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The two-dimensional magneto-polaron in the strong-coupling regime

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Abstract. Within the framework of the strong-coupling polaron theory the problem of a two-dimensional electron coupled to LO phonons under an external magnetic field is studied. When a suitably modified coherent phonon state interrelating the magnetic field and the polaron counterparts of the problem is adopted, it is seen that the theory reproduces the desirable asymptotic limits attained by the perturbation or the usual adiabatic theories. Moreover, the theory indicates that an abrupt 'stripping transition' in the internal structure of the magneto-polaron with varying magnetic field intensity is favoured as investigated by Wu, Peeters and Devreese.

1. Introduction

Even though the problem of a polaron in a magnetic field is a rather old subject, it has recently received increasing attention in the context of quasi-two-dimensionally confined quantum systems. In view of the innumerable studies devoted to both three-dimensional (3D) and two dimensional (2D) magneto-polarons, we see that the problem, besides displaying distinctive qualitative features in the different regimes of the magnetic field intensity and the electron–phonon coupling strength, is also attractive from a formal point of view. Among various methods developed on the basis of existing polaron theories, the Feynman path-integral formulation is intended to be the most powerful technique interpolating between all the regimes of the problem. Wu *et al* (1985) have elaborated the ground-state property of the 2D polaron by generalising the Feynman variational theory so as to include the influence of an external magnetic field of arbitrary strength. They have raised the possibility that, similar to the bulk case (Peeters and Devreese 1982, Lépine 1985), the 2D polaron may undergo an abrupt 'stripping transition' in its internal structure at sufficiently strong electron–phonon couplings and high magnetic fields. Whether or not the change in the state of the system as a function of the magnetic field is in fact abrupt is, however, controversial. The regime of strong electron–phonon interactions and/or large magnetic fields therefore deserves special emphasis.

In order to investigate the possibility of discontinuous behaviour of the magneto-polaron, we would like to consider the strongly coupled case within a Buimistrov–Pekar (Buimistrov and Pekar 1957, 1958) type of variational scheme modified so as to account for the distinctive regimes where the effect of either the electron–phonon coupling or the magnetic field dominates over the other. Although most of the formulation that we follow in this work applies to any type of polaron, for the present we restrict our considerations to polar optical mode coupling and, for simplicity, ignore motion in the direction parallel to the magnetic field.

2. Theory

Using the symmetric gauge for the vector potential, i.e. $A = (B/2)(-y, x, 0)$, the Hamiltonian describing an electron (in the x–y plane) coupled to bulk LO phonons with a frequency $\omega_Q = \omega_0$ is given by

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

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

where $\boldsymbol{\rho} = x\hat{\boldsymbol{x}} + y\hat{\boldsymbol{y}}$, $l_z = xp_y - yp_x$ and ω_c is the dimensionless cyclotron frequency expressed in units of ω_0. 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 $V_Q = (4\pi\alpha)^{1/2}/Q$. It should be noted that all physical quantities and operators have been written in dimensionless form with $\hbar\omega_0$ being selected as a unit of energy and $(\hbar/2m\omega_0)^{1/2}$ as a unit of length.

The variational procedure followed in this work assumes the electron and lattice variables to be totally separable (Pekar 1954) with the phonon part of the wavefunction given as

$$\varphi_{\mathrm{ph}} = \exp(S)\,|0\rangle \tag{3}$$

with $\exp(S)$ being a coherent state operator which creates the optimal lattice deformation surrounding the mean charge density of the electron or of its orbit.

Before setting up the coherent phonon state appropriate to the present problem, we would like to re-emphasise that the combined effect of the magnetic field and the Fröhlich interaction leads to rather involved and totally different features depending on the strength of electron–phonon interaction and the magnetic field. The qualitative aspects of the system become simple, however, in two extremes.

For large α and $\omega_c \ll 1$ the problem simplifies to an almost free strongly coupled polaron in which the lattice deformation is taken to be centred around the average electron position. Clearly, in the other extreme of a large magnetic field the situation is somewhat different. In this limit 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 reached when $\omega_c \gg 1$.

