Perturbation theory for the two-dimensional polaron in a magnetic field

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The ground-state energy of a two-dimensional polaron in a magnetic field is evaluated in fourth-order perturbation theory by a novel method. In this method complicated sums over products of matrix elements and energy denominators are replaced by simple algebraic manipulations of operators. An analytical expression is derived for the high-magnetic-field limit; in that limit the sixth-order perturbation contribution is also determined.

One of the most powerful mathematical techniques for finding the ground-state energy of polarons is the Feynman path-integral method.[1] In the absence of magnetic fields this method, which involves minimizing an energy expression with respect to variational parameters, is known to produce an approximate ground-state energy which is an upper bound to the true energy. Furthermore, it is believed that the Feynman energy is an accurate approximation to the true energy for all values of the Fröhlich electron—LO-phonon coupling constant, α, in both two and three dimensions.

Less well understood is the situation when a magnetic field is present. The Feynman method has been generalized by Peeters and Devreese[2] (PD) in an attempt to provide a theory which approaches the Feynman theory at zero field and which does not lose appreciable accuracy in the presence of a magnetic field of arbitrary strength. Although PD employed a path-integral variational method similar to that of Feynman, they were unable to prove that the approximate ground-state energy obtained from their calculation is an upper bound to the exact ground-state energy. Indeed, if for some range of field strengths the PD energy were to lie below the exact ground state, then it would seem difficult to justify a variational calculation for this energy and to attach physical significance to the associated wave function.

Remarkably, the PD theory gives, both in two[3] and three dimensions, cusps in the ground-state energy at sufficiently large α values and high magnetic fields. It would be interesting to know whether the energies where the cusps occur are above or below the exact energy.

In a first attempt to investigate this question, exact ground-state-energy calculations were carried out for the two-dimensional polaron in various limits. These calculations lead to the conclusion, presented in Ref. 4, that for sufficiently strong magnetic fields the PD energy lies below the exact ground-state energy. This conclusion was buttressed in part by weak-coupling perturbation-theory results quoted in Ref. 4 but not derived there. The derivation is presented in the present paper.

Both the Feynman and PD theories have the desirable property that in the weak-coupling limit ($\alpha\rightarrow 0$, magnetic field held constant) the approximate ground-state energies of those theories agree to order α with the result of second-order perturbation theory. Thus to test the accuracy of either theory for weak coupling, one must evaluate the next term of the expansion of the ground-state energy in powers of α. In this paper the ground-state energy of the two-dimensional polaron is evaluated in fourth-order perturbation theory for arbitrary magnetic field strength. (The results of this calculation have already been quoted, in graphical form, in Ref. 4.) For the special case of weak coupling and high magnetic field the perturbation theory is carried out to sixth order.

The Hamiltonian H employed in this paper can be written

$$\begin{aligned}
&H=H_u+H_{e\text{-ph}} ,\\
&H_u=H_0+\sum_k b_k^\dagger b_k ,\\
&H_{e\text{-ph}}=\sum_k v_k(e^{-i\mathbf{k}_\perp\cdot\boldsymbol{\rho}}b_k^\dagger+e^{i\mathbf{k}_\perp\cdot\boldsymbol{\rho}}b_k) ,\\
&H_0=\left[p_x-\frac{\lambda^2}{4}y\right]^2+\left[p_y+\frac{\lambda^2}{4}x\right]^2 ,\\
&v_k=\left[\frac{4\pi\alpha}{\Omega}\right]^{1/2}\Big/k , \qquad (1)\\
&\lambda^2=(eB_M/mc)/\omega_{\mathrm{LO}} ,\\
&\boldsymbol{\rho}=(x,y,0) ,\\
&\mathbf{k}=(k_x,k_y,k_z) ,\\
&\mathbf{k}_\perp=(k_x,k_y,0) ,
\end{aligned}$$

where Ω is the volume of the crystal in which the three-dimensional LO phonons are confined, $b_k^\dagger$ creates an LO phonon with three-dimensional wave vector $\mathbf{k}$, $h\omega_{\mathrm{LO}}$ is the LO phonon energy, m is the band mass of the electron, and B_M is the static uniform magnetic field applied perpendicular to the x-y plane, the plane of the electronic motion. All lengths are in units of the polaron radius, $(\hbar/2m\omega_{\mathrm{LO}})^{1/2}$ and energies are in units of $\hbar\omega_{\mathrm{LO}}$. We shall take H_u as the unperturbed Hamiltonian and $H_{e\text{-ph}}$ as the perturbation.

I. PERTURBATION THEORY IN THE HIGH-FIELD LIMIT

The perturbation calculation is simplest in the high-field limit, defined by

$$\lambda^2 \to \infty, \quad \alpha\lambda \to 0 . \tag{2}$$

The unperturbed eigenstates, which are, in general, products of a Landau level and a phonon state of the form

$$b_{k_1}^\dagger b_{k_2}^\dagger \cdots b_{k_N}^\dagger |0\rangle , \tag{3}$$

where $|0\rangle$ is the zero-phonon state, only involve, in the limit defined in (2), Landau levels belonging to the $n=0$ (or lowest-lying) manifold of Landau states. These states, omitting normalization, have the form

$$\chi_M = (x-iy)^M e^{-\lambda^2\rho^2/8} \tag{4}$$

with

$$H_0 \chi_M = (\lambda^2/2)\chi_M ,$$

where the z-angular momentum quantum number M is an arbitrary positive integer or zero. (Note, in this notation the z-angular momentum is actually $-M$.) Excited eigenstates of H_0, which are orthogonal to the χ_M's, contribute terms to the ground-state energy which are smaller by order λ^{-2} than those contributed by the χ_M's.

