# A variational approach for the two-dimensional magnetopolaron



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# A variational approach for the two-dimensional magnetopolaron

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**Abstract.** The problem of a two-dimensional magnetopolaron is investigated on the basis of a variational theory consisting of an adiabatic polaronic wavefunction combined with a perturbative correction by which it is possible to interrelate the strong and weak coupling counterparts of the coupled electron–phonon system. It is seen that the theory conveniently reproduces the desirable asymptotic limits in the different regimes of the problem. Furthermore, it is suggested that a satisfying improvement should be achieved if one adopts a suitably modified coherent phonon state operator which takes into account the fractional admixture of whether the lattice deformation tends to cover the entire Landau orbit or the mean electron position.

## 1. Introduction

In view of the innumerable amount of papers focused on the study of magnetopolarons we observe that the problem is not only interesting in laying out quite distinguishing features depending on the magnetic field intensity and the strength of electron–phonon coupling, but is also attractive formally. The interpretation of the problem and its mathematical structure are relatively simple and well understood in the asymptotic limits. At weak phonon coupling the most usual approach is the perturbation theory (see Larsen 1986, for instance), and moreover if the magnetic field is also weak, the problem can be visualised as consisting of an electron orbiting together with its concomitant lattice deformation with an effective polaron mass rather than the band mass. A contrasting aspect to such a description of the polaron is the case where the electron goes into a bound state with a highly localised wavefunction in the deep potential well induced by the lattice polarisation. A way to reach this totally distinct 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 mean charge density of the rapidly orbiting electron and hence acquire a static deformation clothing the entire Landau orbit. In both situations a satisfying approach can most readily be attained by the strong coupling–adiabatic theory (Pekar 1954).

For a more general view of the problem, not restricted to the limiting regimes, one requires more powerful methods or interpolating approximations. The purpose of this paper is to refer to such a technique so as to display a broader insight into the ground state behaviour of the magnetopolaron beyond that given in the weak and strong coupling extremes. The formalism we follow in this work was previously used by Devreese *et al* (1982) in their study of a polaron bound to a Coulomb centre. The procedure is an extension of the adiabatic approximation in the sense that a strongly coupled polaronic state combined with a first-order perturbative correction is used as

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a variational trial function by which it is possible to achieve a satisfying extrapolation towards the weak coupling regime.

In the following we specialise our considerations to an idealised two-dimensional (2D) system by taking the electronic wavefunction strictly planar lying in the directions perpendicular to the magnetic field, and thus ignore the charge density fluctuations of the electron in the longitudinal dimension which is not very crucial in the discussion of the formalism we follow in this work. A description of the 2D approximation and the rationale behind it has already been given by Das Sarma and Mason (1985) in their study of the free polaron problem in two-dimensionally confined quantum structures. The purely 2D characterisation of the dynamical behaviour of the electron, besides facilitating our computations, provides a means by which a correspondence of our 2D results can be made with some of the recent papers along the same line (Larsen 1984, 1986, Das Sarma 1984, Wu *et al* 1985).

Apart from its formal interest, the 2D model lends some insight into the significance, or at least the order of magnitude of, the polaron effect in confined structures such as, for instance, when the magnetopolaron gets compressed between the confining barriers of a quantum well. It should, however, be noted that a more appropriate approach would be to account for the possibility that the transverse coordinates may become incorporated with the longitudinal direction via coupling to the phonon field. In fact, the salient features which may be brought about by the mutual interrelation between the transverse and longitudinal directions was exemplified previously in the study of the quasi-2D polaron bound to a Coulomb centre (Erçelebi and Süalp 1987). Nevertheless, for the present we still adopt the 2D model of a polaron in a magnetic field so as to eliminate any complications comprised by the third dimension and give most emphasis on the formal viewpoint of the problem.

