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Energy and mass of 3D and 2D polarons in the overall range of the electron–phonon coupling strength

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Abstract. The ground-state characterization of the polaron problem is retrieved within the framework of a variational scheme proposed previously by Devreese *et al* for the bound polaron. The formulation is based on the standard canonical transformation of the strong coupling *ansatz* and consists of a variationally determined perturbative extension serving for the theory to interpolate in the overall range of the coupling constant. Specializing our considerations to the bulk and strict two-dimensional polaron models we see that the theory yields significantly improved energy upper bounds in the strong coupling regime and, moreover, extrapolates itself successfully towards the well-established weak coupling limits for all polaron quantities of general interest.

1. Introduction

In view of the innumerable amount of papers focused on the study of polarons, we observe that the problem, apart from its solid state interpretation, is of more general theoretical interest and attractive formally. (For a general review of the subject and the relevant approximation methods, see [1, 2].) The interpretation of the problem and its mathematical structure are relatively simple and well understood in the asymptotic limits. One of the basic points of view is the case where the kinetic energy of the electron is much smaller than the energy of the phonon modes. In this case the lattice deformation tends to follow the electron as it moves through the crystal. A reasonable treatment in such a case is to take the electron–phonon interaction as a perturbation and to calculate the corrections to the energy eigenvalues brought about by the polaron effect. Another approach which successfully gives a good description of the behaviour of the electron and its concomitant lattice deformation at weak coupling has been developed by Lee *et al* [3]. This theory is of variational nature and leads to essentially the same results as the perturbation theory.

A contrasting point of view originates from the idea that for a strong enough electron–phonon interaction the electron goes into a bound state with a highly localized wavefunction in the self-induced potential which is built up by the field of correlated virtual phonons [4]. If the electron is really deeply bound one expects the lattice deformation to react back and produce some structure in the electronic wavefunction, and the presence of the electron in turn determines and maintains the size and shape of the deformation. The point of view presented by these arguments is referred to as the strong coupling (adiabatic) theory.

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 an approximation so as to display a broader insight into the ground-state property of the polaron problem beyond that given in the weak and strong coupling

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extremes. The formalism we adopt in this work is based on the method introduced previously by Devreese *et al* [5] in their study of the problem of a bulk polaron bound to a Coulomb centre. The procedure is an extension of the adiabatic approximation in the sense that a strongly coupled polaron state combined with a first-order perturbative extension is used as a variational trial state by which it is possible to achieve a satisfying extrapolation towards the weak coupling regime. Since the rationale behind this approximation has already been given in detail [5], only the essential points and modifications in the formulation will be presented.

In the following we give all emphases on the formal viewpoint of the problem and specialize our considerations to the bulk (3D) and the strict two-dimensional (2D) [6, 7] optical polaron models which have been well established and well understood in the literature.

2. Theory

2.1. Formal preliminaries

Regardless of the strength of the electron–phonon coupling we start with a strongly coupled polaron state given as a product *ansatz* of the form

$$\Psi = \Phi_0 \Phi_{ph} \tag{1}$$

where Φ_0 is the localized electron wavefunction. For an electron trapped about the origin, the optimal lattice wavefunction describing the deformation surrounding the electronic charge density can be derived through the displaced oscillator representation

$$\Phi_{ph} = \mathcal{U}|0\rangle \tag{2}$$

where $|0\rangle$ is the phonon vacuum, and

$$\mathcal{U} = \exp \sum_{Q} u_Q(\Phi_0)[a_Q - a_Q^\dagger] \tag{3}$$

in which $u_Q(\Phi_0)$ is to be adjusted variationally. It should be noted that simultaneous optimizations with respect to $u_Q(\Phi_0)$ and Φ_0 correspond to the self-trapping picture of the polaron where the electron distribution and the lattice polarization influence each other in such a way that a stable relaxed state is eventually attained. Under the canonical transformation $H \rightarrow \mathcal{U}^{-1}H\mathcal{U}$, the Fröhlich polaron Hamiltonian (in usual polaron units: $\hbar = 2m_e^* = \omega_{LO} = 1$) conforms to

