k}U_{2} = a_{k} + f_{k}$$
 (26)

A derivation of (24) is given in Appendix A. Taking the expectation value of (18) by (19) leads to the following expression:

$$E = \langle \Psi | H | \Psi \rangle$$

= $m (s_1^2 d_1^2 + s_2^2 d_2^2 + s_3^2 d_3^2) + \sum_{\mathbf{k}} (\hbar \omega_k + 2m s_1^2 d_1^4 k^2) | f_{\mathbf{k}} |^2$
+ $\sum_{\mathbf{k}} V_{\mathbf{k}} \exp \left[-(d_2^2 + d_3^2) k^2 / 2 - 2 \sum_{\mathbf{k}'} | f_{\mathbf{k}'} |^2 \sin^2 \Delta(\mathbf{k}, \mathbf{k}') \right] (f_{\mathbf{k}} + f_{-\mathbf{k}}^*).$ (27)

Here we have used the following equations under the assumption that $|f_k|^2 = |f_{-k}|^2$:

$$\langle 0 | \mathbf{R}_{j}^{2} | 0 \rangle = \langle 0 | 4d_{j}^{2}(C_{j}^{\dagger}C_{j} + \frac{1}{2}) | 0 \rangle$$

= $2d_{j}^{2}$, (28)
$$\langle 0 | e^{i\mathbf{k}\cdot\mathbf{R}_{j}} | 0 \rangle = \langle 0 | \exp(\kappa C_{j}^{\dagger} - \kappa^{*}C_{j}) | 0 \rangle$$

= $e^{-k^{2}d_{j}^{2}/2}$ (29)

with $\kappa = id_j \{k_x + i(-1)^j k_y\}$, and

$$\langle 0 \mid U_{2}^{\dagger} \exp \left[2i \sum_{\mathbf{k}'} \Delta(\mathbf{k}, \mathbf{k}') a_{\mathbf{k}'}^{\dagger} a_{\mathbf{k}'} \right] U_{2} \mid 0 \rangle$$

$$= \exp \left[-2 \sum_{\mathbf{k}'} \left| f_{\mathbf{k}'} \right|^{2} \sin^{2} \Delta(\mathbf{k}, \mathbf{k}') \right].$$
(30)

To obtain (29) and (30) we utilize the following identities:

$$e^{\gamma b^{\dagger} - \gamma^{*} b} = e^{-|\gamma|^{2}/2} e^{\gamma b^{\dagger}} e^{-\gamma^{*} b}$$
, (31)

$$e^{xb^{\dagger}b} = \sum_{n=0}^{\infty} \frac{1}{n!} (e^{x} - 1)^{n} b^{\dagger n} b^{n} , \qquad (32)$$

where b and b^{\dagger} satisfy the relation $[b, b^{\dagger}] = 1$.

In the following two limits we can neglect the term $2\sum_{\mathbf{k}'} |f_{\mathbf{k}'}|^2 \sin^2 \Delta(\mathbf{k}, \mathbf{k}') \ (\equiv T')$ compared with the term $(d_2^2 + d_3^2)k^2/2 \ (\equiv T)$ in (27). (1) Weak-magnetic-field limit: In this limit T and T' are reduced to

$$T \rightarrow \frac{k^2 \hbar}{4mv} \left[1 - \frac{w^2}{v^2} \right],$$

$$T' \rightarrow k^2 \left[\frac{3\hbar w^2}{4mv^4} \left[1 - \frac{w^2}{v^2} \right] \omega_c \right]^2 \sum_{\mathbf{k}'} k'^2 |f_{\mathbf{k}'}|^2.$$
(33)

For sufficiently small ω_c it holds that T >> T'. (2) Strong-magnetic-field limit: In this limit T and T' are reduced to

$$T \rightarrow k^{2} \frac{\hbar}{4m\omega_{c}} ,$$

$$T' \rightarrow k^{2} \left[\frac{\hbar}{2m\omega_{c}} \right]^{2} \sum_{\mathbf{k}'} k'^{2} |f_{\mathbf{k}'}|^{2} .$$
(34)

