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A variational study of the ground Landau level of the 2D Fröhlich polaron in a magnetic field

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Abstract. The problem of a two-dimensional polaron in a magnetic field is retrieved within the framework of an improved variational approximation which sets up a fractional admixture of the strong- and weak-coupling counterparts of the coupled electron–phonon system. The formulation is based on the usage of an adiabatic polaronic wavefunction corrected by a variationally determined perturbative extension enabling the adiabatic *ansatz* to be extrapolated towards the weak-coupling regime. The trial state derived here accounts for the magnetic field intensity not only in the electron part of the Hamiltonian, but also within the context of the part of the Hamiltonian describing the coupling of the electron to the phonon field.

1. Introduction

Even though the polaron problem is a rather old subject, it has recently excited renewed interest in the context of low-dimensionally confined quantum systems. Of particular interest are idealized strict two-dimensional (2D) models accounting for the almost-two-dimensional generic aspect of an electron in a thin quantum well and yet interacting with the bulk phonon modes of the well material [1–9]. Studies along these lines have revealed that the effective electron–phonon coupling becomes enhanced by a factor of $\pi/2$ over its bulk value in the weak-coupling regime relevant to most interesting compound semiconductors. For the case of a polaron under a magnetic field the binding gets even deeper due to the additional degree of localization brought about by the magnetic field [3–9]. It has been noted that for intense magnetic fields the phonon part of the ground-state energy grows at a rate $\sqrt{B}$, which is much faster than in 3D where the magnetic field dependence is of $\ln B$ form.

In view of the innumerable papers devoted to magnetopolarons, we see that the problem is not only interesting in laying out distinctive qualitative features in the different regimes of the magnetic field intensity and the electron–phonon coupling strength, but is also attractive from a formal point of view. The visualization of the problem as a whole is not very immediate due to the roles which the magnetic field and phonon coupling play in the polaron binding being not completely independent: they are interrelated, each sometimes dominating over the other, and yet they act together to enhance the phonon coupling. The qualitative aspects of the problem become simple, however, in some extreme cases.

For weak phonon coupling the most sensible approach is via the perturbation theory (see Larsen [4, 5], for instance), and moreover if the magnetic field is also weak, the problem can be characterized as consisting of an electron orbiting together with its concomitant lattice deformation with an effective polaron mass rather than the band mass. In this limit the ground-state energy can readily be written as the sum of the polaron self-energy

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$-(\pi/2)\alpha\hbar\omega_{LO}$ and of the lowest Landau energy $eB/2m^*c$ in which m^*, corrected up to first order in the coupling constant, scales to $m^*(1+(\pi/8)\alpha)$. Introducing the dimensionless cyclotron frequency ω_c expressed in units of ω_{LO} (the LO-phonon frequency), the ground-state energy (in usual polaron units: $\hbar = 2m^* = \omega_{LO} = 1$) is given approximately by

$$E_g \approx \frac{1}{2}\omega_c - \frac{\pi}{2}\alpha\left(1+\frac{\omega_c}{8}\right). \tag{1}$$

A contrasting aspect to such a description of the polaron is the case where the electron goes into a bound state with a highly localized wavefunction in a deep self-induced potential well of the lattice polarization. A way to investigate this totally distinctive aspect is either to imagine a rather strong coupling to the lattice or to go over to the high-magnetic-field limit where the lattice can only respond to the mean charge density of the rapidly orbiting electron and hence acquire a static deformation over the entire Landau orbit. Thus, one readily notes that, in spite of a small coupling constant, a pseudo-adiabatic condition can be attained when $\omega_c \gg 1$.

A complementary remark in this regard is that in the high-field limit and for weak polar coupling ($\alpha \ll 1$), the usual adiabatic theory gives

$$E_g = \frac{1}{2}\omega_c - \frac{1}{2}\alpha\sqrt{\pi\omega_c/2} \tag{2}$$

for the ground-state energy which differs from the perturbation theory estimate by a factor of $2^{-1/2}$ in the polaronic term [5]. The reason for the inconsistency lies in the fact that the most efficient coherent phonon state should not be taken as centred on the average electron position but instead on the orbit centre [10] $\rho_0 = x_0\hat{x} + y_0\hat{y}$, where

$$x_0 = \frac{1}{2}x - \frac{2}{\omega_c}p_y y_0 = \frac{1}{2}y + \frac{2}{\omega_c}p_x. \tag{3}$$

In fact, the role which the orbit centre coordinates play in the theory and, for large ω_c, the necessity of imposing a coherent phonon state operator leading to a deformation centred at ρ_0 were emphasized earlier in an elaborate discussion by Whitfield, Parker and Rona [11].

In this report we retrieve the magnetopolaron problem within a generalized variational scheme and give emphasis to the case where the effect of electron–phonon coupling is dominated by the magnetic field counterpart of the problem. We shall totally disregard the phonon-coupling-dominated ($\alpha \gg 1$) characterization of the polaron consisting of a deep self-induced potential well confining the rapid random charge density fluctuations of the electron which is furthermore under the influence of a relatively weak magnetic field. In the following we take the lattice deformation as centred essentially at ρ_0 rather than at the mean electron position and think of the electron as rotating on a complete Landau orbit.

Even though for somewhat strong field intensities the problem shows a vague strong-coupling aspect, a pure adiabatic approach fails to reflect a correct description of the system other than for infinitely large magnetic field strengths. On the other hand, a pure perturbation treatment may also be not perfectly appropriate other than for too small α. We are therefore tempted to formulate the magnetic-field-dominated regime of the magnetopolaron within the framework of a more convenient approach accounting for the fractional admixture of the weak- and strong-coupling aspects simultaneously. The formalism that we follow in this work consists of the usage of a variational *ansatz* introduced previously by Devreese *et al* [12] in their application to the bulk optical polaron bound to a Coulomb potential. The procedure is to start with the standard canonical transformation of the strong-coupling formulation and then modify the adiabatic polaron state via a variationally determined perturbative extension serving for the theory to interpolate in the overall range of the coupling constant.

