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Rapid Communications

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Upper bound to the polaron ground state in a magnetic field using the Feynman path-integral method

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It is shown that for sufficiently strong magnetic fields the Feynman path-integral method can give a ground-state energy lying below the exact ground-state energy of the two-dimensional polaron.

In an important paper,[1] henceforth denoted I, Peeters and Devreese employed the Feynman path-integral method to devise an algorithm for practical numerical calculations of the ground state (and free energy) of a polaron in magnetic fields of arbitrary strength. By minimizing the ground-state energy with respect to parameters characterizing their trial action, they found, remarkably, discontinuities in the ground-state polaron wave function which occurred at sufficiently large values of the dimensionless magnetic field λ^2 and of the Fröhlich coupling constant α, both in two[2] and three dimensions.[1] Peeters and Devreese recognized that a potential logical difficulty arises in justifying their minimization procedure for a polaron in a magnetic field since they were unable to prove that their ground-state energy (GSE) is an upper bound to the exact GSE. If, in fact, some of the minima of energy found in I were to lie below the exact energy, then it would seem difficult to attach any particular physical significance to such minima.

In this Rapid Communication we show that for two-dimensional polarons and for sufficiently strong magnetic fields, the GSE of I lies below the exact GSE and, in the weak-coupling limit, we give an upper bound to the magnetic field strength at which the GSE of I drops below the exact GSE.

The Hamiltonian H for a polaron moving in the x-y plane with a uniform magnetic field in the z direction, can be written

$$H_0=\left[p_x-\frac{\lambda^2}{4}y\right]^2+\left[p_y+\frac{\lambda^2}{4}x\right]^2 ,$$
$$H=H_0+\sum_{\mathbf{k}} b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}+\sum_{\mathbf{k}}\nu_k(e^{-i\mathbf{k}\cdot\boldsymbol{\rho}}b_{\mathbf{k}}^{\dagger}+e^{i\mathbf{k}\cdot\boldsymbol{\rho}}b_{\mathbf{k}}) , \quad (1)$$

where $\nu_k=(4\pi\alpha/\Omega)^{1/2}/k$, Ω is the volume of the crystal in which the LO phonons are confined, $b_{\mathbf{k}}^{\dagger}$ is the creation operator for an LO phonon of wave vector $\mathbf{k}$, $\lambda^2=\omega_c/\omega_{\mathrm{LO}}$, $\omega_c=eB/mc$ is the electron cyclotron frequency when $\alpha=0$, ω_{LO} is the LO-phonon frequency, and $\boldsymbol{\rho}$ is the electron displacement in the plane, $\boldsymbol{\rho}=(x,y)$. All lengths are in units of the polaron radius, $(\hbar/2m\omega_{\mathrm{LO}})^{1/2}$ and energies are in units of $\hbar\omega_{\mathrm{LO}}$.

In general, the GSE of H, E_G, has the form $E_G=E_G(\alpha,\lambda^2)$, but, for the very high fields defined by

$$\lambda^2 >> 1 \text{ and } \lambda^2 >> \alpha , \quad (2)$$

E_G becomes a function of the single dimensionless parameter[3] $\alpha\lambda$.

We begin by showing that the GSE as calculated in I never can be greater than the second-order perturbation-theory energy,[4] E_{UBF}, given by

$$E_{\mathrm{UBF}}=\tfrac{1}{2}\lambda^2-\frac{\pi\alpha}{2\lambda}\Gamma(1/\lambda^2)/\Gamma(1/\lambda^2+\tfrac{1}{2})$$
$$\underset{\lambda^2\to\infty}{\longrightarrow}\tfrac{1}{2}\lambda^2-\frac{\sqrt{\pi}}{2}\alpha\lambda . \quad (3)$$

We then present various cases in which the exact GSE is greater than E_{UBF}.

To demonstrate that E_{UBF} is an upper bound to the GSE of I we specialize the results of I to two dimensions by omitting all contributions to the energy from motion parallel to z, and then showing that E_{UBF} is the GSE, which results in I when the variational parameters $v_\perp$ and $w_\perp$ are set equal to zero. Our starting point is Eq. (60) of I, from which we omit terms proportional to s_0, $w_\parallel$, and $c_\parallel$; those terms arise from motion along z. The resulting equation is

$$E_{\mathrm{as}}=\tfrac{1}{2}\sum_{u=1}^{3}s_u-w_\perp+\frac{v_\perp^2-w_\perp^2}{4v_\perp}\sum_{j=1}^{3}\partial s_j/\partial v_\perp$$
$$-\frac{1}{\sqrt{2}}\int_0^\infty du\, e^{-u}\sum_{\mathbf{k}}\nu_k e^{-k_z^2D(u)}e^{-k_\perp^2D_H(u)} . \quad (4)$$