For sufficiently large ω_c it holds that $T \gg T'$. If we neglect T', the expression (27) becomes a quadratic form with respect to f_k . Minimizing (27) with respect to f_k leads to

$$f_{\mathbf{k}} = -\frac{V_{-\mathbf{k}} \exp[-(d_{2}^{2} + d_{3}^{2})k^{2}/2]}{\hbar \omega_{\mathbf{k}} + 2ms_{1}^{2}d_{1}^{4}k^{2}}$$
(35)

Substitution of (35) into (27) yields

$$E = m (s_1^2 d_1^2 + s_2^2 d_2^2 + s_3^2 d_3^2) - \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2 \exp[-(d_2^2 + d_3^2)k^2]}{\hbar \omega_{\mathbf{k}} + 2m s_1^2 d_1^4 k^2} .$$
(36)

In the next section we minimize (36) with respect to v and w and obtain the explicit analytic expressions for the ground-state energy. We introduce the polaron radius r_p and the cyclotron radius of the polaron r_c , which are easily calculated in terms of d_j ,

$$r_{p} \equiv (\langle 0 \mid \frac{1}{2} (\mathbf{R}_{2} + \mathbf{R}_{3})^{2} \mid 0 \rangle)^{1/2} = (d_{2}^{2} + d_{3}^{2})^{1/2} , \qquad (37)$$

$$r_c \equiv (\langle 0 \mid \frac{1}{2} \mathbf{R}_1^2 \mid 0 \rangle)^{1/2} = d_1 .$$
(38)

In the absence of a magnetic field we obtain from (36)

$$E = \frac{\hbar v}{2} \left[1 - \frac{w^2}{v^2} \right] - \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2 \exp[-(1 - w^2/v^2)\hbar k^2/2mv]}{\hbar \omega_k + (w^2/v^2)^2 \hbar^2 k^2/2m} .$$
 (39)

This expression is equivalent to the early result obtained by a modified variational scheme of the Lee-Low-Pines theory.^{6,7}

III. ANALYTIC EXPRESSIONS FOR THE GROUND-STATE ENERGY

In this section we minimize (36) with respect to v and w and obtain the explicit analytic expressions for the ground-state energy for the limiting values of the electron-ripplon coupling and the magnetic field. Substitution of (4) and (5) into (36) yields

$$E(\alpha, \omega_{c}, v, w) = s_{1}^{2} d_{1}^{2} + s_{2}^{2} d_{2}^{2} + s_{3}^{2} d_{3}^{2} - \alpha s \int_{0}^{1} dk \frac{k \exp[-(d_{2}^{2} + d_{3}^{2})k^{2}]}{s + 2s_{1}^{2} d_{1}^{4} k} , \qquad (40)$$

where we have used units such that $\hbar = m = k_c = 1$.

A. Weak-magnetic-field limit

Assuming that $\omega_c \ll 1$ ($\omega_c \ll v$) and retaining terms to the second order in ω_c , we reduce Eq. (40) to

$$E = \frac{v}{2}(1-u) - \alpha \left[\frac{v}{1-u} (1-e^{-(1-u)/2v}) - \frac{u^2}{2s} \int_0^1 dk \, k^2 e^{-(1-u)k^2/2v} \right] + \frac{\omega_c}{2} u^2 + \frac{\omega_c^2}{8} \frac{1-u}{v} \left\{ \frac{3}{2} - \frac{\alpha}{(1-u)^2} \left[1 - \left[1 + \frac{1-u}{2v} \right] e^{-(1-u)/2v} \right] \right\},$$
(41)

where *u* is defined by $u = w^2/v^2$.