## 2. Formulation

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

$$H = H_0 + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q (a_Q \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{\rho}) + a_Q^\dagger \exp(-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{\rho})) \tag{1}$$

$$H_0 = p_x^2 + p_y^2 + \tfrac{1}{4}(\omega_c/2)^2(x^2 + y^2) + (\omega_c/2)l_z \tag{2}$$

in which energies have been scaled by the phonon energy $\hbar\omega_0$, and lengths by the polaron radius $(\hbar/2m\omega_0)^{1/2}$. In the above, $\boldsymbol{\rho} = (x, y)$ denotes the electron position in the transverse plane, $l_z = xp_y - yp_x$ is the angular momentum, and $\omega_c = (eB/mc)/\omega_0$ is the dimensionless cyclotron frequency. The interaction amplitude is related to the electron–phonon coupling constant $\alpha$ and the phonon wavevector $\boldsymbol{Q} = \boldsymbol{q} + q_z\hat{\boldsymbol{z}}$ through $V_Q = (4\pi\alpha)^{1/2}/Q$.

In the following we shall not take any explicit functional form for the electron part of the trial state, but instead use the linear combinations of the coordinates and momenta of the electron as operators:

$$b_\mu = (1/\sqrt{\sigma})(p_\mu - \tfrac{1}{2}\mathrm{i}\sigma x_\mu) \qquad [b_\mu, b_{\mu'}^\dagger] = \delta_{\mu\mu'} \tag{3}$$

where the index $\mu$ refers to the $x$ and $y$ directions, and $\sigma$ is an adjustable parameter. For the electron Hamiltonian we then have

$$H_0 = \left[\frac{\sigma}{2} + \frac{1}{2\sigma}\left(\frac{\omega_c}{2}\right)^2\right]\left(1 + \sum_\mu b_\mu^\dagger b_\mu\right) + \frac{1}{2}\left[\frac{\sigma}{2} - \frac{1}{2\sigma}\left(\frac{\omega_c}{2}\right)^2\right]\sum_\mu (b_\mu b_\mu + b_\mu^\dagger b_\mu^\dagger) - \mathrm{i}\frac{\omega_c}{2}(b_x^\dagger b_y - b_x b_y^\dagger). \tag{4}$$

Defining the ground state $|\,0\rangle$ by

$$b_\mu\,|\,0\rangle = 0 \qquad a_Q\,|\,0\rangle = 0 \qquad \langle 0\,|\,0\rangle = 1 \tag{5}$$

we find that with no phonon coupling yet introduced into the problem, the optimal $\sigma$-value is $\omega_c/2$, yielding $e_0 = \langle 0\,|\,H_0\,|\,0\rangle = \omega_c/2$ as expected.

Turning on the phonon coupling the problem becomes somewhat complicated owing to the combined effect of the magnetic field and the Fröhlich interaction. We therefore choose to begin with the weak coupling extreme where at high magnetic fields the adiabatic approach is expected to give the same result obtained from the second-order perturbation theory. Setting up the most efficient coherent phonon state as centred on the orbit centre (Whitfield *et al* 1976)

$$\boldsymbol{\rho}_0 = [x/2 - (2/\omega_c)p_y]\hat{\boldsymbol{x}} + [y/2 + (2/\omega_c)p_x]\hat{\boldsymbol{y}} \tag{6}$$

the Hamiltonian transforms to

$$H' = H_0 + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q^2\sigma_Q^2 - \sum_Q V_Q^2\sigma_Q[\exp(\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}_0)) + \exp(-\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}_0))] + \sum_Q V_Q(\eta_Q a_Q + \eta_Q^* a_Q^\dagger) \tag{7}$$

where

$$\eta_Q = \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{\rho}) - \sigma_Q\exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{\rho}_0) \tag{8}$$

$$\sigma_Q = \langle 0\,|\,\exp(\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}_0))\,|\,0\rangle = \exp(-q^2/2\omega_c) \tag{9}$$

and, for the ground-state energy we obtain

$$\epsilon_0 = \langle 0\,|\,H'\,|\,0\rangle = \frac{\omega_c}{2} + e_p \qquad e_p = -\sum_Q V_Q^2\sigma_Q^2 = -\frac{\alpha}{2}\sqrt{\pi\omega_c} \tag{10}$$

which is identical to the perturbation result of Larsen (1986) to leading order in $\alpha$.

Obviously, for not too strong magnetic fields the adiabatic condition and hence (10) loses its validity. This, however, can be corrected using the improved trial state (Devreese *et al* 1982)

$$|\,0'\rangle = c\,|\,0\rangle + \sum_Q V_Q g_Q \eta_Q^* a_Q^\dagger\,|\,0\rangle \tag{11}$$

in which $c$ is a constant which serves for normalisation, and $g_Q$ is a variational parameter determining the fractional admixture of the strong and weak coupling counterparts of the problem.