$$H' = p^2 + \sum_{Q} u_Q^2 - \sum_{Q} \Gamma_Q u_Q(\exp(iQ \cdot r) + \exp(-iQ \cdot r)) + \sum_{Q} a_Q^\dagger a_Q + \sum_{Q}[(\Gamma_Q \exp(iQ \cdot r) - u_Q)a_Q + \text{HC}] \tag{4}$$

where p and r denote the electron momentum and position, and Q is the phonon wavevector, all of which are to be regarded as three (two) dimensional for the 3D (2D) polaron. With

the normalization volume (area) set to unity for notational convenience, the interaction amplitude is related to the electron–phonon coupling constant α through

$$\Gamma_Q = \begin{cases} \sqrt{4\pi\alpha}/Q & \text{in three dimensions} \\ \sqrt{2\pi\alpha}/Q & \text{in two dimensions.} \end{cases} \tag{5}$$

Since the polaron Hamiltonian is invariant to translations of the electron and the lattice distortion together, the total momentum

$$P = p + \sum_Q Q a_Q^\dagger a_Q \tag{6}$$

must be conserved. The variation thus requires an optimization of the polaron state Ψ which minimizes $\langle \Psi \mid H \mid \Psi \rangle$ subject to the constraint that $\langle \Psi \mid P \mid \Psi \rangle$ is a constant of motion.

In the calculations 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:

$$b_\mu = (1/\sqrt{\sigma})(p_\mu - \tfrac{1}{2}i\sigma x_\mu) - \tfrac{1}{2}p_{0\mu} \qquad [b_\mu, b_{\mu'}^\dagger] = \delta_{\mu\mu'} \tag{7}$$

where the index μ refers to the cartesian directions, and σ is an adjustable parameter with $\sigma^{-1/2}$ yielding a measure of the spatial extent of the electron. The vector p_0 is introduced as a further variational quantity in the theory so as to account for the composite inertia of the electron dressed by the cloud of virtual phonons.

Defining the ground state of the coupled electron–phonon system by

$$b_\mu |0\rangle = 0 \qquad a_Q |0\rangle = 0 \qquad \langle 0|0\rangle = 1 \tag{8}$$

and minimizing the functional

$$\phi(\sigma, v; p_0, u_Q) \equiv \langle 0|\mathcal{U}^{-1}(H - v \cdot P)\mathcal{U}|0\rangle \tag{9}$$

with respect to p_0 u_Q yields

$$p_0 = (1/\sqrt{\sigma})v \qquad \text{and} \qquad u_Q = \Gamma_Q s_Q \rho_Q \tag{10}$$

where

$$s_Q = \langle 0 \mid \exp(\pm iQ \cdot r) \mid 0 \rangle = \exp(-Q^2/2\sigma) \tag{11}$$

$$\rho_Q = (1 - v \cdot Q)^{-1} \tag{12}$$

in which the Lagrange multiplier v is to be identified as the polaron velocity (see, e.g., [8]).

In what follows we shall consider the case of a stationary polaron, i.e. take $\langle 0 \mid \mathcal{U}^{-1}P\mathcal{U} \mid 0 \rangle = 0$, and thus regard v as a virtual velocity which we retain in our calculations to keep track of the effective mass of the coupled electron–phonon system.

In complete form, with the optimal fits for p_0 and u_Q substituted in, the Hamiltonian which we shall be referring to hereafter is

$$H' = p^2 + \sum_Q a_Q^\dagger a_Q + \sum_Q \Gamma_Q^2 s_Q^2 \rho_Q^2 - \sum_Q \Gamma_Q^2 s_Q \rho_Q (\exp(iQ \cdot r) + \exp(-iQ \cdot r)) + \sum_Q \Gamma_Q (\eta_Q a_Q + \eta_Q^* a_Q^\dagger) \tag{13}$$

where

$$\eta_Q = \exp(\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}) - s_Q\rho_Q \tag{14}$$

$$p^2 = e_0 + \tfrac{1}{4}\sigma\sum_\mu (2b_\mu^\dagger b_\mu + b_\mu b_\mu + b_\mu^\dagger b_\mu^\dagger) + \tfrac{1}{4}v^2 + \tfrac{1}{2}\sqrt{\sigma}\sum_\mu v_\mu(b_\mu + b_\mu^\dagger) \tag{15}$$

in which e_0 takes the value $\frac{3}{4}\sigma$ in three dimensions and $\frac{1}{2}\sigma$ in two dimensions.