In the weak-coupling limit ($\alpha \ll 1$) the electron is almost free so that the ground state is obtained by taking the variational parameters v and w such that v = w, implying that the mass of the fictitious particle m' is zero. Then Eq. (41) becomes

$$E = \omega_c / 2 - \alpha s \int_0^1 dk \frac{k}{s + k/2}$$

= $\omega_c / 2 - 2s \alpha \{ 1 - 2s \ln[(1 + 2s)/2s] \}$. (42)

The first term in (42) is the zero-point energy of an electron in a magnetic field and the second term is the polaron energy in a free state without a magnetic field. This expression is almost equivalent to one obtained by the second-order perturbation theory except the modulation of the zero-point energy due to the mass renormalization by the electron-ripplon coupling (see Appendix B). To understand this effect we present an improved argument in Appendix B. From Eq. (42) we can construct a physical image for the polaron such that an electron interacting with virtual ripplons is on a free Landau orbit. This image is suggested by the fact that in this limit the polaron radius is given with $r_p = 0$ and the cyclotron radius is $r_c = (1/2\omega_c)^{1/2}$. This image may be depicted in Fig. 2(a).

In the strong-coupling limit $(\alpha \gg 1)$ the electron motion is strongly restricted within the ripplon cloud. Minimizing (38) with respect to v and u we obtain to the first order in ω_c

$$v = \left(\frac{\alpha}{4}\right)^{1/2}, \quad u = \left(\frac{9s^2}{4\alpha}\right)^{1/2} \left(1 - \frac{3s}{\alpha}\omega_c\right). \tag{43}$$

then the ground-state energy becomes

$$E = -\frac{\alpha}{2} + \frac{\sqrt{\alpha}}{2} - \frac{1}{12} - \frac{3s}{8} + \frac{\omega_c}{2m_c} + \frac{\omega_c^2}{8v} , \qquad (44)$$

with $m_c = 4\alpha/9s^2$. The polaron radius and the cyclotron radius are, respectively, given by $r_p = (1/2v)^{1/2}$ and $r_c = (1/2\omega_c)^{1/2}$. The first four terms in (44) give the

7882



FIG. 1. The coordinates of the coupled particles in a magnetic field. The circle and the square represent an electron and a fictitious particle, respectively. Definition of \mathbf{R}_j and κ_j (j = 0, 1, 2, 3) are given in the text.

ground-state energy of the strongly coupled polaron without a magnetic field, the fifth term is the zero-point energy of a free particle (with mass m_c) in a magnetic field, and the last term is due to the diamagnetic motion of the electron in a potential well of the ripplon cloud surrounding the electron. This image is depicted in Fig. 2(b).

B. Strong-magnetic-field limit

In the strong-magnetic-field limit ($\omega_c >> 1$) assuming that v = w and $\omega_c > v$, we obtain from (41) irrespective of α

$$E = \frac{1}{2}\omega_{c} - \alpha\omega_{c}(1 - e^{-1/2}\omega_{c}) .$$
 (45)

In this limit the polaron radius is given by $r_p = (1/2\omega_c)^{1/2}$ and the cyclotron radius is $r_c = 0$. In the strongmagnetic-field limit the cyclotron radius of the electron becomes very small and the region in which the electron moves around is so small that the coherent ripplon cloud can be created even if α is small. The first term in (45) is the energy of an electron on a free Landau orbit and the second term is the energy due to the ripplon cloud. This image is depicted in Fig. 2(c). Jackson and Peeters⁴ called this state as a quasifree state because the Feynman mass, reduces to the bare electron mass. Within our theory the model mass v^2/w^2 also reduces to the bare electron mass, but this does not mean that the polaron is in a free state. The model mass is only a parameter to determine the motion of the electron. If the model mass reduces to the bare electron mass the electron motion is of course equivalent to a free electron motion, but it does not neces-



FIG. 2. Sketch for the states of the 2D polaron in a uniform magnetic field. The electron is described by the small circle with its locus. The mesh shows the helium surface. (a) Free state for $\omega_c \ll 1$ and $\alpha \ll 1$, (b) self-trapped state for $\omega_c \ll 1$ and $\alpha \gg 1$, (c) magnetically trapped state for $\omega_c \gg 1$.

sarily mean that there is no ripplon cloud around the electron.