The perturbation calculation is greatly facilitated by representing the Landau levels as products of two independent one-dimensional harmonic oscillator states. Following Suzuki and Hensel,[5] we introduce harmonic oscillator operators

$$A = \left[\left[p_x - \frac{\lambda^2}{4} y \right] - i \left[p_y + \frac{\lambda^2}{4} x \right] \right] \Big/ \lambda ,$$
$$B = A^\dagger - \frac{i\lambda}{2}(x+iy) , \tag{5}$$

with the properties

$$[A,A^\dagger] = [B,B^\dagger] = 1 \text{ and } [A,B] = [A,B^\dagger] = 0 . \tag{6}$$

Here $A^\dagger$ lowers the quantum number M and raises the Landau quantum number n by one unit, while $B^\dagger$ raises M by one unit but has no effect on n. Thus, if $|0\rangle_A$ and $|0\rangle_B$ are the vacuum states of the A and B operators, respectively, then

$$\chi_M = \text{const} \times (B^\dagger)^M |0\rangle_B |0\rangle_A \tag{7}$$

and

$$H_0 = \lambda^2 (A^\dagger A + \tfrac{1}{2}) ,$$
$$H_{e\text{-ph}} = \sum_k v_k (L_k M_k b_k^\dagger + L_k^{-1} M_k^{-1} b_k) , \tag{8}$$

where

$$L_k = \exp\left[-\frac{1}{\lambda}(k_x+ik_y)A + \frac{1}{\lambda}(k_x-ik_y)A^\dagger \right]$$
$$= \exp\left[\frac{1}{\lambda}(k_x-ik_y)A^\dagger \right] \times \exp\left[-\frac{1}{\lambda}(k_x+ik_y)A \right] e^{-k_\perp^2/2\lambda^2} ,$$
$$L_k^{-1} = \exp\left[-\frac{1}{\lambda}(k_x-ik_y)A^\dagger \right] \times \exp\left[\frac{1}{\lambda}(k_x+ik_y)A \right] e^{-k_\perp^2/2\lambda^2} , \tag{9}$$
$$M_k = \exp\left[\frac{1}{\lambda}(k_x-ik_y)B - \frac{1}{\lambda}(k_x+ik_y)B^\dagger \right] .$$

Since in the limit of Eq. (2) the electronic states can be restricted to the $n=0$ Landau state, one need consider only the effective Hamiltonian (10) for calculating the energy to lowest nontrivial order in λ^{-2},

$$H_{\text{eff}} = {}_A\langle 0|H|0\rangle_A$$
$$= \tfrac{1}{2}\lambda^2 + \sum_k b_k^\dagger b_k + \sum_k v_k e^{-k_\perp^2/2\lambda^2} (M_k b_k^\dagger + M_k^{-1} b_k) , \tag{10}$$

where L_k has been replaced using

$${}_A\langle 0|L_k|0\rangle_A = e^{-k_\perp^2/2\lambda^2} .$$

The normalized unperturbed states of H_{eff} are denoted

$$|M;k_1,k_2,\ldots,k_N\rangle = (M!)^{-1/2}(B^\dagger)^M |0\rangle_B b_{k_1}^\dagger b_{k_2}^\dagger \cdots b_{k_N}^\dagger |0\rangle \equiv |M\rangle_B b_{k_1}^\dagger b_{k_2}^\dagger \cdots b_{k_N}^\dagger |0\rangle ,$$

and the ground state is obtained by perturbing any of the states

$$|M;0\rangle = (M!)^{-1/2}(B^\dagger)^M |0\rangle_B |0\rangle ,$$

where M is 0 or a positive integer.

The perturbed ground-state energy is found by expanding first in Wigner-Brillouin perturbation theory (WBPT), then the energy denominators appearing are expanded to obtain a power series in the relevant small parameter of the problem, which, in this case, turns out to be not α but $\alpha\lambda$.[6]

Measuring the perturbed ground-state energy E_p from $\lambda^2/2$, one has in second order

$$\begin{aligned}\Delta E_p^{(2)} &= (E_p-1)^{-1}\sum_k v_k^2 e^{-k_\perp^2/\lambda^2}\sum_{J'}\langle J;0\,|\,M_k^{-1}b_k\,|\,J';k\rangle\langle J';k\,|\,M_k b_k^\dagger\,|\,J;0\rangle \\ &= (E_p-1)^{-1}\sum_k v_k^2 e^{-k_\perp^2/\lambda^2}\,|\langle k\,|\,b_k^\dagger\,|\,0\rangle|^2\sum_{J'}{}_B\langle J\,|\,M_k^{-1}\,|\,J'\rangle_B\,{}_B\langle J'\,|\,M_k\,|\,J\rangle_B \\ &= (E_p-1)^{-1}\sum_k v_k^2 e^{-k_\perp^2/\lambda^2}\,{}_B\langle J\,|\,M_k^{-1}M_k\,|\,J\rangle_B \\ &= (E_p-1)^{-1}\alpha\int_0^\infty dk_\perp\, e^{-k_\perp^2/\lambda^2} = \tfrac{1}{2}\sqrt{\pi}\alpha\lambda/(E_p-1)\;. \end{aligned} \tag{11}$$

In obtaining (11) the passage from summation to integration

$$\sum_k v_k^2 \to \alpha\int_0^\infty dk_\perp \frac{1}{2\pi}\int_0^{2\pi} d\phi_k$$

is employed.