Similarly, for the total momentum transformed accordingly, $\boldsymbol{P} \to \mathcal{U}^{-1}\boldsymbol{P}\mathcal{U}$, we have

$$\boldsymbol{P}' = \boldsymbol{p} + \sum_Q \boldsymbol{Q}a_Q^\dagger a_Q + \sum_Q \boldsymbol{Q}\Gamma_Q^2 s_Q^2\rho_Q^2 - \sum_Q \boldsymbol{Q}\Gamma_Q s_Q\rho_Q(a_Q + a_Q^\dagger) \tag{16}$$

where the components of the electron momentum are given through

$$p_\mu = \tfrac{1}{2}\sqrt{\sigma}(b_\mu + b_\mu^\dagger) + \tfrac{1}{2}v_\mu. \tag{17}$$

2.2. The variational trial state

If what interested us was solely the strong coupling regime, all that would remain would consist of a further optimization of $\langle 0 \mid (H' - \boldsymbol{v}\cdot\boldsymbol{P}') \mid 0\rangle$ with respect to σ. We retain the results pertaining to the large-α limit until later and point them out as a special case of the more general results which we derive in the next section. Here, our concern is to adopt the variational scheme of Devreese *et al* [5] where the adiabatic polaron trial state is modified accordingly so as to cover the overall range of the coupling strength. For the sake of completeness, in this and the following subsections we choose to include a brief revision of the basic essentials in the variational *ansatz* advanced in [5]. The major distinction which sets the present concern apart from that in [5] is that we confine ourselves to a totally free polaron model with a virtual momentum imposed to the coupled electron–phonon complex through the factor ρ_Q multiplying the term s_Q in the Hamiltonian (13).

Regardless of the value of α, no matter how small it is, the procedure is still to continue with our considerations from equation (13), since with decreasing α the degree of localization of the electron becomes reduced in a significant manner; eventually s_Q tends to zero on the average and thus H' converts back to the starting Hamiltonian H in which for weak α the Fröhlich interaction $\sum_Q \Gamma_Q[\exp(\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r})a_Q + \mathrm{HC}]$ should serve as the perturbing term. In view of this reasoning one is led to treat the last term in equation (13) as a perturbation. Since at present we limit ourselves to the case of a stationary polaron, we first would like to bring about an insight into the problem with ρ_Q in equation (13) set to unity, thereby obtaining a means of characterizing the polaron (i.e. calculating the optimal σ value and hence the binding energy, for instance) for the case when $\boldsymbol{v} = 0$. Thereafter we shall turn on the velocity to keep track of the polaron mass under a virtual translation of the electron and the lattice distortion together.

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 trial state defined through equation (8) is of first order. The ground-state trial wavefunction for H' and for the constraint that the total momentum $\boldsymbol{P}'$ be conserved then becomes extended to

$$|0'\rangle = c\,|0\rangle + \sum_Q \Gamma_Q \sum_i |i\rangle \frac{\langle i \mid (\exp(-\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}) - s_Q)a_Q^\dagger \mid 0\rangle}{\Delta\varepsilon_{i-o}}. \tag{18}$$