The optimal fit to $g_Q$ is achieved by minimising $\langle 0' \mid H' \mid 0' \rangle$ subject to the constraint

$$\langle 0' \mid 0' \rangle = c^2\left(1 + \sum_Q V_Q^2 (g_Q/c)^2 h_Q\right) = 1 \tag{12}$$

in which

$$h_Q = \langle 0 \mid \eta_Q \eta_Q^* \mid 0 \rangle = 1 - \sigma_Q^2. \tag{13}$$

For the energy we then have

$$E_a = \epsilon_0 + \epsilon \tag{14}$$

where $\epsilon$ is a Lagrange multiplier depending on $\alpha$ and $\omega_c$ through the transcendental equation

$$\epsilon = \sum_Q V_Q^2 (g_Q/c) h_Q \tag{15}$$

where

$$g_Q/c = -h_Q[e_Q + f_Q + (1 - \epsilon - \tfrac{1}{2}\omega_c - 2e_p)h_Q]^{-1} \tag{16}$$

with

$$e_Q = \langle 0 \mid \eta_Q H_0 \eta_Q^* \mid 0 \rangle = \tfrac{1}{2}\omega_c h_Q + q^2 \tag{17}$$

and

$$\begin{aligned} f_Q &= -\sum_{Q'} V_{Q'}^2 \sigma_{Q'} \langle 0 \mid \eta_Q \{\exp[i\boldsymbol{q}' \cdot (\boldsymbol{\rho} - \boldsymbol{\rho}_0)] + \exp[-i\boldsymbol{q}' \cdot (\boldsymbol{\rho} - \boldsymbol{\rho}_0)]\} \eta_Q^* \mid 0 \rangle \\ &= 2e_p \sigma_Q [I_0(q^2/8\omega_c) - \sigma_Q] \end{aligned} \tag{18}$$

in which $I_0$ is the modified Bessel function of order zero.

In order to find a solution for $\epsilon$ in (15) in the overall range of the magnetic field one requires numerical techniques. Taking a small coupling constant ($\alpha = 0.01$), in figure 1 we plot the polaronic correction to the ground state energy as a function of the cyclotron frequency. Starting from the high-field extreme and going to the weak-field limit we observe that the improved state (11) gives a satisfying description of the ground state in that it does not only yield better results, but indeed approaches asymptotically to the well established value, $\epsilon_p = -(\pi/2)\alpha$, for a weakly coupled polaron. In order to test the degree of validity of this formulation we make some correspondence with the generalised path-integral results of Wu *et al* (1985), hereafter referred to as WPD.

A comparison of the present work with the WPD theory for $\alpha = 0.1$ is given in table 1 which also includes the strong coupling results (with $\epsilon = 0$) for completeness. We observe that the improvement achieved by the trial state (11) is promising. For $\omega_c = 1$, for instance, the deviation from the path-integral value is less than 4%, whereas in the strict adiabatic treatment the discrepancy is as large as 28%.

For a comparatively large $\alpha$ however, the theory we follow in its present form is observed to fail to reflect a correct description of the ground state except for sufficiently large magnetic fields. In table 2 we tabulate our results together with the available data

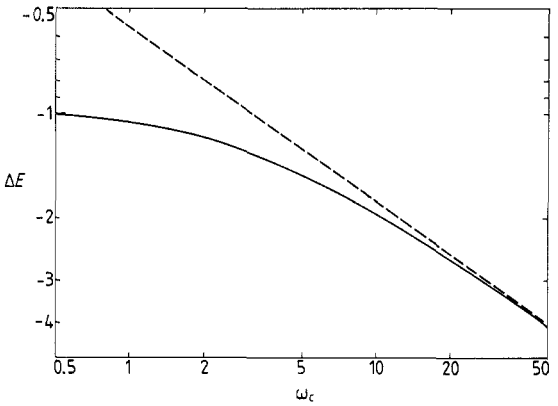


**Figure 1.** The polaronic correction $\Delta E = (E_a - \frac{1}{2}\omega_c)/\frac{1}{2}\pi\alpha$ as a function of $\omega_c$ at weak coupling for $\alpha = 0.01$. The full and broken curves refer to the present and the strong coupling approximations with $\epsilon$ in (14) taken as non-zero and zero, respectively.