It is easy to see that the factorization of the M and b operators performed above can be done in any order of perturbation theory for $H_{\rm eff}$. This is because the M and b operators commute and the electronic intermediate states are degenerate. Thus in fourth order one has

$$\begin{aligned}\Delta E_p^{(4)} &= (E_p-1)^{-2}(E_p-2)^{-1}\sum_{k,l} v_k^2 v_l^2 e^{-(k_\perp^2+l_\perp^2)/\lambda^2}\,{}_B\langle J\,|\,(M_k^{-1}M_l^{-1}+M_l^{-1}M_k^{-1})M_l M_k\,|\,J\rangle_B \\ &= \sum_{k,l} v_k^2 v_l^2 e^{-(k_\perp^2+l_\perp^2)/\lambda^2}\left[1+\exp\left[\frac{2i}{\lambda^2}l_\perp k_\perp \sin(\phi_k-\phi_l)\right]\right]\,, \end{aligned} \tag{12}$$

where we have used

$$M_l^{-1}M_k = M_k M_l^{-1}\exp\left[\frac{2i}{\lambda^2}(l_x k_y - k_x l_y)\right]\,, \tag{13}$$

which is a special case of the operator identity

$$\exp(\gamma_+A^\dagger+\gamma_-A)\exp(\xi_+A^\dagger+\xi_-A) = \exp(\xi_+A^\dagger+\xi_-A)\exp(\gamma_+A^\dagger+\gamma_-A)\exp(\gamma_-\xi_+-\gamma_+\xi_-) \tag{14a}$$

where the γ's and ξ's are c numbers. A closely related identity, which was used in (9), is

$$e^{\gamma_+A^\dagger+\gamma_-A} = e^{\gamma_+A^\dagger}e^{\gamma_-A}e^{\gamma_+\gamma_-/2}\;. \tag{14b}$$

Converting the summations to integrations in (12) and integrating over k_z, l_z, and the angles ϕ_k and ϕ_l gives

$$\begin{aligned}\Delta E_p^{(4)} &= (E_p-1)^{-2}(E_p-2)^{-1}\alpha^2\int_0^\infty dk_\perp e^{-k_\perp^2/\lambda^2}\int_0^\infty dl_\perp e^{-l_\perp^2/\lambda^2}\left[1+J_0\left[\frac{2k_\perp l}{\lambda^2}\right]\right] \\ &= (E_p-1)^{-2}(E_p-2)^{-1}(\alpha\lambda)^2[\pi/4+K(0.5)/\sqrt{8}] \\ &\cong 1.440\,91(\alpha\lambda)^2/(E_p-1)^2(E_p-2)\,, \end{aligned} \tag{15a}$$

where $K(z)$ is the complete elliptic integral of the first kind,

$$K(z) \equiv \int_0^{\pi/2}(1-z\sin^2\theta)^{-1/2}d\theta\;. \tag{15b}$$

The correction in sixth order is

$$\begin{aligned}\Delta E_p^{(6)} = \sum_k v_k^2 v_l^2 v_q^2 e^{-(k_\perp^2+l_\perp^2+q_\perp^2)/\lambda^2}\Bigg[&\left\langle J\left|\sum_p (M_k^{-1}M_l^{-1}M_q^{-1})M_q M_l M_k\right|J\right\rangle(E-1)^{-2}(E-2)^{-2}(E-3)^{-1} \\ &+\langle J\,|\,(M_k^{-1}M_q^{-1}+M_q^{-1}M_k^{-1})M_q M_l^{-1}(M_l M_k+M_k M_l)\,|\,J\rangle \\ &\times(E-1)^{-3}(E-2)^{-2}\Bigg]\,, \end{aligned} \tag{16}$$

where $\sum_p(\ )$ means a sum on all permutations of indices of operators enclosed in the parentheses. The indicated expectation values in (16) can all be evaluated by moving M^{-1} operators to the right (until they annihilate their matching M operator) and using (13).

Introducing the shorthand notation

$$(l\times k)_z \equiv l_x k_y - k_x l_y ,$$

one can write

$$\begin{aligned}
\Delta E_p^{(6)} &= (I_0^3+2I_0I_1+2I_2+I_3)/(E_p-1)^2(E_p-2)^2(E_p-3)+(I_0^3+2I_0I_1+I_2)/(E_p-1)^3(E_p-2)^2 ,\\
I_0 &= \sum_k v_k^2 e^{-k_1^2/\lambda^2} = \alpha\lambda\sqrt{\pi}/2 = 0.881\,627\alpha\lambda ,\\
I_1 &= \sum_{k,l} v_k^2 v_l^2 e^{-(k_1^2+l_1^2)/\lambda^2} \exp\left[\frac{2i}{\lambda^2}(k\times l)_z\right] = (\alpha\lambda)^2 K(0.5)/\sqrt{8} = 0.655\,514(\alpha\lambda)^2 ,\\
I_2 &= \sum_{k,l,q} v_k^2 v_l^2 v_q^2 e^{-(k_1^2+l_1^2+q_1^2)/\lambda^2} \exp\left[\frac{2i}{\lambda^2}[k\times(l+q)]_z\right] \cong 0.505\,09(\alpha\lambda)^3 ,\\
I_3 &= \sum_{k,l,q} v_k^2 v_l^2 v_q^2 e^{-(k_1^2+l_1^2+q_1^2)/\lambda^2} \exp\left[\frac{2i}{\lambda^2}[k\times(l+q)+l\times q]_z\right] \cong 0.447\,47(\alpha\lambda)^3 .
\end{aligned} \tag{17}$$