In equation (18), c is a constant which serves for normalization, and the index i refers to the intermediate states consisting of the electron and one phonon with wavevector $\boldsymbol{Q}$. The summation over the intermediate states is a rather difficult task since now the states themselves and the corresponding energies depend on α and the lattice coordinates in involved manners. Nevertheless, this shortcoming can be eliminated by replacing the energy denominator $\Delta\varepsilon_{i-o}$ by an average quantity which in the calculation will be determined variationally. Using completeness the i summation can be projected out to yield [5]

$$|0'\rangle = c\,|0\rangle + \sum_{\boldsymbol{Q}} \Gamma_{\boldsymbol{Q}} g_{\boldsymbol{Q}} (\exp(-\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}) - s_{\boldsymbol{Q}}) a_{\boldsymbol{Q}}^{\dagger}\,|0\rangle. \tag{19}$$

The variational parameter $g_{\boldsymbol{Q}}$ sets up a fractional admixture of the strong and weak coupling counterparts of the coupled electron–phonon system and thus is expected to serve for the theory to interpolate between the extreme limits of the coupling constant.

2.3. Formulation

The requirement that the trial state $|\,0'\rangle$ be normalized poses yet a further constraint, interrelating the parameters c and $g_{\boldsymbol{Q}}$ through

$$f(c, g_{\boldsymbol{Q}}) = c^2 + \sum_{\boldsymbol{Q}} \Gamma_{\boldsymbol{Q}}^2 g_{\boldsymbol{Q}}^2 h_{\boldsymbol{Q}} - 1 = 0 \tag{20}$$

in which

$$h_{\boldsymbol{Q}} = \langle 0|\,(\exp(\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}) - s_{\boldsymbol{Q}})(\exp(-\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}) - s_{\boldsymbol{Q}})\,|0\rangle = 1 - s_{\boldsymbol{Q}}^2. \tag{21}$$

In order to find the optimal fit to $g_{\boldsymbol{Q}}$ one has to minimize the expectation value of $H' - \boldsymbol{v}\cdot\boldsymbol{P}'$ in the trial state (19) subject to the constraint (20). Within the framework of the modified trial state $|\,0'\rangle$ the functional (9) now takes the form

$$\begin{aligned}\phi(\sigma, \boldsymbol{v}; c, g_{\boldsymbol{Q}}) &= c^2(e_0 + \tfrac{1}{4}v^2) - \tfrac{1}{2}v^2 + (1 - 2c^2)\chi \\ &\quad + 2c \sum_{\boldsymbol{Q}} \Gamma_{\boldsymbol{Q}}^2 g_{\boldsymbol{Q}} h_{\boldsymbol{Q}} + \sum_{\boldsymbol{Q}} \Gamma_{\boldsymbol{Q}}^2 g_{\boldsymbol{Q}}^2 (e_{\boldsymbol{Q}} - \delta_{\boldsymbol{Q}} + h_{\boldsymbol{Q}})\end{aligned} \tag{22}$$

where

$$\chi = \sum_{\boldsymbol{Q}} \Gamma_{\boldsymbol{Q}}^2 s_{\boldsymbol{Q}}^2 \rho_{\boldsymbol{Q}} \tag{23}$$

$$\begin{aligned}e_{\boldsymbol{Q}} &= \langle 0|\,(\exp(\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}) - s_{\boldsymbol{Q}})p^2(\exp(-\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}) - s_{\boldsymbol{Q}})\,|0\rangle \\ &= e_{\boldsymbol{Q}}^{(0)} - \boldsymbol{v}\cdot(\boldsymbol{Q} - \tfrac{1}{4}\boldsymbol{v})h_{\boldsymbol{Q}} e_{\boldsymbol{Q}}^{(0)} = \tfrac{1}{2}\boldsymbol{Q}^2 + (e_0 + \tfrac{1}{2}\boldsymbol{Q}^2)h_{\boldsymbol{Q}}\end{aligned} \tag{24}$$

$$\delta_{\boldsymbol{Q}} = \sum_{\boldsymbol{Q}'} \Gamma_{\boldsymbol{Q}'}^2 s_{\boldsymbol{Q}'} \Delta_{\boldsymbol{Q}\boldsymbol{Q}'} \rho_{\boldsymbol{Q}'} \tag{25}$$

with

$$\Delta_{\boldsymbol{Q}\boldsymbol{Q}'} = \langle 0|\,(\exp(\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}) - s_{\boldsymbol{Q}})(\exp(\mathrm{i}\boldsymbol{Q}'\cdot\boldsymbol{r}) + \exp(-\mathrm{i}\boldsymbol{Q}'\cdot\boldsymbol{r}))(\exp(-\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}) - s_{\boldsymbol{Q}})\,|0\rangle. \tag{26}$$