**Table 1.** The ground state energy $E_a$ against the cyclotron frequency for $\alpha = 0.1$. The first and the third rows display the results of the generalised path integral approach of Wu *et al* (1985) and the strong coupling approximation.

| $\omega_c$ | 0.1 | 1 | 10 |
|---|---|---|---|
| $E_{WPD}$ | −0.1095 | 0.3225 | 4.6827 |
| $E_a$ | −0.0989 | 0.3343 | 4.6901 |
| $\epsilon_0$ | −0.0220 | 0.4114 | 4.7198 |

**Table 2.** The ground state energy $E_a$ against $\omega_c$ for $\alpha = 4$. The upper (lower) values for $E_{WPD}$ refer to the Gaussian (generalised) path integral calculations of Wu *et al* (1985).

| $\omega_c$ | 0.1 | 0.2 | 1 | 2 | 10 |
|---|---|---|---|---|---|
| $E_a$ | −3.531 | −3.761 | −4.780 | −5.477 | −7.069 |
| $E_{WPD}$ | −7.694 | −7.694 | −7.683 | −7.650 | −6.729 |
| $E_{WPD}$ | −8.207 | −8.206 | −8.190 | −8.150 | −7.700 |

of WPD for $\alpha = 4$. We at once note that the present values deviate rather drastically from those of WPD except the one for $\omega_c = 10$. The reason for the fault lies in that the transformed Hamiltonian (7) involves the coherent phonon state centred on the orbit centre $\boldsymbol{\rho}_0$ which obviously is misleading since for strong phonon coupling and not too large $\omega_c$, the polaronic aspect overcompensates the magnetic field counterpart of the problem. An insight to overcome the drawback encountered here can readily be achieved by making reference to the extreme limit of $\alpha \gg 1$ and $\omega_c \ll 1$ where now the lattice deformation should be thought as surrounding the mean charge density of the electron itself rather than its overall motion in a Landau orbit. Selecting the displaced (coherent) phonon state to be centred on the origin, i.e. setting $\boldsymbol{\rho}_0 = \mathbf{0}$ in (7)–(9) and (18), we obtain the following alternative form for the energy

$$E_b = e_0 + e_p + \epsilon \tag{19}$$

where

$$e_0 = \sigma/2 + (1/2\sigma)(\omega_c/2)^2 \qquad e_p = -(\alpha/2)\sqrt{\pi\sigma} \tag{20}$$

and $\epsilon$ is to be evaluated in an iterative scheme through

$$\epsilon = -\sum_Q V_Q^2 h_Q^2 [e_Q + f_Q + (1 - \epsilon - e_0 - 2e_p)h_Q]^{-1} \tag{21}$$

in which

$$e_Q = (e_0 + q^2)h_Q + (e_0/\sigma)q^2\sigma_Q^2 \tag{22}$$

$$f_Q = 2e_p[1 + \sigma_Q^2 - 2\sigma_Q^{7/4} I_0(q^2/8\sigma)] \tag{23}$$

with

$$\sigma_Q = \exp(-q^2/2\sigma). \tag{24}$$

Unlike the former case, the variational parameter $\sigma$ does not depend only on $\omega_c$ but on $\alpha$ as well. Optimising (19) with respect to $\epsilon$ and $\sigma$ we find that for all cases when the magnetic field loses its dominating strength over the coupled electron–phonon system, the ground state energy is more appropriately given by $E_b$, and approaches the well established asymptotic value $-(\pi/8)\alpha^2$ for $\alpha \gg 1$ and $\omega_c \to 0$. In order to give a pictorial view of the ground state energy calculated with both choices for the set of coordinates about which the lattice deformation forms, we display $E_a$ and $E_b$ against the cyclotron frequency for $\alpha = 4$ (cf figure 2).