In fact, the problem that we refer to here has already been discussed earlier within almost the same variational approach in a paper by Erçelebi and Saqqa [9]. The major distinction which sets the present concerns apart is that the variational state derived here is of a more general content, accounting for the magnetic field parameter ω_c not only in the electron part of the Hamiltonian, but also within the context of the part of the Hamiltonian describing the coupling of the electron to the phonon field. Performing the two studies separately with identical numerical precisions, we have observed that one reaches significantly improved energy upper bounds in the present case and this provides the motivation for readdressing the problem.

2. Formal preliminaries

Employing the symmetric gauge, $\boldsymbol{A} = (B/2)(-y, x, 0)$, for the vector potential, the Hamiltonian of a 2D electron immersed in the field of bulk LO phonons is given by

$$H = H_{\rm el} + \sum_{Q} a_Q^\dagger a_Q + \sum_{Q} \Gamma_Q [a_Q \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{\rho}) + a_Q^\dagger \exp(-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{\rho})] \tag{4}$$

$$H_{\rm el} = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + \frac{1}{4}\left(\frac{1}{2}\omega_c\rho\right)^2 - \frac{\mathrm{i}}{2}\omega_c\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \tag{5}$$

in which a_Q ($a_Q^\dagger$) is the phonon annihilation (creation) operator, and $\boldsymbol{\rho} = (x, y)$ denotes the electron position in the transverse plane. The interaction amplitude is related to the electron–phonon coupling constant α and the phonon wavevector $\boldsymbol{Q} = \boldsymbol{q} + q_z\hat{\boldsymbol{z}}$ through $\Gamma_Q = \sqrt{4\pi\alpha}/Q$. In the above, all physical quantities and operators have been written in dimensionless form with $(\hbar/2m^*\omega_{\rm LO})^{1/2}$ being selected as the unit of length and the phonon quantum $\hbar\omega_{\rm LO}$ as the unit of energy.

2.1. Electron eigenstates

Before proceeding with our main theme we first put the electron part of the Hamiltonian and its eigenstates into a transparent and convenient form where the relevant algebra is well known and calculations are easily made. To this end we follow the representation advanced in the papers by Malkin and Man'ko [13] and Whitfield, Parker and Rona [11]. Setting

$$z = \frac{1}{2}\sqrt{\frac{\omega_c}{2}}(x + \mathrm{i}y)$$

and introducing the operators

$$\begin{aligned} u &= \frac{1}{\sqrt{2}}\left(\bar{z} + \frac{\partial}{\partial z}\right) \qquad & u^\dagger &= \frac{1}{\sqrt{2}}\left(z - \frac{\partial}{\partial \bar{z}}\right) \\ v &= \frac{1}{\sqrt{2}}\left(z + \frac{\partial}{\partial \bar{z}}\right) \qquad & v^\dagger &= \frac{1}{\sqrt{2}}\left(\bar{z} - \frac{\partial}{\partial z}\right) \end{aligned} \tag{6}$$

with

$$[u, u^\dagger] = [v, v^\dagger] = 1 \qquad [u, v] = [u, v^\dagger] = 0 \tag{7}$$

one obtains

$$H_{\rm el} = \left(u^\dagger u + \frac{1}{2}\right)\omega_c. \tag{8}$$

It is evident that $u^\dagger$ (u) steps up (down) both the energy and the angular momentum:

$$l_z = -\mathrm{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = u^\dagger u - v^\dagger v.$$

On the other hand, $v^\dagger$ and v step only the angular momentum and not the energy. It thus follows that the energy eigenvalues of H_{el} are infinite-fold degenerate and, therefore, one is led to represent the corresponding eigenstates as

$$|n_u n_v\rangle = \chi_{n_u,n_v}|00\rangle \qquad n_u, n_v = 0, 1, 2, \ldots \tag{9}$$

where

$$\chi_{n_u,n_v} = (n_u!n_v!)^{-1/2}(u^\dagger)^{n_u}(v^\dagger)^{n_v}. \tag{10}$$

2.2. *The displaced oscillator transformation*

No matter how small α is, the starting idea in the foregoing approximation is to contemplate a very strong magnetic field to which the lattice responds by acquiring a relaxed static deformation clothing the entire Landau orbit. The adiabatic polaron ground state thus formed can be written in a product *ansatz* consisting of the electron and lattice parts, i.e.,

$$\Psi_g = |00\rangle \mathrm{e}^S|0_{\mathrm{ph}}\rangle \tag{11}$$

where $|0_{\mathrm{ph}}\rangle$ is the phonon vacuum and e^S is a unitary displacement operator changing the reference system of virtual particles by an amount $\Gamma_Q\sigma_{Q0}$. The most appropriate lattice wavefunction corresponding to the relaxed state of the electron–lattice system is determined to be

$$\Phi_{\mathrm{ph}} = \exp\left[\sum_Q \Gamma_Q\sigma_{Q0}(a_Q\mathrm{e}^{\mathrm{i}q\cdot\rho_0} - \mathrm{HC})\right]|0_{\mathrm{ph}}\rangle \tag{12}$$

with

$$\sigma_{Q0} = \langle 00|\mathrm{e}^{\pm\mathrm{i}q\cdot(\rho-\rho_0)}|00\rangle = \exp(-q^2/2\omega_c). \tag{13}$$

Thus, with the most efficient coherent phonon state as centred on the orbit centre, the Hamiltonian transforms to

$$\begin{aligned} H' &= \mathrm{e}^{-S}H\mathrm{e}^S \\ &= H_{\mathrm{el}} + \sum_Q a_Q^\dagger a_Q + \sum_Q \Gamma_Q^2\sigma_{Q0}^2 - \sum_Q \Gamma_Q^2\sigma_{Q0}[\mathrm{e}^{\mathrm{i}q\cdot(\rho-\rho_0)} + \mathrm{CC}] \\ &\quad + \sum_Q \Gamma_Q(\eta_Q a_Q + \eta_Q^* a_Q^\dagger) \end{aligned} \tag{14}$$

where

$$\eta_Q = \mathrm{e}^{\mathrm{i}q\cdot\rho_0}\{\mathrm{e}^{\mathrm{i}q\cdot(\rho-\rho_0)} - \sigma_Q\}. \tag{15}$$

If we were interested only in the adiabatic high-field limit, all that would remain would be the calculation of the expectation value of H' in the state $|00\rangle|0_{\mathrm{ph}}\rangle$, and we would readily obtain

$$E_g = \frac{1}{2}\omega_c - \Lambda_0 \tag{16}$$

where

$$\Lambda_0 = \sum_Q \Gamma_Q^2\sigma_{Q0}^2 = \frac{1}{2}\alpha\sqrt{\pi\omega_c} \tag{17}$$

which is identical to the perturbation result of Larsen [5] to leading order in α.