The variational procedure requires

$$\frac{\partial}{\partial g_Q}\{\phi(\sigma, v; c, g_Q) - \lambda f(c, g_Q)\} = 0 \tag{27}$$

where λ is a Lagrange multiplier. It then follows that the functional ϕ is given by

$$\phi(\sigma, v) = e_0 - \chi - \tfrac{1}{4}v^2 + \lambda \tag{28}$$

where λ is derived through the transcendental equation

$$\lambda = \sum_Q \Gamma_Q^2 (g_Q/c) h_Q \tag{29}$$

in which

$$g_Q/c = -h_Q/D_Q \qquad D_Q = e_Q - \delta_Q + (1 - e_0 - \tfrac{1}{4}v^2 + 2\chi - \lambda)h_Q. \tag{30}$$

In order to trace out the polaron mass from equation (28) we have to split $\phi(\sigma, v)$ into its parts, consisting of the binding energy of the polaron alone and the additional kinetic contribution which shows up after imposing a virtual momentum on the polaron. We are thus tempted to expand equations (23), (25) and the summand in equation (29) in a power series up to second order in v. Letting

$$\chi = \chi^{(0)} + \tfrac{1}{4}v^2\chi^{(v)} \qquad \delta_Q = \delta_Q^{(0)} + \tfrac{1}{4}v^2\delta_Q^{(v)} \tag{31}$$

and, furthermore, setting

$$D_Q^{(0)} = e_Q^{(0)} - \delta_Q^{(0)} + (1 - e_0 + 2\chi^{(0)} - \lambda)h_Q \tag{32}$$

we obtain

$$\phi(\sigma, v) = E_g(\sigma) - \tfrac{1}{4}v^2 m_p \tag{33}$$

where

$$E_g(\sigma) = e_0 - \chi^{(0)} + \lambda \tag{34}$$

refers to the ground-state energy and the factor m_p multiplying $\frac{1}{4}v^2$ is identified as the polaron mass, given by

$$m_p = 1 + \chi^{(v)} + \sum_Q \Gamma_Q^2 \frac{h_Q^2}{D_Q^{(0)}} \left(\frac{4}{d} Q^2 (h_Q/D_Q^{(0)})^2 + \frac{\delta_Q^{(v)} - 2\chi^{(v)} h_Q}{D_Q^{(0)}} \right) \tag{35}$$

with d standing for the dimensionality (i.e. $d = 3$ or 2 for the 3D or 2D polarons, respectively).

For the set of parameters $\chi^{(0)}$, $\chi^{(v)}$, $\delta_Q^{(0)}$ and $\delta_Q^{(v)}$, we have

$$\chi^{(0)} = \sum_Q \Gamma_Q^2 s_Q^2 = \begin{cases} \alpha\sqrt{\sigma/\pi} & \text{in three dimensions} \\ (\alpha/2)\sqrt{\pi\sigma} & \text{in two dimensions} \end{cases} \tag{36}$$

$$\chi^{(v)} = (4/d) \sum_Q \Gamma_Q^2 s_Q^2 Q^2 = (2/d)\sigma\chi^{(0)} \tag{37}$$

and

$$\delta_Q^{(0)} = \sum_{Q'} \Gamma_{Q'}^2 s_{Q'} \Delta_{QQ'}$$

$$= 2\chi^{(0)}(1+s_Q^2) - \begin{cases} (4/\mathrm{i})\sqrt{\pi\sigma}\, s_Q^2 \operatorname{erf}(\mathrm{i}2\sqrt{\xi}) & \text{in three dimensions} \\ 4\chi^{(0)} s_Q^{3/2} \mathrm{e}^{-\xi} I_0(\xi) & \text{in two dimensions} \end{cases} \tag{38}$$