The integrals I_2 and I_3 in (17) were reduced to three-dimensional integrals and performed by computer; the last quoted digit in their numerical coefficients has an estimated uncertainty of ± 1.

Inserting values for the integrals gives finally

$$\Delta E_p^{(6)} = 3.315\,56(\alpha\lambda)^3/(E_p-1)^2(E_p-2)^2(E_p-3) + 2.363\,00(\alpha\lambda)^3/(E_p-1)^3(E_p-2)^2 . \tag{18}$$

The expansion of the ground-state energy in powers of $\alpha\lambda$ is obtained from the sum $\Delta E_p^{(2)}+\Delta E_p^{(4)}+\Delta E_p^{(6)}$ by expanding the energy denominators of (11) and (15) to the appropriate order and setting $E_p=0$ in (18). One obtains

$$\begin{aligned}
E &= -\frac{\sqrt{\pi}}{2}\alpha\lambda + \tfrac{1}{2}[\pi/4 - K(0.5)/\sqrt{8}](\alpha\lambda)^2\\
&\quad -0.024\,42(5)(\alpha\lambda)^3\\
&\simeq -0.886\,227\alpha\lambda + 0.064\,941\,9(\alpha\lambda)^2\\
&\quad -0.024\,42(5)(\alpha\lambda)^3 .
\end{aligned} \tag{19}$$

Extension of this series to higher order in $\alpha\lambda$ is feasible but requires the evaluation of additional integrals which are of higher dimension than those of (17).

II. FOURTH-ORDER PERTURBATION THEORY FOR ARBITRARY MAGNETIC FIELDS

In the more general situation in which magnetic fields of arbitrary strength are considered, it is not possible to restrict the intermediate states to the $n=0$ Landau levels and to replace the Hamiltonian by H_{eff} of (10). Instead, the full Hamiltonian H of (1) is required and the perturbation $H_{e\text{-ph}}$ takes the form given by (8). The intermediate states can be written

$$(n!M!)^{-1/2}(A^\dagger)^n\,|0\rangle_A\,(B^\dagger)^M\,|0\rangle_B\, b_{k_1}^\dagger b_{k_2}^\dagger \cdots b_{k_N}^\dagger\,|0\rangle$$

with the initial unperturbed state taken as

$$|0\rangle_A\ |J\rangle_B\ |0\rangle .$$

Again setting the unperturbed $n=0$ Landau state energy as the zero of energy, the second-order correction becomes

$$\begin{aligned}
\Delta E_p^{(2)} &= \sum_k v_k^2\,|\langle k|b_k^\dagger|0\rangle|^2\,{}_B\langle J|M_k^{-1}M_k|J\rangle_B\\
&\quad\times\sum_n {}_A\langle 0|L_k^{-1}|n\rangle_A \frac{1}{E_p-n\lambda^2-1}\\
&\quad\times {}_A\langle n|L_k|0\rangle_A ,
\end{aligned} \tag{20}$$

where

$$|n\rangle_A = (n!)^{-1/2}(A^\dagger)^n|0\rangle_A$$

and the M operators have been factored out as before.

Anticipating that $E_p\le 0$, one can write

$$E_p - n\lambda^2 - 1 = -\int_0^\infty dt\, e^{-(1+n\lambda^2-E_p)t} ,$$

so that (20) can be written

$$\Delta E_p^{(2)} = -\sum_k v_k^2 \int_0^\infty dt\, e^{-(1-E_p)t} \times {}_A\langle 0|L_k^{-1} e^{-\lambda^2 t A^\dagger A} L_k|0\rangle_A , \tag{21}$$

where the relation

$$A^\dagger A\,|n\rangle_A = n\,|n\rangle_A$$

has been used. From (9) we obtain

$$_A\langle 0|L_k^{-1}e^{-\lambda^2 t A^\dagger A}L_k|0\rangle_A = e^{-k_\perp^2/\lambda^2}\left\langle 0\left|\exp\left[\frac{1}{\lambda}(k_x+ik_y)A\right]e^{-\lambda^2 t A^\dagger A}\exp\left[\frac{1}{\lambda}(k_x-ik_y)A^\dagger\right]\right|0\right\rangle_A . \tag{22}$$