IV. RESULT AND DISCUSSION

In this paper the 2D polaron in the electron-ripplon system under a uniform magnetic field is studied with an extended variational scheme of the modified Lee-Low-Pines theory. To describe the motion of the electron we used a model in which an electron is coupled to a fictitious particle by a spring. In this model the mass of the coupled particles does not always represent the mass of the polaron.

The polaron takes three kinds of states for the limiting values of the electron-ripplon coupling constant and the magnetic field as summarized in Fig. 2: (a) The free state in which an electron interacting with virtual ripplons is on a free Landau orbit realized when $\omega_c \ll 1$ and $\alpha \ll 1$. (b) The self-trapped state in which an electron trapped by a ripplon cloud is in a diamagnetic motion in the potential well of the cloud realized when $\omega_c \ll 1$ and $\alpha \gg 1$. (c) The magnetically trapped state in which an electron on a free Landau orbit is surrounded and trapped by a ripplon cloud realized when $\omega_c \gg 1$ irrespective of the value of α .

The limiting expressions (42), (44), and (45) are essentially equivalent to those obtained by Jackson and Peeters⁴ (notice that their unit for the energy is $\hbar^2 k_c^2/2m$ but ours is $\hbar^2 k_c^2/m$). This suggests that, in spite of Larsen's criticism,¹³ their formulation gives the correct result so far as the magnetic field and the electron-ripplon coupling constant take the limiting values. This does not mean, however, that we can use the path-integral formalism assuming the validity of the Feynman-Jensen inequality in the presence of a magnetic field. If we apply our method to the optical polaron in a magnetic field, the results do not agree with those obtained in terms of the path-integral formalism.

To obtain the magnetically trapped state we use the condition that the term T' should be negligibly small as compared with T in (27) based on the limiting expressions (34). This condition is not satisfied for the 2D optical polaron (i.e., $\omega_k = 1$ and $V_k = \{\sqrt{2}\pi\alpha/k\Omega\}^{1/2}$ in the strong-coupling regime. For the 2D optical polaron the term $\sum_{k} k^2 |f_k|^2$ in T' is proportional to $\alpha \omega_c$ if we use (35) for f_k , therefore T and T' become the same order in ω_c and moreover T' becomes larger than T for the strong-coupling limit. The magnetically trapped state for the 2D optical polaron, therefore, does not appear in the strong-coupling regime, which is a different result from that of Peeters and Devreese. By the same reason the 3D optical polaron cannot take the magnetically trapped state in the strong-coupling regime. We think that the selftrapped state and the magnetically trapped state are responsible for a phase-transition-like behavior of the strongly coupled polaron, if it exists. As the magnetic field increases the polaron changes its state from a selftrapped state to a magnetically trapped state. Based on this consideration we are doubtful about the presence of a phase-transition-like behavior induced by a magnetic field in the 3D optical polaron discussed by Peeters and Devreese.12

APPENDIX A

In this appendix we give a proof for (24). The following formula is essential for the proof.

$$e^{S}Ae^{-S} = A + [S, A] + [S, [S, A]]/2! + [S, [S, [S, A]]]/3! + \cdots,$$

$$e^{A}e^{B} = \exp\{A + B + [A, B]/2 + ([A, [A, B]])$$
(A1)

$$e^{A}e^{B} = \exp\{A + B + [A,B]/2 + ([A,[A,B]])\}$$

+[[
$$A,B$$
], B])/12+···}.
(A2)

Equation (23) is obtained by straightforward application of (A1). We denote $\mathbf{R}_0 + \mathbf{R}_1$ by \mathbf{R} and $d_0^2 - d_1^2$ by d^2 . Then the operator U_1 is described by

$$U_1 = \exp\left[-\sum_{\mathbf{k}} i\mathbf{R} \cdot \mathbf{k} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}\right].$$
(A3)