$$\delta_Q^{(v)} = (4/d)\sum_{Q'} \Gamma_{Q'}^2 s_{Q'} \Delta_{QQ'} Q'^2 = 2\chi^{(v)}(1+s_Q^2)$$

$$= -\begin{cases} 4d\chi^{(v)} s_Q^{3/2} (\hat{v}\cdot\hat{Q})^2 & \text{in three dimensions} \\ 4d\chi^{(v)} s_Q^{3/2} \mathrm{e}^{-\xi}[(\xi+\tfrac{1}{2})I_0(\xi) + \xi I_1(\xi)] & \text{in two dimensions} \end{cases} \tag{39}$$

where $\xi = Q^2/8\sigma$, and the symbols I_0 and I_1 denote the zeroth- and first-order modified Bessel functions, respectively.

It should be clear that in deriving equation (33) we have regarded the parameter λ, involved in equations (34) and (35), as to be obtained from equation (29) for when $g_Q/c = -h_Q/D_Q^{(0)}$, i.e. for the case where the polaron is taken as stationary.

3. *Results and conclusions*

Due to the analytic complexity, the optimal fits to λ and σ are to be performed by numerical methods within an iterative scheme. The results incorporating equations (34) and (35) become more comprehensive and immediate, however, in the extreme limits of strong and weak coupling. (For the corresponding asymptotic limits in three dimensions the reader is refered to [5].)

When the binding is very deep one expects the energy eigenvalues of the unperturbed 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 are applying were ordinary perturbation theory the only significant contribution in the perturbation sum would come from the leading term $i = 0$, for this term has the smallest energy denominator. Dropping all terms except $i = 0$, we arrive at exactly the same expression obtained by the present calculation with $\lambda = 0$. This verifies the equivalence of the two approaches in the limit of large α. On the other hand, as the coupling constant is made smaller, the corresponding perturbation series becomes slowly convergent and one needs to include the remaining terms, apart from $i = 0$, as well. This is accomplished in the present formalism by simply solving the transcendental equation (29) for the Lagrange multiplier λ.

For large coupling constants the electron gets highly localized ($\sigma = \mathrm{O}(\alpha^2) \gg 1$), s_Q becomes unity on the average, and thus h_Q, and hence λ, tend to zero and the strong coupling limit is readily attained. For a loosely bound electron, however, the role λ plays becomes very prominent and the polaron binding is dominantly determined by this term.

In the limit $\alpha \ll 1$, equations (34) and (35) simplify greatly. In this extreme, $s_Q \approx 0$ ($h_Q \approx 1$) and, moreover, the quantities σ, e_0, $\chi^{(0)}$ and $\delta_Q^{(0)}$ fall off rather rapidly with an order of magnitude of α^2. The decay rates of $\chi^{(v)}$ and $\delta_Q^{(v)}$ are even faster, going as α^3 on

the average. Omitting the contributions coming from such terms and retaining terms up to order α only, equation (34) reduces to

$$E_g \approx \lambda \approx -\sum_Q (\Gamma_Q^2/D_Q^{(0)})$$
$$\approx -\sum_Q \Gamma_Q^2 \frac{1}{1+Q^2} = \begin{cases} -\alpha & \text{in three dimensions} \\ -(\pi/2)\alpha & \text{in two dimensions.} \end{cases} \tag{40}$$

Similarly, equation (35) conforms to

$$m_p \approx 1 + \frac{4}{d}\sum_Q \Gamma_Q^2 \frac{Q^2}{(1+Q^2)^3} = \begin{cases} 1+(1/6)\alpha & \text{in three dimensions} \\ 1+(\pi/8)\alpha & \text{in two dimensions.} \end{cases} \tag{41}$$