One way to evaluate (22) is to expand exponentials in the matrix element on the right-hand side to obtain

$$e^{-k_\perp^2/\lambda^2}\sum_{n=0}^{\infty}\frac{1}{(n!)^2}\left[\frac{k_\perp^2}{\lambda^2}\right]^n e^{-n\lambda^2 t}{}_A\langle 0|A^n(A^\dagger)^n|0\rangle_A = e^{-k_\perp^2/\lambda^2}\sum_{n=0}^{\infty}\frac{1}{n!}\left[\frac{k_\perp^2}{\lambda^2}\right]^n e^{-n\lambda^2 t} \tag{23}$$

$$= \exp[-(k_\perp^2/\lambda^2)(1-e^{-\lambda^2 t})] . \tag{23}$$

This result is inserted into (21) and the sum converted to an integral to give

$$\Delta E_p^{(2)} = -\alpha\int_0^\infty dt\, e^{-(1-E_p)t}\int_0^\infty dk_\perp \exp[-(k_\perp^2/\lambda^2)(1-e^{-\lambda^2 t})]$$
$$= -\frac{\sqrt{\pi}\alpha\lambda}{2}\int_0^\infty dt\, e^{-(1-E_p)t}(1-e^{-\lambda^2 t})^{-1/2} \tag{24}$$

in agreement with Eq. (2) of Ref. 7 if E_p on the right-hand side above is set equal to zero.

Another way of evaluating the matrix element of (22) is to apply the operator identity (25), derived in Appendix A, to the left-hand side,

$$e^{-\tau A^\dagger A}\exp(\gamma_+ A^\dagger + \gamma_- A) = \exp(\gamma_+ e^{-\tau}A^\dagger + \gamma_- e^{\tau}A)e^{-\tau A^\dagger A} , \tag{25}$$

where γ_+ and γ_- are c numbers. The resulting matrix element becomes

$$_A\left\langle 0\left|L_k^{-1}\exp\left[\frac{1}{\lambda}(k_x-ik_y)e^{-\lambda^2 t}A^\dagger - \frac{1}{\lambda}(k_x+ik_y)e^{\lambda^2 t}A\right]\right|0\right\rangle_A$$
$$= e^{-k_\perp^2/\lambda^2}{}_A\left\langle 0\left|\exp\left[\frac{1}{\lambda}(k_x+ik_y)A\right]\exp\left[\frac{1}{\lambda}(k_x-ik_y)e^{-\lambda^2 t}A^\dagger\right]\right|0\right\rangle_A$$
$$= \exp[-(k_\perp^2/\lambda^2)(1-e^{-\lambda^2 t})]{}_A\left\langle 0\left|\exp[\tfrac{1}{2}(k_x-ik_y)e^{-\lambda^2 t}A^\dagger]\exp\left[\frac{1}{\lambda}(k_x+ik_y)A\right]\right|0\right\rangle_A$$
$$= \exp[-(k_\perp^2/\lambda^2)(1-e^{-\lambda^2 t})] .$$

The identity of (25), while offering no major simplification for second-order perturbation theory, is very useful for evaluating matrix elements appearing in fourth order.

One finds that the fourth-order term in Wigner-Brillouin perturbation theory, $\Delta E^{(4)}$, can be expressed as

$$\Delta E^{(4)} = \mathcal{I}_1 + \mathcal{I}_2 ,$$
$$\mathcal{I}_j = -\int_0^\infty dt_1\, e^{-(1-E_p)t_1}\int_0^\infty dt_2\, e^{-(2-E_p)t_2}\int_0^\infty dt_3\, e^{-(1-E_p)t_3}\widetilde{I}_j \quad (j=1,2) , \tag{26}$$
$$\widetilde{I}_1 = \sum_{k,l} v_k^2 v_l^2\, {}_A\langle 0|L_k^{-1}e^{-\tau_3 A^\dagger A}L_l^{-1}e^{-\tau_2 A^\dagger A}L_l e^{-\tau_1 A^\dagger A}L_k|0\rangle_A\, {}_B\langle 0|M_k^{-1}M_l^{-1}M_l M_k|0\rangle_B , \tag{27}$$
$$\widetilde{I}_2 = \sum_{k,l} v_k^2 v_l^2\, {}_A\langle 0|L_k^{-1}e^{-\tau_3 A^\dagger A}L_l^{-1}e^{-\tau_2 A^\dagger A}L_k e^{-\tau_1 A^\dagger A}L_l|0\rangle_A\, {}_B\langle 0|M_k^{-1}M_l^{-1}M_k M_l|0\rangle_B ,$$
$$\tau_i \equiv \lambda^2 t_i .$$

It is convenient to introduce

$$x = (k_x - ik_y)/\lambda, \quad y = (l_x - il_y)/\lambda .$$

Consider first $\widetilde{I}_1$ and apply (25) to obtain

$$L_l e^{-\tau_1 A^\dagger A}L_k|0\rangle_A = L_l\exp(xe^{-\tau_1}A^\dagger - x^* e^{\tau_1}A)|0\rangle_A$$
$$= L_l\exp(xe^{-\tau_1}A^\dagger)|0\rangle_A\, e^{-|x|^2/2}$$
$$= \exp(yA^\dagger)\exp(-y^*A)\exp(xe^{-\tau_1}A^\dagger)|0\rangle_A\, e^{-(|x|^2+|y|^2)/2}$$
$$= \exp[(y+xe^{-\tau_1})A^\dagger]|0\rangle_A\exp[-y^* x e^{-\tau_1} - (|x|^2+|y|^2)/2] .$$

Similarly

$$ {}_A\langle 0|L_k^{-1}e^{-\tau_3 A^\dagger A}L_l^{-1} = {}_A\langle 0|\exp(-xe^{\tau_3}A^\dagger + x^*e^{-\tau_3}A)L_l^{-1} $$
$$ = \exp[-x^*ye^{-\tau_3} - (|x|^2+|y|^2)/2]\, {}_A\langle 0|\exp[(y^*+x^*e^{-\tau_3})A] . $$

Here the operator identity of (14b) has been employed.