A further important remark concerning the high-field limit is that, at weak polar couplings ($\alpha \ll 1$), the usual adiabatic theory gives $E = \frac{1}{2}\omega_c - \frac{1}{2}\alpha\sqrt{\pi\omega_c/2}$ for the ground-state energy which differs from the correct value by a factor of $2^{-1/2}$ in the polaronic term (see Larsen (1986) for instance). The reason for the fault lies in the fact that the most efficient coherent phonon state should not be taken as centred on the average electron position but on the orbit centre $\boldsymbol{\rho}_0 = x_0\hat{\boldsymbol{x}} + y_0\hat{\boldsymbol{y}}$ (Landau and Lifshitz 1965) where

$$x_0 = x/2 - (2/\omega_c)p_y \qquad y_0 = y/2 + (2/\omega_c)p_x. \tag{4}$$

In fact, the role which the orbit centre coordinates play in the theory and, for large ω_c, the necessity of making the deformation centred at $\boldsymbol{\rho}_0$ were emphasised earlier in an elaborate discussion by Whitfield *et al* (1976).

Therefore, in an attempt to bring about a unified scheme in the overall range of ω_c, we propose a coherent phonon state where the operator S in equation (3) has the form

$$S = \sum_Q \{[F_Q + G_Q \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{\rho}_0)]a_Q - [F_Q + G_Q \exp(-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{\rho}_0)]a_Q^\dagger\} \tag{5}$$

in which the variational weights F_Q and G_Q are intended to interrelate the polaron and magnetic field counterparts of the problem. Clearly one expects either F_Q or G_Q to dominate over the other in weak or large magnetic fields, respectively. For a sufficiently large ω_c the theory is expected to conform totally to that suggested by Whitfield *et al* (1976).

For the electron part of the trial state, we use the linear combinations of the positions and momenta of the electron as operators:

$$x_j = (i/\sqrt{\sigma})(b_j - b_j^\dagger) \qquad p_j = (\sqrt{\sigma}/2)(b_j + b_j^\dagger) \qquad [b_j, b_{j'}^\dagger] = \delta_{jj'}. \tag{6}$$

The index j refers to the x and y directions, and σ is an adjustable parameter.

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

$$a_Q|0'\rangle = b_j|0'\rangle = 0 \qquad \langle 0'|0'\rangle = 1 \tag{7}$$

and optimising the expectation value of $H' = \exp(-S)\, H \exp(S)$ with respect to F_Q and G_Q, we obtain

$$F_Q = V_Q f_Q \qquad G_Q = V_Q g_Q \tag{8}$$

where

$$f_Q = (s - s_0^2)/(1 - s_0^2) \qquad g_Q = s_0(1-s)/(1-s_0^2) \tag{9}$$

with

$$s = \langle 0'|\exp(\mathrm{i}\,\boldsymbol{q}\cdot\boldsymbol{\rho}|0'\rangle = \exp(-q^2/2\sigma) \tag{10}$$

$$\begin{aligned} s_0 &= \langle 0'|\exp(\mathrm{i}\,\boldsymbol{q}\cdot\boldsymbol{\rho}_0|0'\rangle = \langle 0'|\exp[\mathrm{i}\,\boldsymbol{q}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}_0)]|0'\rangle \\ &= \exp[-\tfrac{1}{2}(1/4\sigma + \sigma/\omega_c^2)q^2]. \end{aligned} \tag{11}$$

The ground-state energy is then given by

$$E = \tfrac{1}{2}\sigma + \tfrac{1}{8}\omega_c^2\sigma^{-1} - \sum_Q V_Q^2(f_Q^2 - g_Q^2 + 2s_0 g_Q) \tag{12}$$

which has to be further minimised with respect to σ.

3. Results and conclusions

In the extreme limits of strong and weak fields, we attain explicit asymptotic expressions for the ground-state energy. For weak electron–phonon coupling and large magnetic fields, we achieve the 'stripped' polaron state where the lattice is thought to be responding only to the overall motion of the electron in its Landau orbit. For the parameters in equation (12), we obtain $f_Q \to 0$, $g_Q \simeq s_0$ with $\sigma = \omega_c/2$, and

$$E = \tfrac{1}{2}\omega_c - \alpha \int_0^\infty \mathrm{d}q\, s_0^2 = \tfrac{1}{2}\omega_c - \tfrac{1}{2}\alpha(\pi\omega_c)^{1/2} \tag{13}$$

which is identical with the second-order perturbation result of Larsen (1986).