As a further polaron quantity of general interest, we also calculate the mean number of phonons, $n_{ph} = \langle 0' \,|\, \mathcal{U}^{-1} \sum_Q a_Q^\dagger a_Q \mathcal{U} \,|\, 0' \rangle$, clothing the electron. Using equation (20) we obtain

$$n_{ph} = \chi^{(0)} + \sum_Q \Gamma_Q^2 g_Q^2 h_Q = \chi^{(0)} + \nu(1+\nu)^{-1} \qquad \nu = \sum_Q \Gamma_Q^2 (g_Q/c)^2 h_Q \tag{42}$$

which, in the limit $\alpha \to 0$, simplifies to

$$n_{ph} \approx \nu \approx \sum_Q \Gamma_Q^2 \frac{1}{(1+Q^2)^2} = \begin{cases} (1/2)\alpha & \text{in three dimensions} \\ (\pi/4)\alpha & \text{in two dimensions.} \end{cases} \tag{43}$$

The asymptotic expressions (40), (41) and (43) thus exemplify the essential role which λ plays in making the adiabatic approximation go over to the results derived from the ordinary perturbation theory.

In order to provide a general display of our results (beyond those for $\alpha \gg 1$ and $\alpha \ll 1$), we minimize equation (34) numerically over a reasonably broad range of α for the 3D and 2D polarons. In figure 1 we plot the binding energy ($\varepsilon_p = |E_g|$) and the phonon contribution to the effective mass ($\mu = m_p - 1$) as a function of the coupling constant, including also a comparison of the present results with those of the strong coupling and perturbation theories. An immediate glance at the set of curves on the large-α site reveals that the strong coupling theory deviates considerably from the present formalism except in the extreme limit $\alpha \gg 1$. The reason is that the pure strong coupling treatment of the problem is totally inadequate to reflect any weak coupling aspect for not too strong α. This shortcoming is, however, eliminated in the present approach by preserving λ in equation (34), since it is only through this term that a detailed interbalance is set up between the strong and weak coupling counterparts of the problem.

A further feature pertaining to the regime of strong phonon coupling is that, with growing α, the rate at which the the strong coupling and present theories approach one another and eventually match is relatively faster in two dimensions than in three. For $\alpha = 10$, for instance, we find $\varepsilon_p = 12.30$ for the 3D polaron, whereas the corresponding strong coupling value is $\alpha^2/3\pi = 10.61$, yielding a deviation somewhat close to 14%. The discrepancy for the 2D polaron, while still not negligible, is, however, not more than 3%. This is merely a consequence of the general trend that the electron–phonon interaction is inherently stronger in systems of lower dimensionality. For the 2D polaron, the theory therefore puts