The above results are inserted into $\tilde{I}_1$ to give

$$ \tilde{I}_1 = \sum_{k,l} v_k^2 v_l^2 \exp[-(|x|^2+|y|^2+x^*ye^{-\tau_3}+xy^*e^{-\tau_1})]\, {}_A\langle 0|\exp[-(y^*+x^*e^{-\tau_3})A] \times \exp(-\tau_2 A^\dagger A)\exp[-(y+xe^{-\tau_1})A^\dagger]|0\rangle_A . \quad (28) $$

Notice that the matrix element in (28) is very similar to the one already considered in (22); it can be evaluated in a similar way, giving

$$ \exp[(y^*+x^*e^{-\tau_3})(y+xe^{-\tau_1})e^{-\tau_2}] , $$

so that

$$ \tilde{I}_1 = \sum_{k,l} v_k^2 v_l^2 \exp[-|y|^2(1-e^{-\tau_2}) - |x|^2(1-e^{-\tau_1-\tau_2-\tau_3})]\exp[(-xy^*e^{-\tau_1}-x^*ye^{-\tau_3})(1-e^{-\tau_2})] . \quad (29) $$

The same kind of calculation leading to (29) gives, for $\tilde{I}_2$,

$$ \tilde{I}_2 = \sum_{k,l} v_k^2 v_l^2\, {}_B\langle J|M_k^{-1}M_l^{-1}M_kM_l|J\rangle_B \exp[-|y|^2-|x|^2-x^*y(e^{-\tau_3}+e^{-\tau_1})] \times {}_A\langle 0|\exp[-(y^*+x^*e^{-\tau_3})A]e^{-\tau_2 A^\dagger A}\exp[-(x+ye^{-\tau_1})A^\dagger]|0\rangle_A , $$

$$ {}_B\langle J|M_k^{-1}M_l^{-1}M_kM_l|J\rangle_B = \exp(x^*y - xy^*) . $$

Thus

$$ \tilde{I}_2 = \sum_{k,l} v_k^2 v_l^2 \exp[-|y|^2(1-e^{-\tau_2-\tau_1}) - |x|^2(1-e^{-\tau_2-\tau_3})]\exp[qx^*y-(1-e^{-\tau_2})xy^*] , $$
$$ q = 1-e^{-\tau_1}-e^{-\tau_3}+e^{-\tau_1-\tau_2-\tau_3} . \quad (30) $$

Appendix B shows how $\tilde{I}_1$ and $\tilde{I}_2$ can be evaluated analytically as functions of τ_1, τ_2, and τ_3. The expressions obtained are then inserted into (26) which is integrated numerically.

For purposes of expanding the ground-state energy to order α^2, E_p is set equal to zero in (26) and to $E_G^{(2)}$, given by[7]

$$ E_G^{(2)} = -\frac{\pi\alpha}{\lambda}\Gamma(1/\lambda^2)/\Gamma(1/\lambda^2+\tfrac{1}{2}) , \quad (31) $$

in (24).

The correction to order α^2 arising from $\Delta E_G^{(2)}$ in (24) can be obtained by expanding

$$ \exp[-(1-E_G^{(2)})t] \cong e^{-t}(1+E_G^{(2)}t) , $$

which contributes in order α^2 the term

$$ \mathscr{I}_3 \equiv -\frac{\sqrt{\pi}\alpha\lambda}{2}E_G^{(2)}\int_0^\infty dt\, t\, e^{-t}(1-e^{-\lambda^2 t})^{-1/2} $$
$$ = (E_G^{(2)})^2\frac{1}{\lambda^2}[\psi(1/\lambda^2+\tfrac{1}{2})-\psi(1/\lambda^2)] , \quad (32) $$

where ψ is the digamma function, defined by

$$ \psi(z) = \frac{1}{\Gamma(z)}\frac{d\Gamma(z)}{dz} . $$

The total fourth-order correction to the ground-state energy of the two-dimensional polaron in a magnetic field is $\mathscr{I}_1+\mathscr{I}_2+\mathscr{I}_3$. In general, $\mathscr{I}_1$ and $\mathscr{I}_2$ are both negative, whereas $\mathscr{I}_3$ is positive. For strong fields $\mathscr{I}_3$ exceeds

TABLE I. Numerical values for $\Delta E_G^{(4)}$, the fourth-order Rayleigh-Schrödinger perturbation correction to the ground-state energy of a two-dimensional polaron, and the various energies $\mathscr{I}$ which contribute, versus the dimensionless magnetic field, λ^2. The energies $\mathscr{I}_j$ are defined by Eqs. (26), (27), (31), and (32). See also Eqs. (B4) and (B5) of Appendix B. All energies are in units of $\alpha^2\hbar\omega_{LO}$.