In the remaining extreme of weak fields ($\alpha \gg 1$, $\omega_c \ll 1$), we have $g_Q \to 0$, $f_Q \simeq s$ and

$$E = \tfrac{1}{2}\sigma + \tfrac{1}{8}\omega_c^2\sigma^{-1} - \tfrac{1}{2}\alpha(\pi\sigma)^{1/2} \tag{14}$$

in which the dominant terms are the first and the third, and the second term is only a small correction. We find that the optimal σ-value which minimises the dominant part is $(\pi/4)\alpha^2$. Substitution into equation (14) yields

$$E = -\tfrac{1}{8}\pi\alpha^2[1 - (2\omega_c/\pi\alpha^2)^2] \tag{15}$$

which is the 2D analogue of the corresponding bulk value. In fact, the corresponding 3D ground-state energy can readily be obtained from equation (14) by including $\langle 0'|p_z^2|0'\rangle = \sigma/4$ and further making the 2D electron position $\boldsymbol{\rho}$ in equation (1) of a 3D type so that Q^2 replaces q^2 in equation (10). The third term in equation (14) then conforms to $-\alpha(\sigma/\pi)^{1/2}$ and one obtains

$$E = -(\alpha^2/3\pi)[1 - \tfrac{3}{2}(3\pi\omega_c/4\alpha^2)^2] \tag{16}$$

which is the same as that given by Lépine (1985) and Tokuda and Kato (1987) for large α and small ω_c.

An interesting remark concerning this limit is that equation (15) gives a self-energy correction of order $\omega_c^2\alpha^{-2}$ whereas the corresponding term reported by Wu *et al* (1985) is proportional to $\omega_c\alpha^{-4}$. In our opinion the distinction encountered here is because the present approximation leads to a qualitatively distinguishing characterisation of the system other than that of a strongly coupled polaron orbiting as a rigid entity as an effective particle. We think that the description displayed by the present model consists of a deep self-induced potential well confining the charge-density fluctuations of the electron which is further under the influence of a weak magnetic field. The polaron thus formed is stationary and centred essentially at the mean electron position rather than the centre of a complete Landau orbit as implied by the fact that G_Q in equation (5) becomes zero in the limit $\alpha \gg 1$, $\omega_c \ll 1$. We refer to this situation as the 'self-trapped' phase with the ground-state energy $(-\pi\alpha^2/8)$ being modified only slightly by the magnetic field.

In order to explore the ground-state property in the overall range of the magnetic field, one requires numerical techniques. In view of our results, we find that the theory is a fairly good approximation not only in the asymptotic limits of weak and strong fields but also for intermediate field strengths, giving a description of the change in the system as a function of ω_c. It should be pointed out that equation (12) does not always have a unique minimum. Below a certain value of the cyclotron frequency, we observe that a second locally stable minimum appears, indicating that in the transition region both types of phase (stripped and self-trapped) may coexist.

Taking a large enough coupling constant ($\alpha = 4$), in figure 1 we plot the ground-state energy against ω_c in the region where the polaron changes its state. Starting from the high-field limit, the only σ-value minimising equation (12) is $\frac{1}{2}\omega_c$ relevant to the stripped phase of polaron where the lattice deformation is over the entire electron orbit rather

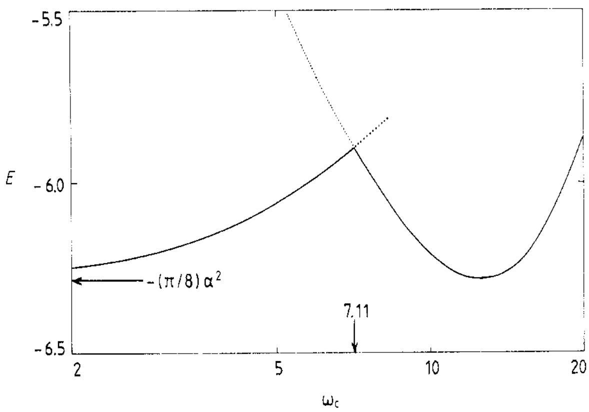

Figure 1. The ground-state energy (in $\hbar\omega_0$) as a function of ω_c for $\alpha = 4$: ...., metastable state.

than the electron itself. At about $\omega_c \simeq 8.6$ the minimum corresponding to the self-trapped phase starts to appear, and at $\omega_c \simeq 7.11$ the two distinct solutions cross over. Below the crossing point the energy of the self-trapped phase is found to be lower than that in the stripped phase and, as the cyclotron frequency is reduced even more, the energy profile displays dominantly the trapped state of the system as given by equation (15).