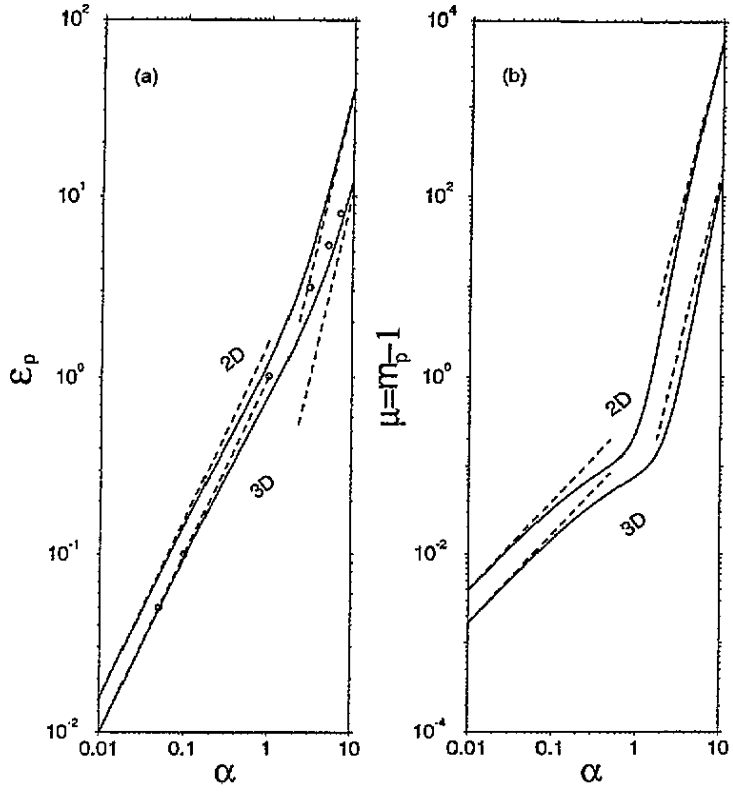

Figure 1. (*a*) The binding energy and (*b*) the phonon contribution to the effective mass as a function of α for the 3D and 2D polarons. The broken lines refer to the results of the strong coupling and second-order perturbation theories. The centred dots display the 3D results of the generalized path integral formalism of [9].

comparatively less weight on the role which the parameter λ plays in equation (34), thus adding somewhat more emphasis to the strong coupling counterpart of the problem.

A complementary remark in connection with the improvement achieved through the perturbative extension in the trial state (19) is that the theory gives very satisfying results in the strong coupling regime. For the 2D polaron for example, the bare strong coupling theory (under a Gaussian electron profile) gives $E_g = -(\pi/8)\alpha^2 = -0.3927\alpha^2$. The presumably exact upper bound for the ground-state energy has been obtained as $-0.4047\alpha^2$ by Wu *et al* [10], utilizing what they refer to as the modified Pekar-type *ansatz*:

$$\Phi_0 \sim (1 + br + a(br)^2 + c(br)^3 + d(br)^4)e^{-br}. \tag{44}$$

Even though the usage of such a four-parameter form for the electron wavefunction would have been more appropriate, in equation (19) we have chosen to use the approximate Gaussian form (via the set of operators b_μ and $b_\mu^\dagger$) to facilitate our calculations which would be very tedious otherwise. Yet, in spite of this simplification, we see that, for large but finite α, the trial state (19) yields far better results compared with those obtained from the expression $-(\pi/8)\alpha^2$. For $\alpha = 10$, for instance, the energy value we attain is -40.43, which is fairly close to the exact upper bound within 0.1%. Clearly, in the limit $\alpha \to \infty$,

the present results asymptotically tend to the usual approximate value $-(\pi/8)\alpha^2$ due to the *a priori* Gaussian type character embedded in our trial wavefunction.

In view of the results we have obtained, we see that the formulation we have considered is quite successful, in that the theory, starting from an *a priori* strongly coupled polaron state and generating fairly good results for large α, extrapolates towards the opposite extreme and yields the correct perturbation values within first-order α. We should, however, note that the theory is quite poor in characterizing the free polaron in the intermediate coupling regime (cf figure 1(*a*)). We feel that the drawback encountered here stems from the fact that, in arriving at equation (19), the variational parameter g_Q is introduced to replace the energy denominator $\Delta\varepsilon_{i-o}$ as averaged out over the intermediate state index i, thus containing only an average of the detailed content of the Fröhlich interaction interrelated to each of the intermediate states involved in the perturbation sum in equation (18).

With respect to the discontinuous phase-transition-like behaviour of the polaron (from the quasi-free to the self-trapped state), as suggested by a number of works in the literature (cf [11, 12], for instance), we should point out that no evidence in favour of such a phase transition has shown up in the present treatment of the polaron problem. To understand whether or not the polaron conforms from one phase to the other in an abrupt manner has always been a challenging and controversial aspect of the problem in both three and two dimensions. It has, however, been well established now that the qualitative changes in the polaron quantities do actually take place in a smooth and continuous way, and that any non-analytic behaviour encountered is an artefact of the approximating theory rather than an intrinsic property of the Fröhlich Hamiltonian [13, 14].

In summary, this work revises the free-polaron problem within the framework of the variational theory of Devreese *et al*, consisting of an adiabatic polaron wavefunction combined with a first-order perturbative extension, by means of which it is possible to interrelate the weak and strong coupling counterparts of the system in the overall range of the electron–phonon coupling strength. We see that the theory, besides yielding significantly improved energy upper bounds for strong phonon coupling, is well capable of extrapolating itself towards the weak coupling regime within leading-order perturbation calculations.

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