λ^2	$\mathscr{I}_1$	$\mathscr{I}_2$	$\mathscr{I}_3$	$\Delta E_G^{(4)}$
0	−0.8229	−0.4747	1.233 70	−0.0639
0.2	−0.9028	−0.5191	1.361 37	−0.0605
0.4	−0.9862	−0.5661	1.496 30	−0.0560
1.0	−1.2452	−0.7208	1.928 01	−0.0380
1.5	−1.4625	−0.8598	2.303 88	−0.0184
1.8	−1.5921	−0.9462	2.532 88	−0.0055
2.0	−1.6780	−1.0048	2.686 49	0.0037
3.0	−2.1018	−1.3057	3.460 99	0.0534
4.0	−2.5179	−1.6154	4.240 97	0.1077
10.0	−4.9403	−3.5362	8.945 11	0.4686

$|\mathscr{I}_1+\mathscr{I}_2|$ and the fourth-order correction is positive, whereas it is negative at weak fields. Results for $\mathscr{I}_1$, $\mathscr{I}_2$, and $\mathscr{I}_3$ and their sum are presented in Table I. Values listed there for $\mathscr{I}_1$, $\mathscr{I}_2$, and $\mathscr{I}_3$ are believed to be accurate to within ± 2 units in the last quoted digit.

The zero-field correction of Ref. 8 is recovered here to within the claimed accuracy of the present calculation as is the fourth-order correction of (19) in the limit $\lambda^2 \to \infty$.

It would be of interest to apply the perturbation method described above to the problem of calculating the perturbed $n=1$ level energy so that the relative accuracies of various theories of the cyclotron resonance frequency could be compared in the weak-coupling limit.

The extension of the present method to three dimensions seems straightforward, but the required integrals appear to be much more difficult to evaluate.

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APPENDIX A

Since the commutation relationship of Eq. (25) may not be well known, a derivation is presented here. The vector space with basis comprised of the harmonic-oscillator operators $A^\dagger + A$, $-A^\dagger + A$, $AA^\dagger$, and 1 is closed under commutation, where 1 denotes an operator which commutes with all of the others in the basis. These operators can be represented by 3×3 matrices which are isomorphic to the operators under commutation. The representation is given by

$$A^\dagger + A \leftrightarrow P = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix},$$

$$-A^\dagger + A \leftrightarrow R = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{bmatrix},$$

$$AA^\dagger \leftrightarrow Q = \begin{bmatrix} -\frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & -\frac{1}{2} \end{bmatrix}, \qquad \text{(A1)}$$

$$1 \leftrightarrow S = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Assume that there exist constants ξ_+ and ξ_- such that

$$e^{-\tau AA^\dagger}\exp(\gamma_+ A^\dagger + \gamma_- A) = \exp(\xi_+ A^\dagger + \xi_- A)e^{-\tau AA^\dagger}. \qquad \text{(A2)}$$

By substituting for the operators in (A2) their corresponding matrices from (A1) and explicitly exponentiating, one can solve for ξ_+ and ξ_- in terms of γ_+, γ_-, and τ. Thus

$$e^{-\tau AA^\dagger} = \sum_n \frac{1}{n!}(-\tau Q)^n = \begin{bmatrix} e^{\tau/2} & 0 & 0 \\ 0 & e^{-\tau/2} & 0 \\ 0 & 0 & e^{\tau/2} \end{bmatrix}, \qquad \text{(A3)}$$

$$\exp(\gamma_+ A^\dagger + \gamma_- A) = \sum_n \frac{1}{n!}\left[\frac{(\gamma_- - \gamma_+)}{2}R + \frac{(\gamma_- + \gamma_+)}{2}P\right]^n = \begin{bmatrix} 1 & \gamma_- & \frac{1}{2}\gamma_-\gamma_+ \\ 0 & 1 & \gamma_+ \\ 0 & 0 & 1 \end{bmatrix},$$

so that Eq. (A2) becomes

$$e^{-\tau AA^\dagger}\exp(\gamma_+ A^\dagger + \gamma_- A) = \begin{bmatrix} e^{\tau/2} & \gamma_- e^{\tau/2} & \frac{1}{2}\gamma_-\gamma_+ e^{\tau/2} \\ 0 & e^{-\tau/2} & \gamma_+ e^{-\tau/2} \\ 0 & 0 & e^{\tau/2} \end{bmatrix} = \begin{bmatrix} e^{\tau/2} & \xi_- e^{-\tau/2} & \frac{1}{2}\xi_-\xi_+ e^{\tau/2} \\ 0 & e^{-\tau/2} & \xi_+ e^{\tau/2} \\ 0 & 0 & e^{\tau/2} \end{bmatrix}.$$

By inspection, a solution is

$$\xi_- = \gamma_- e^{\tau}, \quad \xi_+ = \gamma_+ e^{-\tau}. \qquad \text{(A4)}$$

Substituting (A4) back into (A2) and replacing $AA^\dagger$ by $A^\dagger A$ gives Eq. (25).

It is worth pointing out that Eqs. (14) can also be derived using the representation (A1). For example, an ansatz of the form

$$\exp(\gamma_+ A^\dagger + \gamma_- A) = e^{\gamma_+ A^\dagger} e^{\gamma_- A^\dagger} e^{zS}$$

is assumed for (14b) with z the unknown parameter. Explicit matrix exponentiation of both sides shows that $z = \gamma_+\gamma_-/2$ is the solution. Finally, one should note that Eq. (25) can also be derived from an identity given in Ref. 9.

APPENDIX B

Both integrals $\tilde{I}_1$ of Eq. (29) and $\tilde{I}_2$ of Eq. (30) are very similar in structure. It will suffice to describe the evaluation of $\tilde{I}_2$.