3. Theory

Obviously, for magnetic fields that are not too strong the adiabatic condition (and hence equation (16)) loses its validity, and one is tempted to consider the perturbation approach, whose applicability, however, is confined to the region where $\alpha \ll 1$. A theory which is capable of yielding the effective phonon coupling, not restricted solely to the weak α-limit, can be based on variational grounds. We thus choose to continue from equation (14), and modify the state $\Phi_0 = |00\rangle|0_{ph}\rangle$ accordingly by conforming it to a generalized form:

$$\Phi_0 \rightarrow \Phi_0' = \Omega(\alpha, \omega_c)\Phi_0 \tag{18}$$

where the operator $\Omega(\alpha, \omega_c)$ is intended to interrelate the weak- and strong-coupling counterparts of the problem depending on the strength of phonon coupling and the magnetic field intensity.

3.1. The variational trial state

On taking an already small α and further shifting ω_c down to small values, the degree of localization of the electron becomes reduced in a significant manner; σ_{Q0} in equation (14) tends to become zero on average and thus H' converts back to its original form as given by equation (4). In view of this reasoning one is led to treat the last term in equation (14) as a perturbation [12].

In the perturbation treatment of the Fröhlich interaction, the first non-vanishing contribution to the ground-state energy comes from the term which is of second order in the interaction amplitude. Correspondingly, the leading correction to the ground state is of first order and is given by the sum

$$\Delta\Phi_0 = \sum_{Q}\sum_{n} \frac{1}{\varepsilon_n - \varepsilon_0 + 1}|\varphi_n\rangle|1_Q\rangle\langle\varphi_n|\langle 1_Q|\sum_{Q'}\Gamma_{Q'}\eta^*_{Q'}a^\dagger_{Q'}|\Phi_0\rangle \tag{19}$$

in which the index n refers to the intermediate states consisting of those of the electron and one phonon with wavevector Q. In the above, φ_n and ε_n are to be thought of as the eigenstates and the eigenvalues of the unperturbed part of the transformed Hamiltonian (14). In order to calculate the perturbation sum (19) one needs to know the explicit functional forms of φ_n and the energies ε_n which, however, is a rather difficult task since now they depend in general on α and the lattice coordinates in an involved manner. Nevertheless, for the energy correction to be retained up to first order in α, we choose φ_n as the set of eigenfunctions of the bare-electron problem and ignore any α-dependence in either φ_n or ε_n, i.e., we take

$$\varphi_n \equiv \chi_{n_u,n_v}|00\rangle \qquad \varepsilon_n = \left(n_u + \frac{1}{2}\right)\omega_c. \tag{20}$$

Making a correspondence with the perturbation treatment of the problem one readily notes that the only thing we should do is account for the momentum conservation of the scattered electron–phonon system. We are thus tempted to write the energy difference as

$$\varepsilon_n - \varepsilon_0 \approx n_u\omega_c + \delta_n(Q) \tag{21}$$

where $\delta_n(Q)$ is introduced so as to bear any necessary phonon wavevector dependence.

Using the identity

$$s^{-1} = \int_0^\infty d\xi\ e^{-s\xi}$$

we set

$$\frac{1}{\varepsilon_n - \varepsilon_0 + 1} \approx g_Q J(\omega_c, n_u) \tag{22}$$

where

$$J(\omega_c, n_u) \equiv \int_0^\infty \mathrm{d}\xi \ \mathrm{e}^{-\xi} \exp(-\omega_c n_u \xi) \tag{23}$$

and g_Q stands for the exponential $\mathrm{e}^{-\delta_n(Q)\xi}$ factored out as an averaged quantity which, in the calculation, will be determined variationally. Substituting (15) and (22) into equation (19) we obtain

$$\Delta\Phi_0 = \sum_Q \Gamma_Q g_Q \sum_n J(\omega_c, n_u)\tilde{\sigma}_{Qn}\{\sigma_{Qn} - \sigma_{Q0}\delta_{n_u,0}\}\chi_{n_u,n_v} a_Q^\dagger \Phi_0 \tag{24}$$

where

$$\sigma_{Qn} = \langle\Phi_n|\mathrm{e}^{-\mathrm{i}q\cdot(\rho-\rho_0)}|\Phi_0\rangle = (n_u!)^{-1/2}[-\mathrm{i}(q_x - \mathrm{i}q_y)\omega_c^{-1/2}]^{n_u}\sigma_{Q0} \tag{25}$$

$$\tilde{\sigma}_{Qn} = \langle\Phi_n|\mathrm{e}^{-\mathrm{i}q\cdot\rho_0}|\Phi_0\rangle = (n_v!)^{-1/2}[-\mathrm{i}(q_x + \mathrm{i}q_y)\omega_c^{-1/2}]^{n_v}\sigma_{Q0}. \tag{26}$$

Using equations (10), (25) and (26) we see that the extended state $\Phi_0' = c\Phi_0 + \Delta\Phi_0$ can indeed be written in the form (18) with

$$\Omega(\alpha, \omega_c) = c + \sum_Q \Gamma_Q g_Q \lambda_Q^* a_Q^\dagger \tag{27}$$

in which c is a constant to serve for normalization, and

$$\lambda_Q = \sigma_{Q0}^2 \sum_{n_u}\sum_{n_v} \frac{(-\mathrm{i}\omega_c^{-1/2})^{n_u+n_v}}{n_u!n_v!} J(\omega_c, n_u)\{(q_x - \mathrm{i}q_y)^{n_u} - (q_x + \mathrm{i}q_y)^{n_v}\delta_{n_u,0}\}(u^\dagger)^{n_u}(v^\dagger)^{n_v}. \tag{28}$$