We note that in most respects the present model is capable of reproducing similar qualitative features to those obtained by Wu *et al* (1985); however, it yields energy upper bounds considerably above the results of the Feynman variational approach (cf table 1). The reason for the discrepancy is mostly due to the superiority of the Feynman path-integral theory to the strong-coupling approximation. Therefore, rather than making full correlation with the numerical values attained by the path-integral treatment, we give most emphasis to the qualitative description of the strongly coupled magneto-polaron within the framework of the coherent phonon state introduced through equation (5).

In addition to the ground-state energy, we have also plotted the magnetisation $\mu = -\partial E/\partial \omega_c$, and the susceptibility $\chi = -\partial^2 E/\partial \omega_c^2$ as a function of ω_c for $\alpha = 4$ (cf figures 2 and 3). We see that, as the polaron undergoes a change of state as described above, both μ and χ exhibit an abrupt behaviour at almost the same place as obtained by Wu *et al* (1985). The discontinuities encountered here and the cusp in the energy profile at the crossover point can be regarded as giving further insight into the complicated nature of the problem, confirming the possibility in favour of a phase-transition-like behaviour of

Table 1. The ground-state energy (in $\hbar\omega_0$) against ω_c for $\alpha = 4$. The upper energy values refer to the present work and the lower to the Feynman path-integral approach of Wu *et al* (1985).

ω_c	0.1	0.2	1	2	10
E (present work)	−6.2836	−6.2833	−6.2738	−6.2445	−6.2105
E (Wu *et al* 1985)	−8.2074	−8.2067	−8.1899	−8.1502	−7.7004

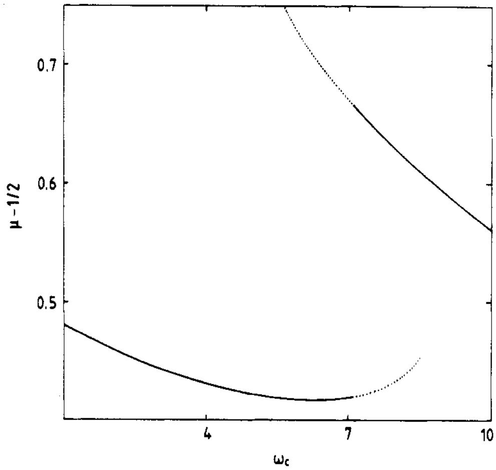

Figure 2. Magnetisation $\mu - \frac{1}{2}$ referred to the free-electron value as a function of ω_c for $\alpha = 4$.

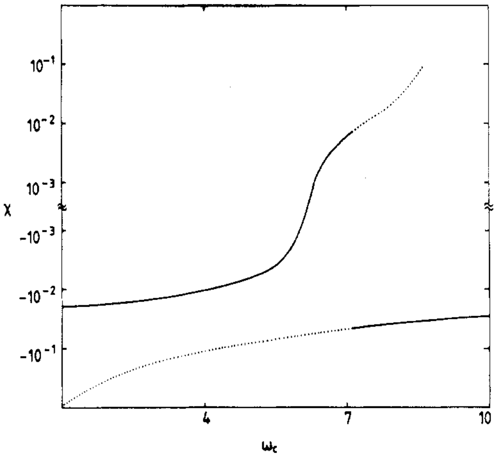

Figure 3. Susceptibility as a function of ω_c for $\alpha = 4$.

the system. Whether or not a 'stripping' phase transition indeed takes place is, however, still an open question.

In summary, this work revises the problem of a 2D polaron in a magnetic field within a generalised variational scheme in the strong-coupling regime. Adopting a suitably modified coherent phonon state the theory is seen to give an intuitive description which takes into account the fractional admixture of whether the lattice deformation tends to cover the entire Landau orbit or the mean electron position. The conclusion which we draw is that the adiabatic treatment of the problem requires the displaced (coherent) phonon state to be in a form incorporating the two competitive contributions coming from the phonon coupling alone and the magnetic field alone.

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