Note first that $x^*y = k_\perp l_\perp e^{i(\phi_k - \phi_l)}/\lambda^2$ and $xy^* = k_\perp l_\perp e^{-i(\phi_k - \phi_l)}/\lambda^2$. Also note that

$$\sum_{k,l} v_k^2 v_l^2 \to \alpha^2 \int_0^\infty dk_\perp \int_0^\infty dl_\perp \frac{1}{2\pi}\int_0^{2\pi} d\phi_k \frac{1}{2\pi}\int_0^{2\pi} d\phi_l .$$

When one expands the exponential in (30) which involves x^*y and xy^*, all terms drop upon the angular integration except those with $e^{i(\phi_k-\phi_l)}$ raised to the zero power. Thus one can make the replacement

$$\exp[qx^*y-xy^*(1-e^{-\tau_2})] \rightarrow \sum_{n=0}^{\infty} \frac{[-q(1-e^{-\tau_2})k_\perp^2 l_\perp^2/\lambda^4]^n}{(n!)^2} . \quad \text{(B1)}$$

The power series in (B1) is equal to

$$J_0(2q^{1/2}(1-e^{-\tau_2})^{1/2}k_\perp l_\perp/\lambda^2) \text{ if } q \geq 0 ,$$

and to

$$I_0(2|q|^{1/2}(1-e^{-\tau_2})^{1/2}k_\perp l_\perp/\lambda^2) \text{ if } q \leq 0 .$$

With the change of variable $w=k_\perp/\lambda$, $v=l_\perp/\lambda$, one has

$$\tilde{I}_2=(\alpha\lambda)^2 \int_0^\infty dv\, e^{-a^2v^2} \int_0^\infty dw\, e^{-c^2w^2} \begin{bmatrix} J_0(2bvw) \\ I_0(2bvw) \end{bmatrix} , \quad \text{(B2)}$$

where

$$a^2=(1-e^{-\tau_2-\tau_1}) ,$$
$$b^2=(1-e^{-\tau_2})|q| , \quad \text{(B3)}$$
$$c^2=(1-e^{-\tau_2-\tau_3}) .$$

The inner integral is given by[10]

$$\frac{\sqrt{\pi}}{2c}\exp(\pm b^2v^2/2c^2)I_0(b^2v^2/2c^2) \text{ if } q=\mp|q| ,$$

so that

$$\tilde{I}_2=(\alpha\lambda)^2\frac{\sqrt{\pi}}{2c}\int_0^\infty dv \exp[(-a^2\pm b^2/2c^2)v^2] \times I_0(b^2v^2/2c^2) .$$

The change of variables $z=(b^2/2c^2)v^2$ puts this in the standard form[11]

$$\tilde{I}_2=(\alpha\lambda)^2\frac{\sqrt{2\pi}}{4b}\int_0^\infty dz \exp[(-2a^2c^2/b^2\pm 1)z] \times I_0(z)z^{-1/2}$$
$$=\frac{(\alpha\lambda)^2}{2b}Q_{-1/2}(2a^2c^2/b^2\mp 1) \text{ if } 2a^2c^2/b^2\mp 1>1 ,$$

where $Q_{-1/2}$ is a Legendre function. One can show that for all positive values of τ_1, τ_2, and τ_3 such that $q<0$, $2a^2c^2/b^2>2$.

Employing the identity

$$Q_{-1/2}(z)=[2/(z+1)]^{1/2}K(2/(z+1)) ,$$

where K is defined by (15b), one can write, from (26), taking $E_p=0$,

$$\mathscr{I}_2=-(\alpha\lambda)^2\int_0^\infty dt_1\, e^{-t_1}\int_0^\infty dt_3\, e^{-t_3}\left[\int_0^{t_m} dt_2\, e^{-t_2}\frac{K(b^2/(a^2c^2+b^2))}{2(a^2c^2+b^2)^{1/2}}+\int_{t_m}^\infty dt_2\, e^{-2t_2}\frac{K(b^2/a^2c^2)}{2ac}\right] , \quad \text{(B4)}$$

where

$$t_m=-\frac{1}{\lambda^2}\ln[(-1+e^{-\lambda^2 t_1}+e^{-\lambda^2 t_3})e^{\lambda^2(t_1+t_3)}] ,$$

provided that this expression gives a real positive t_m. Otherwise, $t_m=\infty$. The parameters a, b, and c are defined by (B3). A similar expression is obtained for $\mathscr{I}_1$. For that integral the analog of q is, from (29), $-(1-e^{-\tau_2})e^{-\tau_1-\tau_3}$, which is always negative for positive τ_i. One obtains

$$\mathscr{I}_1=-(\alpha\lambda)^2\int_0^\infty dt_1\, e^{-t_1}\int_0^\infty dt_3\, e^{-t_3}\int_0^\infty dt_2\, e^{-2t_2}\frac{K(b^2/a^2c^2)}{2ac} , \quad \text{(B5)}$$

where, for (B5),

$$a^2=1-e^{-\lambda^2 t_2},\quad b^2=(1-e^{-\lambda^2 t_2})^2 e^{-\lambda^2(t_1+t_3)},\quad c^2=1-e^{-\lambda^2(t_1+t_2+t_3)} .$$

Useful approximations to $K(z)$ may be found in Ref. 12.

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