Projecting out the quantum numbers n_u and n_v, and, for notational convenience, writing

$$q(\xi) = q\exp(-\omega_c\xi) \tag{29}$$

we find that λ_Q takes the compact form

$$\lambda_Q = \int_0^\infty \mathrm{d}\xi \ \mathrm{e}^{-\xi}\eta_{Q(\xi)}\varrho_{Q(\xi)} \tag{30}$$

where

$$\eta_{Q(\xi)} = \mathrm{e}^{\mathrm{i}q\cdot\rho_0}\{\mathrm{e}^{\mathrm{i}q(\xi)\cdot(\rho-\rho_0)} - \sigma_{Q(\xi)}\} \tag{31}$$

and

$$\varrho_{Q(\xi)} = \frac{\sigma_{Q0}}{\sigma_{Q(\xi)}} = \exp\left\{-\frac{q^2 - q^2(\xi)}{2\omega_c}\right\} \tag{32}$$

in which

$$\sigma_{Q(\xi)} = \exp(-q^2(\xi)/2\omega_c). \tag{33}$$

It should be remarked that the two individual contributions to the binding coming from the electron–phonon coupling alone and the magnetic field alone are fundamentally incorporated via the operator $\Omega(\alpha, \omega_c)$ and, in particular, via the variational parameter g_Q which also governs the detailed admixture of the strong- and weak-coupling counterparts of the problem.

Due to the complicated nature of equation (27) where, at this stage, g_Q remains undetermined, simple concise predictions are not readily tractable except in the high-field limit where one expects the theory to impart most dominance to the strong-coupling aspect. In this extreme, $\varrho_{Q(\xi)} \to 1$, $\eta_{Q(\xi)} \to 0$, and consequently λ_Q in (27) becomes zero, and hence $\Omega(\alpha, \omega_c)$ conforms to the identity operator where we recover the strong-coupling theory.

3.2. Formulation

In order to reach the optimal fit to g_Q one has to minimize the expectation value of H' in the trial state $\Phi_0' = \Omega(\alpha, \omega_c)\Phi_0$ subject to the constraint that Φ_0' is normalized:

$$F(c, g_Q) \equiv \langle \Phi_0' | \Phi_0' \rangle - 1 = c^2 + \sum_Q \Gamma_Q^2 g_Q^2 h_Q^{(1)} - 1 = 0 \tag{34}$$

where

$$h_Q^{(1)} = \langle \Phi_0 | \lambda_Q \lambda_Q^* | \Phi_0 \rangle. \tag{35}$$

The variational procedure thus requires

$$\frac{\partial}{\partial g_Q}\{E(c, g_Q) - \Lambda F(c, g_Q)\} = 0 \tag{36}$$

where Λ is a Lagrange multiplier, and $E(g_Q, c)$ refers to the ground-state energy given as

$$\begin{aligned} E(c, g_Q) &= \langle \Phi_0' | H' | \Phi_0' \rangle \\ &= \frac{1}{2}\omega_c - \Lambda_0 + 2c \sum_Q \Gamma_Q^2 g_Q h_Q^{(0)} + \sum_Q \Gamma_Q^2 g_Q^2 [e_Q + h_Q^{(1)}(1 + 2\Lambda_0) - \delta_Q] \end{aligned} \tag{37}$$

in which

$$h_Q^{(0)} = \langle \Phi_0 | \eta_Q \lambda_Q^* | \Phi_0 \rangle \tag{38}$$

$$e_Q = \omega_c \langle \Phi_0 | \lambda_Q u^\dagger u \lambda_Q^* | \Phi_0 \rangle \tag{39}$$

and

$$\delta_Q = \sum_{Q'} \Gamma_{Q'}^2 \sigma_{Q'0} \langle \Phi_0 | \lambda_Q \{\exp[iq' \cdot (\rho - \rho_0)] + \text{cc}\} \lambda_Q^* | \Phi_0 \rangle. \tag{40}$$

The corresponding analytic expressions for $h_Q^{(0)}$, $h_Q^{(1)}$, e_Q and δ_Q are rather lengthy to give here, and therefore we provide them in the appendix.

Carrying out the Lagrange-multiplier-minimization technique we find that the optimal fits to g_Q and Λ can be derived through the set of equations

$$\Lambda = \sum_Q \Gamma_Q^2 [g_Q / c] h_Q^{(0)} \tag{41}$$

$$\frac{g_Q}{c} = -\frac{h_Q^{(0)}}{e_Q - \delta_Q + (1 + 2\Lambda_0 - \Lambda) h_Q^{(1)}} \tag{42}$$

and, further, for the ground-state energy we obtain

$$E_g = \frac{1}{2}\omega_c - \Lambda_0 + \Lambda. \tag{43}$$

4. Remarks and conclusions

In the energy expression (43), the additive term Λ, by means of which the adiabatic theory goes over to the weak-coupling regime, depends implicitly on the magnetic field and phonon coupling strengths through the transcendental equation (41). For a large value of the cyclotron frequency, $h_Q^{(0)}$ in equations (41) and (42) tends to zero; thereby $\Lambda \approx 0$, and hence the strong-coupling limit is readily attained even for $\alpha \ll 1$. As, however, ω_c

is decreased to lower values, the parameter Λ starts to interfere in the theory and strongly modify the results of the adiabatic approximation. In particular, for somewhat small field intensities and weak phonon coupling, the role Λ plays becomes very prominent and the polaron binding is effectively determined by this term. In this limit it is easy to see that the terms δ_Q, Λ_0 and Λ in equation (42) are all proportional to α in leading order and thus become far too small to yield any significant contribution to the summand in the transcendental equation (41). Therefore, retaining only $h_Q^{(0)}$, $h_Q^{(1)}$ and e_Q, and expanding the summand in a power series up to first order in ω_c, we have

$$\frac{g_Q}{c}h_Q^{(0)} \approx \frac{[h_Q^{(0)}]^2}{e_Q + h_Q^{(1)}} \approx \frac{1}{1+q^2} + \omega_c \left\{ 4\frac{q^2}{(1+q^2)^3} - 3\frac{q^2+q^4}{(1+q^2)^4} \right\} - \sigma_{Q0}^2. \tag{44}$$