If we write the x and y component of \mathbf{R} by X and Y, then these operators satisfy

$$[X,Y] = 2id^2 . \tag{A4}$$

Utilizing (A2) we rewrite the operator U_1 as

$$U_1 = U_1' U_1'' , (A5)$$

with

$$U'_{1} = \exp[-iXA_{x}]\exp[-iYA_{y}],$$
$$U''_{1} = \exp[id^{2}A_{x}A_{y}].$$

Here $A_x = \sum_k k_x a_k^{\dagger} a_k$ and $A_y = \sum_k k_y a_k^{\dagger} a_k$ commute each other. Using (A1), we obtain

$$e^{iYA_y}Xe^{-iYA_y} = X - 2d^2 \sum_{\mathbf{k}} k_y a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}$$
 (A6)

The transformation of a_k by U'_1 is given as follows,

$$U_{1}^{\dagger}a_{\mathbf{k}}U_{1}^{\prime} = e^{iYA_{y}}e^{iXA_{x}}a_{\mathbf{k}}e^{-iXA_{x}}e^{-iYA_{y}}$$

$$= e^{iYA_{y}}\exp[-ik_{x}X]a_{\mathbf{k}}e^{-iYA_{y}}$$

$$= \exp[-ik_{x}e^{iYA_{y}}Xe^{-iYA_{y}}]e^{iYA_{y}}a_{\mathbf{k}}e^{-iYA_{y}}$$

$$= \exp[-i\mathbf{k}\cdot\mathbf{R} - id^{2}k_{x}k_{y} - ik_{x}A_{y}]a_{\mathbf{k}} . \quad (A7)$$

Here for the step from the first to the second line Eq. (A1) is used and from the third to the fourth line Eq. (A6) is used. Using the formula (A1) and the relation

$$[A_x A_y, a_k] = -(k_x k_y + k_x A_x + k_y A_y) a_k , \qquad (A8)$$

we obtain

$$U_1''^{\dagger} a_k U_1'' = \exp[id^2(k_x k_y + k_x A_y + k_y A_x)]a_k .$$
 (A9)

Then the transformation of a_k by U_1 becomes

$$U_{1}^{\dagger}a_{\mathbf{k}}U_{1} = U_{1}^{\prime\prime\dagger}U_{1}^{\prime\dagger}a_{\mathbf{k}}U_{1}^{\prime}U_{1}^{\prime\prime}$$

= exp[-*i***k**·**R**-*id*²(*k*_x*A*_y-*k*_y*A*_x)]*a*_k
= exp[-*i***k**·**R**-*id*²\sum_{\mathbf{k}'}\mathbf{k}\cdot\vec{\sigma}\cdot\mathbf{k}^{\prime}a_{\mathbf{k}^{\prime}}^{\dagger}a_{\mathbf{k}^{\prime}}]a_{\mathbf{k}}. (A10)

This is the relation to be demonstrated.

THREE STATES OF A POLARON ON THE SURFACE OF A ...

APPENDIX B

In this appendix we give an improved argument for the weak-coupling regime to obtain the mass renormalization effect in the zero-point energy in (42). We employ the following unitary transformation:

$$\widetilde{U}_2 = \exp\left[\sum_{\mathbf{k}} \left[(f_{\mathbf{k}} + \mathbf{g}_{\mathbf{k}} \cdot \mathbf{R}_1) (a_{\mathbf{k}}^{\dagger} - a_{\mathbf{k}}) \right] \right].$$
(B1)

To make the calculation as simple as possible we assume that $f_k = f_k^* = f_{-k}$ and $\mathbf{g}_k = \mathbf{g}_k^* = -\mathbf{g}_{-k}$. In the limit of v = w this operator reduces to the operator given in Eq. (18) of Ref. 18. The operator \tilde{U}_2 transforms a_k and \mathbf{R}_j (j = 0, 1, 2, 3) as follows:

$$\widetilde{U}_{2}^{\dagger} a_{\mathbf{k}} \widetilde{U}_{2} = a_{\mathbf{k}} + f_{\mathbf{k}} + \mathbf{g}_{\mathbf{k}} \cdot \mathbf{R}_{1} + id_{1}^{2} \sum_{\mathbf{k}'} \mathbf{g}_{\mathbf{k}'} \cdot \vec{\sigma} \cdot \mathbf{g}_{\mathbf{k}} (a_{\mathbf{k}'}^{\dagger} - a_{\mathbf{k}'}) ,$$
(B2)