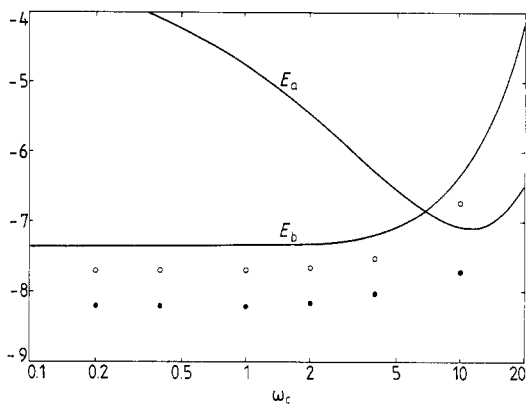


**Figure 2.** The ground state energy versus $\omega_c$ for $\alpha = 4$. $E_a$ and $E_b$ are for when the deformation is taken as centred on the orbit centre coordinates and on the origin, respectively. The open and full circles display the results of the Gaussian and generalised path integral approximations of Wu *et al* (1985).

We note that the two solutions cross over and thus exhibit a cusp in the energy profile at about $\omega_c = 6.85$. For cyclotron frequencies considerably below and above the crossover point the theory is observed to yield predominantly the minimum relevant to two qualitatively distinguishing cases where the lattice polarisation is thought to be clothing the mean electron position or else the lattice acquiring a static deformation over the entire Landau orbit (corresponding to the so-called *dressed* and *stripped*

phases as investigated previously by WPD). This in fact is a further interesting feature of the magnetopolaron pertaining to the combined effect of electron–phonon coupling and the magnetic field. In this context, the understanding of whether or not the system conforms from one phase to the other in an abrupt manner has always been a challenging and controversial aspect of the problem in both two and three dimensions. It has only very recently been reported by Löwen (1988) that the qualitative changes in the polaron quantities as a function of $\alpha$ or $\omega_c$ do actually take place in a smooth and continuous way, and that should any non-analytic behaviour encountered be an artefact of the approximating theory rather than the intrinsic property of the Fröhlich Hamiltonian. For the present we therefore refrain ourselves from giving an elaborate discussion on the ground state behaviour of the magnetopolaron across the transition region since a totally satisfying characterisation of the problem requires the formulation we have utilised to be modified accordingly so as to incorporate the two competitive contributions coming from the phonon coupling alone and the magnetic field alone. Nevertheless, in spite of such a drawback the theory is still promising and conveniently reproduces the desirable asymptotic limits in the different regimes of the problem.

In summary, this work revises the problem of a two-dimensional magnetopolaron within the extended variational scheme of Devreese *et al* (1982). It has been observed that the improved trial state (11) sets up a weighted admixture of the strong and weak coupling counterparts of the problem and thus enables the adiabatic results to conform successfully to those attained from second order perturbation theory. We believe that further improvement and considerably better results should be achieved if one adopts a suitably modified coherent phonon state which takes into account the involved interrelation between whether the lattice deformation tends to cover the entire Landau orbit or the mean electron position. A more appropriate version of the present theory would then consist of utilising the extended trial state (11) together with the Hamiltonian transformed accordingly such as was suggested, for instance, in a previous paper (Erçelebi 1989) concerning the same problem within the strict strong-coupling approximation. Even though the procedure is straightforward, the corresponding algebra is expected to be somewhat tedious. We therefore retain the relevant discussions until a future report.

## References

Das Sarma S 1984 *Phys. Rev. Lett.* **52** 859, 1570(E)
Das Sarma S and Mason B A 1985 *Ann. Phys., NY* **163** 78
Devreese J, Evrard R, Kartheuser E and Brosens F 1982 *Solid State Commun.* **44** 1435
Erçelebi A 1989 *J. Phys.: Condens. Matter* **1** 2321
Erçelebi A and Süalp G 1987 *J. Phys. C: Solid State Phys.* **20** 5517
Larsen D M 1984 *Phys. Rev.* B **30** 4807
—— 1986 *Phys. Rev.* B **33** 799
Löwen H 1988 *J. Math. Phys.* **29** 1498
Pekar S I 1954 *Untersuchungen uber die Elektronentheorie der Kristalle* (Berlin: Akademie)
Whitfield G, Parker R and Rona M 1976 *Phys. Rev.* B **13** 2132
Wu Xiaoguang, Peeters F M and Devreese J T 1985 *Phys. Rev.* B **32** 7964