Finally, projecting out the wavevector sum in (41), we achieve

$$\Lambda \approx -\alpha \int_0^\infty \mathrm{d}q \, \frac{[h_Q^{(0)}]^2}{e_Q + h_Q^{(1)}} \approx -\frac{\pi}{2}\alpha \left(1 + \frac{\omega_c}{8}\right) + \Lambda_0 \tag{45}$$

which, when inserted in equation (43), yields the approximate effective-mass-argument-based energy expression as given in equation (1)—thus exemplifying the essential role which Λ plays in conforming the adiabatic approximation to the results derived from the perturbation theory [4].

It is instructive to note that when the binding is somewhat deep ($\omega_c \gg 1$), one expects the energy eigenvalues of the bare-electron Hamiltonian and hence the differences in them to be significantly larger than the LO-phonon energy, which we take to be unity in our dimensionless units. If what we were really applying was ordinary perturbation theory the only significant contribution in the perturbation sum would come from the leading term $n_u = 0$, for this term has the smallest energy denominator. Dropping all terms except the $n_u = 0$ one, we arrive at exactly the same expression as obtained from the present calculation with $\Lambda = 0$. We thus note that in the extreme regime of highly localized configurations with shrinking cyclotron size the perturbation and strong-coupling theories match and are equally valid. On the other hand, as the magnetic field strength is made smaller, the adiabatic approach rapidly loses its validity since now the Landau levels are closer and even tend to coalesce towards the ground level. The corresponding perturbation series thus becomes slowly convergent and one needs to include the remaining terms—other than $n_u = 0$—as well. This, however, is accomplished in the present formalism by simply solving the transcendental equation (41) for the Lagrange multiplier Λ. Obviously, due to the analytical complexity the optimal fit to Λ (and to g_Q) can only be obtained by numerical techniques.

4.1. An alternative approach

Before presenting a general display of our numerical results we would like to make a small digression on an alternative approach and set up some correspondence with the variational bound-polaron state which has been proposed previously by Devreese *et al* [12], and later, in [9], adapted to the two-dimensional magnetopolaron problem. The basic distinction which sets the present formulation apart from that advanced in papers [12] and [9] stems essentially from the manner in which the perturbation expression (19) is treated in deriving the variational extension to the adiabatic polaron state Φ_0.

A more straightforward and less tedious approach to obtaining an analogous form for the variational state Φ_0', or equivalently for the operator $\Omega(\alpha, \omega_c)$ as defined in equation (18), can be achieved by treating the reciprocal of the total energy denominator $\varepsilon_n - \varepsilon_0 + 1$

in equation (19) as some average c-value, g_Q, and then setting $\sum_n |\varphi_n\rangle\langle\varphi_n|$ to the identity operator. Thus, in complete form, one obtains a simpler structure for the operator Ω as introduced in [12] or [9], i.e.

$$\Omega(\alpha, \omega_c) = c + \sum_Q \Gamma_Q g_Q \eta_Q^* a_Q^\dagger \tag{46}$$

in which the ω_c-dependence is provided only implicitly through parameter g_Q.

In the present treatment of the problem, however, we have found it necessary to conserve the track of the magnetic field parameter ω_c throughout the computational steps taken in reaching the extended variational state Φ_0' (equation (18)), thus accounting for this parameter not solely in the bare-electron part of the Hamiltonian, but also within the context of the part of the Hamiltonian describing the coupling of the electron to the phonon field. A glance at equation (30) reveals that the way in which this is accomplished is through the ξ-integrals involving the modified wavevector $q(\xi) = qe^{-\omega_c\xi}$ which imposes a detailed link incorporating the cyclotron frequency and the electron–phonon coupling. More peculiar in the concern with the weight $e^{-\omega_c\xi}$ is that it further takes part in determining the variational parameter g_Q which sets up the detailed interbalance between the strong- and weak-coupling counterparts of the coupled electron–phonon system. The passage from the form (27) derived in this report to that given in equation (46) can readily be attained by simply deleting the exponential factor $e^{-\omega_c\xi}$ in equation (29), thus replacing $q(\xi)$ by q in the set of equations (30)–(33). The ground-state energy can similarly be derived through equations (41)–(43), where now the parameters $h_Q^{(0)}$, $h_Q^{(1)}$, e_Q and δ_Q simplify to

$$h_Q^{(0)} = h_Q^{(1)} = 1 - \sigma_{Q0}^2 \qquad e_Q = q^2 \qquad \delta_Q = 2\Lambda_0\sigma_{Q0}^2 - 2\Lambda_0\sigma_{Q0}I_0(q^2/8\omega_c) \tag{47}$$

and this facilitates the numerical computations greatly. In contrast, however, the usage of this simplified version (46) is expected to yield somewhat larger energy upper bounds due to the variational parameter g_Q now being introduced to replace the energy denominator as an *average* quantity factored out away from the intermediate Landau level index n_u, thus containing only an *average* of the detailed content of the Fröhlich interaction interrelated to each of the Landau levels involved in the perturbation sum in equation (19).

Hereafter, in our discussions we shall refer to the variational ground-state energy values as $E_g^{(a)}$ and $E_g^{(b)}$, respectively, for the cases where either the form (46) or (27) is adopted. In order to provide a clear insight into the improvement achieved by the present formulation we display our results for the two approaches computed under identical numerical precisions.

Table 1. The ground-state energy versus the cyclotron frequency for $\alpha = 0.01$. The columns (a) and (b) display $E_g^{(a)}$ and $E_g^{(b)}$, and the columns (III) and (IV) display the adiabatic results obtained from equations (2) and (16), (17), respectively.