$$\tilde{U}_{2}^{\dagger}\mathbf{R}_{j}\tilde{U}_{2} = \mathbf{R}_{j} - \delta_{j\,1}i\,2d_{1}^{2}\vec{\sigma}\cdot\sum_{\mathbf{k}'}\mathbf{g}_{\mathbf{k}'}(a_{\mathbf{k}'}^{\dagger} - a_{\mathbf{k}'}) ,$$

$$j = 0, 1, 2, 3 . \quad (\mathbf{B}3)$$

Using \widetilde{U}_2 we define the trial state as follows,

$$|\tilde{\Psi}\rangle = U_1 \tilde{U}_2 |0\rangle . \tag{B4}$$

We assume that f_k and g_k are proportional to $\alpha^{1/2}$. Then the expectation value of the Hamiltonian (1) by (B4) becomes to the order of α as in the following:

$$\widetilde{E} = m \left(s_{1}^{2} d_{1}^{2} + s_{2}^{2} d_{2}^{2} + s_{3}^{2} d_{3}^{2} \right) + \sum_{\mathbf{k}} 2V_{\mathbf{k}} f_{\mathbf{k}} e^{-(d_{2}^{2} + d_{3}^{2})k^{2}/2} + \sum_{\mathbf{k}} \left(f_{\mathbf{k}} \mathbf{g}_{\mathbf{k}} \right) \begin{bmatrix} \hbar \omega_{\mathbf{k}} + 2m s_{1}^{2} d_{1}^{4} k^{2} & 2m s_{1}^{2} d_{1}^{4} \mathbf{k} \cdot \vec{\sigma} \\ 2m s_{1}^{2} d_{1}^{4} \mathbf{k} \cdot \vec{\sigma} & \{ \hbar \omega_{\mathbf{k}} + 2m s_{1}^{2} d_{1}^{2} (k^{2} d_{1}^{2} + 1) \} d_{1}^{2} \end{bmatrix} \begin{bmatrix} f_{\mathbf{k}} \\ \mathbf{g}_{\mathbf{k}} \end{bmatrix}.$$
(B5)

Minimizing (B5) with respect to g_k and f_k , we obtain

$$\mathbf{g}_{\mathbf{k}} = -\frac{2ms_{1}^{2}d_{1}^{2}\mathbf{k}\cdot\vec{\sigma}f_{\mathbf{k}}}{\hbar\omega_{k} + 2ms_{1}^{2}d_{1}^{2}(d_{1}^{2}k^{2} + 1)}$$
(B6)

and

$$f_{\mathbf{k}} = -\frac{V_{-\mathbf{k}} \exp[-(d_{2}^{2} + d_{3}^{2})k^{2}/2]}{\hbar\omega_{k} + 2ms_{1}^{2}d_{1}^{4}k^{2} - \frac{(2ms_{1}^{2}d_{1}^{2})^{2}d_{1}^{2}k^{2}}{\hbar\omega_{k} + 2ms_{1}^{2}d_{1}^{2}(d_{1}^{2}k^{2} + 1)}$$
(B7)

Substituting of (B6) and (B7) into (B5) yields

$$\widetilde{E} = m \left(s_{1}^{2} d_{1}^{2} + s_{2}^{2} d_{2}^{2} + s_{3}^{2} d_{3}^{2} \right) - \sum_{k} \frac{|V_{k}|^{2} \exp[-(d_{2}^{2} + d_{3}^{2})k^{2}]}{\hbar \omega_{k} + 2m s_{1}^{2} d_{1}^{4} k^{2} - \frac{(2m s_{1}^{2} d_{1}^{2})^{2} d_{1}^{2} k^{2}}{\hbar \omega_{k} + 2m s_{1}^{2} d_{1}^{2} (d_{1}^{2} k^{2} + 1)}$$
(B8)