ω_c	(a)	(b)	(III)	(IV)
0.1	0.034 35	0.034 20	0.048 02	0.047 20
0.2	0.084 27	0.083 99	0.097 20	0.096 04
0.5	0.233 88	0.233 36	0.245 57	0.243 73
1	0.483 01	0.482 33	0.493 73	0.491 14
2	0.981 09	0.980 36	0.991 14	0.987 47
5	2.475 82	2.475 20	2.485 99	2.480 18
10	4.968 80	4.968 30	4.980 18	4.971 98
20	9.958 08	9.957 72	9.971 98	9.960 37

4.2. Numerical results

We first refer to the regime of extreme weak coupling and tabulate E_g versus ω_c for $\alpha = 0.01$. An immediate glance at the respective columns for $E_g^{(a)}$ and $E_g^{(b)}$ in table 1 reveals that the improved trial state (27) derived in this work yields significantly lowered energy upper bounds and, moreover, we find that the numerical values produced by the present treatment of the problem are in perfect agreement with those obtained from the second-order perturbation approximation [4]:

$$\Delta E_g^{(\mathrm{pert})} = -\frac{\pi}{2}\alpha\sqrt{\omega_c}\frac{\Gamma(1+1/\omega_c)}{\Gamma(\frac{1}{2}+1/\omega_c)}. \tag{48}$$

We should again draw attention to the facts that, in spite of a small α, a pseudo-adiabatic condition is reached for large ω_c and that the adiabatic limit considered here is the case where the lattice distortion is thought of as centred on the orbit centre coordinates (3) as characterized by equations (16), (17) rather than by equation (2). It is only then that the adiabatic approximation (and hence the present variational approach) fits the second-order perturbation theory for $\alpha \ll 1$ and $\omega_c \gg 1$. Indeed, a careful examination of the numerical values in table 1 confirms that the energies in columns (b) and (IV) (those obtained from (16) and (17)) tend to approach one another and eventually coincide as the magnetic field is made stronger. The energy values obtained from equation (2), however, remain deviated from the correct high-field limit due to the electronic wavefunction in the x–y plane not having to be as broad as depicted when the lattice displacement is set at $\rho = 0$ (cf. section III in [11]). This feature has been made more explicit in figure 1 where ΔE_g is displayed for large cyclotron frequencies.

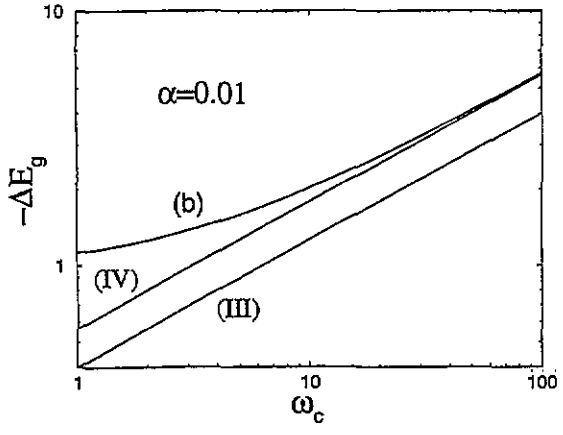

Figure 1. The asymptotic profiles for ΔE_g in the high-field limit. Curve (b) displays the results for the improved version in the present calculation. The straight lines (III) and (IV) are the strong-coupling results plotted from equations (2) and (16), (17), respectively. The energies are expressed in terms of the free-polaron binding energy, $(\pi/2)\alpha$.

In order to provide a pictorial view of the asymptotic energy profile of the system in the low-field limit and, in particular, to give somewhat more impact to the limiting expression for the parameter Λ as derived in equation (45), we also display the polaron-induced shift, $\Delta E_g = E_g - E_g(\alpha = 0)$, in the lowest Landau level calculated from both approaches, (a) and (b), over a reasonably broad range of small ω_c-values. A remarkable feature pertaining to the set of energy values (a) and (b) in figure 2 is that as ω_c tends to small values, $|\Delta E_g^{(a)}|$

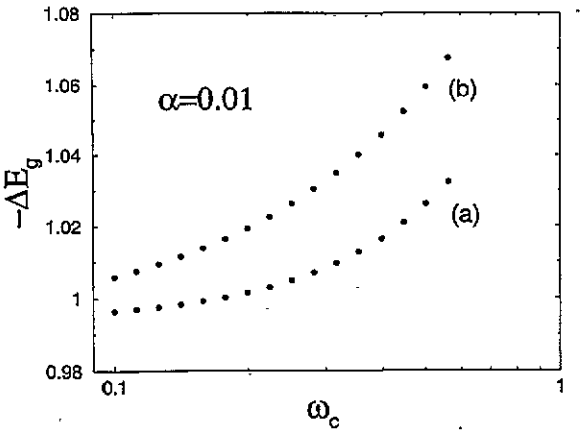

Figure 2. ΔE_g versus ω_c in the low-field regime. The sets of dark circles (a) and (b) display the results for the present formalism for the cases where either the form (46) or the form (27) is adopted. The energies are expressed in terms of the free-polaron binding energy, $(\pi/2)\alpha$.

approaches the free-polaron binding energy, $(\pi/2)\alpha$, from slightly below, which clearly is an incorrect description at least from a qualitative viewpoint—the binding should inherently be stronger under an external magnetic field. The deficiency encountered here, however, is 'cured' on utilizing the improved version (b). Within the framework of the modified trial state (27) we observe that $|\Delta E_g^{(b)}|$ displays instead a monotonically decreasing profile approaching the asymptotic value $(\pi/2)\alpha$ from above, thus being totally consistent with the description implied by equation (1) or, equivalently, by (48).

Going over to stronger-coupling constants a clear and concise description of the polaron state may no longer be readily tractable owing to the combined effect of the magnetic field and the Fröhlich interaction. Depending on the strengths of the parameters ω_c and α, there are two competitive contributions coming from the magnetic field alone and the phonon coupling alone—yet acting in an interrelated manner, thus leading to rather involved and distinguishing characterizations of the magnetopolaron. The treatment of the problem is relatively simple, however, in the extreme regimes where either the magnetic field counterpart or the phonon coupling dominates over the other. It is worthwhile to recall that our present considerations have been focused on the regime in which the magnetic field has the dominating strength over the coupled electron–phonon system where the relevant coherent phonon state is most appropriately structured so as to clothe the entire Landau orbit (with centre at ρ_0) rather than the mean electron position at the origin.

In figure 3 we select the coupling constant as larger by an order of magnitude, $\alpha = 0.1$, and provide plots of the phonon-induced shift in the energy against ω_c together with the available data (cf. dark circles in the figure) taken from the generalized path-integral formalism of Wu, Peeters and Devreese [6] (henceforth denoted as WPD). At this point it should be mentioned that the validity of the WPD theory has remained an open question over almost a decade (since the pioneering conjecture of Larsen [14]) from the formal viewpoint in the sense that their high-field estimates might lie below the actual ground-state energy [8, 14–16]. The controversy in the literature on the applicability of the path-integral formalism for systems with non-zero magnetic fields has been resolved recently in an elaborate discussion by Devreese and Brosens [17, 18] where they have shown that the Jensen–Feynman inequality is not *a priori* justified unless it is extended under additional

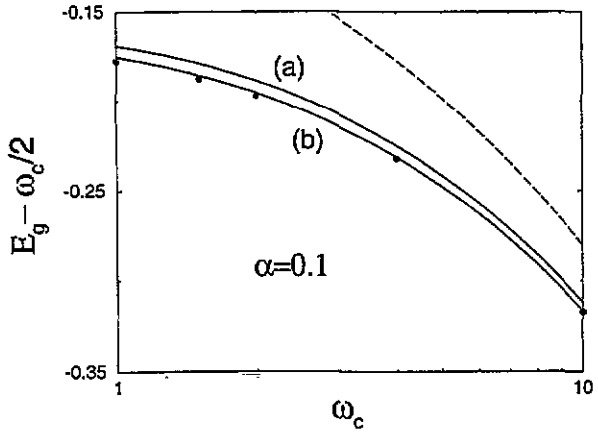

Figure 3. The phonon-induced shift in the lowest Landau level energy as a function of ω_c. Curves (a) and (b) are, respectively, for the cases where the form (46) or the form (27) is used for $\Omega(\alpha, \omega_c)$. The dark circles display the generalized path-integral results for the WPD theory [6], and the dashed line refers to the results of the strong-coupling approximation (17).

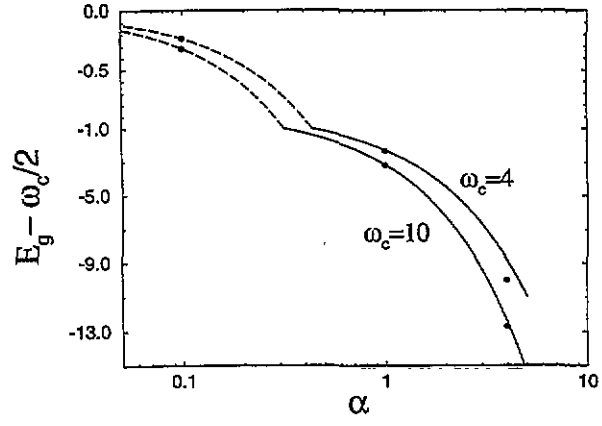

Figure 4. The phonon-induced shift in the lowest Landau level energy as a function of α. The dark circles display the generalized path-integral results for the WPD theory [6]. The plot is expanded in the energy region between -1 and 0, and to avoid confusion the curves are dashed in that region.

constraints when a magnetic field is present. Therefore, a rigorous variational justification of the WPD results can only be made within the framework of the generalized inequality derived in [17]. Nevertheless, we still choose to make a correspondence with the numerical outcomes of the WPD approximation and compare them with those derived from the present approach which has a conventional variational framework.

Referring first to the present results (a) and (b) derived for the variational polaron states given through equations (46) and (27), we infer that $E_g^{(b)}$ drops significantly below $E_g^{(a)}$ and that the usage of the improved trial state (b) gives far more satisfactory energy upper bound values. Comparing our results with those of WPD we find that even though $E_g^{(b)}$ lies consistently above the WPD energies, the discrepancy does not seem to be strikingly prominent especially for large magnetic field strengths. For $\omega_c = 4$, for instance, we obtain

$\Delta E_g^{(b)} = -0.2310$ which is fairly close (within only 0.6%) to the value -0.2324 derived by WPD. Using the form (46) for $\Omega(\alpha, \omega_c)$ however, we obtain $\Delta E_g^{(a)} = -0.2250$ yielding a discrepancy as large as 3.2%. We thus see explicitly that approach (b) gives far better results than (a) and further that the values reached using (b) are in fairly close agreement with those of WPD.

As the adiabatic limit ($\omega_c \gg 1$) is approached, we observe that the present formulation and the WPD theory match and give almost identical results, e.g. for $\omega_c = 10$ we have $\Delta E_g^{(b)} = -0.3170$ and $\Delta E_g^{(\mathrm{WPD})} = -0.3173$. For even larger values of ω_c the theory places comparatively less weight on the role which the parameter Λ plays in equation (43), thus imparting somewhat more dominance to the strong-coupling counterpart of the problem. Therefore, in the limit of intense magnetic fields, one readily expects all theories ((a), (b) and WPD) to duplicate asymptotically the strong-coupling results given by equation (17). Similar conclusions hold true for even stronger values of the coupling constant provided that the magnetic field is sufficiently large as to preserve the validity of the displaced oscillator transformation applied to the starting strong-coupling *ansatz* in the derivation of the present variational formalism. Setting $\omega_c = 10$, we obtain $\Delta E_g^{(b)} = -3.1472$ and -12.4171 for $\alpha = 1$ and $\alpha = 4$, respectively, whereas the corresponding WPD values have been reported to be -3.1737 and -12.7004 which lie below the (b) results by not more than 0.8% and 2.2%.