The ground-state energy in the weak-magnetic-field limit is given by choosing v = w and $\omega_c < v$ in (B8):

$$\widetilde{E} = \frac{\hbar\omega_c}{2} \left[1 - \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{m} \frac{|V_{\mathbf{k}}|^2 \exp[-(d_2^2 + d_3^2)k^2]}{\{\hbar\omega_k + \hbar^2 k^2/2m\}^3} \right] - \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2 \exp[-(d_2^2 + d_3^2)k^2]}{\hbar\omega_k + \hbar^2 k^2/2m} .$$
(B9)

The first term of (B9) is equivalent to the energy of a free particle in a magnetic field with mass m^* given by

$$\frac{m^*}{m} = 1 + \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{m} \frac{|V_{\mathbf{k}}|^2 \exp[-(d_2^2 + d_3^2)k^2]}{\{\hbar\omega_{\mathbf{k}} + \hbar^2 k^2/2m\}^3} .$$
(B10)

This is the same expression for the polaron mass as defined by the Lee-Low-Pines theory.⁷

The energy for the strong-magnetic-field limit is given by taking v = w and $\omega_c > v$ in (B8). The resultant expression is the same as given by (45).

Within the second-order perturbation theory^{13,19} we obtain the ground-state energy

$$E = \frac{\hbar\omega_c}{2} - \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{\hbar\omega_k} \int_0^\infty dt \exp\left[-t - \frac{\hbar k^2}{2m\omega_c} (1 - e^{-t\omega_c/\omega_k})\right].$$
(B11)

From this expression we obtain the same expression as (B9) for the weak-magnetic-field limit and as (45) for the strongmagnetic-field limit.

- *Present address: VLSI Research Center, Toshiba Co., Kawasaki 210, Japan.
- ¹L. M. Sander, Phys. Rev. B 11, 4350 (1975).
- ²S. A. Jackson and P. M. Platzman, Phys. Rev. B 24, 499 (1981); 25, 4886 (1982); Surf. Sci. 142, 125 (1984).
- ³S. A. Jackson, in *Polarons and Excitons in Polar Semiconduc*tors and Ionic Crystals, edited by J. T. Devreese and F. M. Peeters (Plenum, New York, 1984), p. 419.
- ⁴S. A. Jackson and F. M. Peeters, Phys. Rev. B 30, 4196 (1984).
- ⁵O. Hipólito, G. A. Farias, and N. Studart, Surf. Sci. **113**, 394 (1982).
- ⁶N. Tokuda and H. Kato, J. Phys. C 16, 1567 (1983).
- ⁷M. D. Degani and O. Hipólito, Surf. Sci. 142, 107 (1984).
- ⁸H. Kato, E. Takagi, and N. Tokuda, Surf. Sci. 170, 103 (1986).
- ⁹M. Saitoh, J. Phys. C 16, 6995 (1983).

- ¹⁰M. Saitoh, J. Phys. C 16, 6983 (1983).
- ¹¹E. Y. Andrei, Phys. Rev. Lett. 52, 1449 (1984).
- ¹²F. M. Peeters and J. T. Devreese, Phys. Rev. B **25**, 7281 (1982); **25**, 7302 (1982).
- ¹³D. M. Larsen, Phys. Rev. B 32, 2657 (1985); 33, 799 (1986).
- ¹⁴C. H. Anderson and E. S. Sabisky, Phys. Rev. Lett. 24, 1049 (1970).
- ¹⁵R. P. Feynman, Phys. Rev. 97, 660 (1955).
- ¹⁶T. D. Lee, F. E. Low, and D. Pines, Phys. Rev. 90, 297 (1953).
- ¹⁷G. Whitfield, R. Parker, and M. Rona, Phys. Rev. B 13, 2132 (1976).
- ¹⁸D. M. Larsen, Phys. Rev. 135, A419, (1964).
- ¹⁹G. Lindemann, R. Lassing, W. Seidenbusch and E. Gornik, Phys. Rev. B 28, 4693 (1983); F. M. Peeters and J. T. Devreese, *ibid.* 31, 3689 (1985).