In order to provide comprehensive insight into the extent of applicability of the present approach in the large-α regime we display our results together with some of the available WPD data (dark circles) for two different magnetic field strengths (cf. figure 4). We note that as long as the magnetic field is strong enough to dominate over phonon-coupling-induced self-localization of the polaron, the agreement is fairly good in that all the WPD points for $\alpha = 0.1, 1$ and 4 lie only slightly below our calculated values plotted for $\omega_c = 10$ and $\omega_c = 4$, except the one for $\alpha = 4$ and $\omega_c = 4$ which is seen to lie drastically below the present theory values ($\Delta E_g^{(\mathrm{WPD})} = -10.0090$, $\Delta E_g^{(b)} = -8.7823$). The reason for this lies in the transformed Hamiltonian (14) involving the coherent phonon state centred on the orbit centre ρ_0, which is obviously misleading since, for strong phonon coupling but not large enough ω_c, the polaronic aspect overcompensates for the magnetic field counterpart of the problem—this particular situation being beyond the limit of applicability of the present approximation. A way to overcome the drawback encountered here can readily be found by making reference to the extreme limit where $\alpha \gg 1$ and $\omega_c \ll 1$, where now the lattice deformation should be thought of as surrounding the mean charge density of the electron itself rather than its overall motion in a complete Landau orbit (cf. [9]). Discussion pertaining to this totally distinctive aspect of the magnetopolaron is beyond the scope of our present interest.

In summary, this work revises the problem of a polaron in a magnetic field within an improved version of the extended variational scheme of Devreese *et al* [12] proposed for the bulk bound polaron. Although most of the formulation that we have adopted applies to a polaron in any dimensionality, for the present we have restricted our considerations to the 2D model of a magnetopolaron so as to eliminate any complications arising from the third dimension and have given most emphasis to the formal viewpoint of the problem. In view of our numerical results and the asymptotic analytic forms (16) and (45) achieved for $\omega_c \gg 1$ and $\omega_c \ll 1$, we reach the conclusion that the improved trial state introduced through equations (27) and (29)–(33) is rather promising in that it conveniently sets up a weighted admixture of the strong- and weak-coupling counterparts of the problem and thus enables the adiabatic results to conform satisfactorily to those attained from second-order perturbation theory.

Appendix

Referring to the set of equations (30)–(33) and using the integral transform

$$\int_0^\infty d\xi \int_0^\infty d\xi'\ f(\xi,\xi') = \frac{1}{2}\int_0^\infty dt \int_{-t}^{t} dt'\ f\left(\frac{t+t'}{2}, \frac{t-t'}{2}\right) \tag{A1}$$

we obtain the following functional forms for the parameters $h_Q^{(0)}$, $h_Q^{(1)}$, e_Q and δ_Q defined in equations (35) and (38)–(40):

$$h_Q^{(n)} = \int_0^\infty dt\ t^n e^{-t} \exp\left[-\frac{q^2}{\omega_c}(1-e^{-\omega_c t})\right] - \sigma_{Q0}^2 \qquad n = 0, 1 \tag{A2}$$

$$e_Q = q^2 \int_0^\infty dt\ te^{-t}e^{-\omega_c t} \exp\left[-\frac{q^2}{\omega_c}(1-e^{-\omega_c t})\right] \tag{A3}$$

and

$$\begin{aligned}\delta_Q = {} & 2\Lambda_0\sigma_{Q0}^2 - 2\Lambda_0 \int_0^\infty dt\ e^{-t} \int_0^t dt'\ [G(t+t') + G(t-t')] \\ & + 2\Lambda_0 \int_0^\infty dt\ e^{-t} \exp\left[\frac{q^2}{\omega_c}(1-e^{-\omega_c t})\right] \\ & \times \int_0^t dt'\ F\left[\frac{q^2}{4\omega_c}e^{-\omega_c t}(1-\cosh\omega_c t')\right]\end{aligned} \tag{A4}$$

where

$$G(t \pm t') = \exp\left[-\frac{q^2}{\omega_c}(1-e^{-\omega_c(t\pm t')})\right] F\left[\frac{q^2}{8\omega_c}e^{-\omega_c(t\pm t')}\right] \tag{A5}$$

and

$$F(x) = e^{-x} I_0(x)$$

with I_0 denoting the modified Bessel function of order zero.

References

[1] Das Sarma S and Mason B A 1985 *Ann. Phys., NY* **163** 78
[2] Peeters F M and Devreese J T 1987 *Phys. Rev.* B **36** 4442
[3] Das Sarma S 1984 *Phys. Rev. Lett.* **52** 859, 1570(E)
[4] Larsen D M 1984 *Phys. Rev.* B **30** 4807
[5] Larsen D M 1986 *Phys. Rev.* B **33** 799
[6] Wu Xiaoguang, Peeters F M and Devreese J T 1985 *Phys. Rev.* B **32** 7964
[7] Peeters F M and Devreese J T 1985 *Phys. Rev.* B **31** 3689
[8] Ninno D and Iadonisi G 1989 *Phys. Rev.* B **39** 10963
[9] Erçelebi A and Saqqa B 1989 *J. Phys.: Condens. Matter* **1** 10081
[10] Landau L D and Lifshitz E M 1965 *Quantum Mechanics* (Oxford: Pergamon) section 111
[11] Whitfield G, Parker R and Rona M 1976 *Phys. Rev.* B **13** 2132
[12] Devreese J, Evrard R, Kartheuser E and Brosens F 1982 *Solid State Commun.* **44** 1435
[13] Malkin I A and Man'ko V I 1969 *Sov. Phys.–JETP* **28** 527
[14] Larsen D M 1985 *Phys. Rev.* B **32** 2657
[15] Bhatthacharya M, Chatterjee A and Mitra T K 1989 *Phys. Lett.* **134A** 391
[16] Devreese J T and Brosens F 1991 *Solid State Commun.* **77** 583
[17] Devreese J T and Brosens F 1992 *Phys. Rev.* B **45** 6459
[18] Devreese J T and Brosens F 1993 *Lectures on Path Integration (Trieste, 1991)* ed H A Cerdeira, S Lundqvist, D Mugnai, A Ranfagni, V Sa-yakanit and L S Schulman (Singapore: World Scientific) p 109