In writing Eq. (4) we have replaced the integral of Eq. (60) in I by the more general expression from which it originates. If we now omit the factor $e^{-k_z^2D(u)}$ and take the limit as both $v_\perp$ and $w_\perp$ vanish, we obtain, using Eqs. (58), (33), (49b), and (36) of I,

$$E_{\mathrm{as}}\to\frac{\lambda^2}{2}-\frac{\sqrt{\pi}}{2\sqrt{2}}\alpha\int_0^\infty\frac{du\,e^{-u}}{\left[(1/2\lambda^2)(1-e^{-\lambda^2u})\right]^{1/2}}=E_{\mathrm{UBF}} .$$

Next, consider the limit of the exact energy as $\lambda^2 \to \infty$, $\alpha\lambda \to \infty$, and the inequalities of (2) hold. Then only the lowest-lying ($n=0$) Landau levels contribute to leading order in λ^2, and the strong-coupling (SC) condition $\alpha\lambda \to \infty$ leads to a product wave function for the ground state of H. The $n=0$ eigenstates of H_0 have the form, omitting normalization,

$$\psi_M = (x-iy)^M e^{-\lambda^2\rho^2/8} , \tag{5}$$

where the z angular momentum quantum number M is 0 or a positive integer. For $M=0$ ψ_M is most strongly localized, and the trial function $\psi_0\Phi_L(0)$, where L denotes the lattice, produces a lower GSE than that of any other trial function $\psi_M\Phi_L(M)$ by an energy of order $\alpha\lambda$. The required GSE is easily found by taking the expectation value

$$\int \psi_0 H \psi_0 \Big/ \int \psi_0^2 = \lambda^2/2 + \sum_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \sum_{\mathbf{k}} \nu_k e^{-k_\perp^2/\lambda^2}(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}) ,$$

where $\mathbf{k}_\perp = (k_x, k_y, 0)$, and diagonalizing the lattice Hamiltonian in the usual way, leading to the GSE $E_{\rm SC}$, given by

$$E_{\rm SC} - \tfrac{1}{2}\lambda^2 = -\sum_{\mathbf{k}} \nu_k^2 e^{-2k_\perp^2/\lambda^2} = -\alpha \int_0^\infty dk\, e^{-2k_\perp^2/\lambda^2} = -\frac{\sqrt{\pi}}{2\sqrt{2}}\alpha\lambda . \tag{6}$$

[One can show that the leading correction to $E_{\rm SC}$ is of order $(\alpha\lambda)^0$. A variational estimate of this term gives -1.06, although the exact result is probably closer to -1.2.]

Comparison of $E_{\rm SC}$ with $\lim_{\lambda^2\to\infty} E_{\rm UBF}$ from (3) indicates that $E_{\rm SC}$ lies above $E_{\rm UBF}$.

In the opposite limit, $\lambda^2 \to \infty$, $\alpha\lambda \to 0$, the electron-phonon interaction can be treated as a perturbation using initial unperturbed states of the form

$$\psi_M|0\rangle ,$$

where $|0\rangle$ is the LO-phonon vacuum state. Carrying out the perturbation theory to fourth order gives, independent of M,

$$E_G \to E_{\rm UBF} + \frac{(\alpha\lambda)^2}{2}[\pi/4 - K(0.5)/\sqrt{8}] \cong E_{\rm UBF} + 0.064\,941\,9(\alpha\lambda)^2 , \tag{7}$$

where $K(z)$ is the complete elliptic function of the first kind, defined by

$$K(z) = \int_0^{\pi/2} d\theta (1 - z\sin^2\theta)^{-1/2} .$$

Variational calculations which interpolate between small and large $\alpha\lambda$ strongly indicate (but, admittedly, do not prove) that for all $\alpha\lambda$

$$\lim_{\lambda^2\to\infty} E_G > E_{\rm UBF} .$$

At what value of λ^2 does the exact GSE rise above $E_{\rm UBF}$ for given α? We have examined this question in the weak-coupling limit ($\alpha \ll 1$, $\alpha\lambda \ll 1$). By a novel method to be described elsewhere, we have succeeded in evaluating numerically the fourth-order perturbation correction to the ground-state energy of the two-dimensional polaron for arbitrary magnetic field strength. The results are shown in Fig. 1, where the fourth-order correction goes positive and hence the exact energy exceeds $E_{\rm UBF}$ at $\lambda^2 \sim 1.9$. Our calculation confirms the recently reported[5] correction of $-0.064\alpha^2$ at $\lambda^2 = 0$ and approaches $0.064\,941\,9(\alpha\lambda)^2$ as $\lambda^2 \to \infty$, in accord with Eq. (7). Since $E_{\rm UBF}$ exceeds the ground-state energy given by the algorithm of I, the actual value of λ^2 at which the GSE of I lies below the true energy is less than 1.9. We would expect that for stronger coupling the GSE of I crosses below the true energy at higher fields, but the methods employed here do not allow us to make reliable estimates for larger α values.

Details of the variational and perturbation calculations alluded to in this Rapid Communication will be discussed elsewhere.

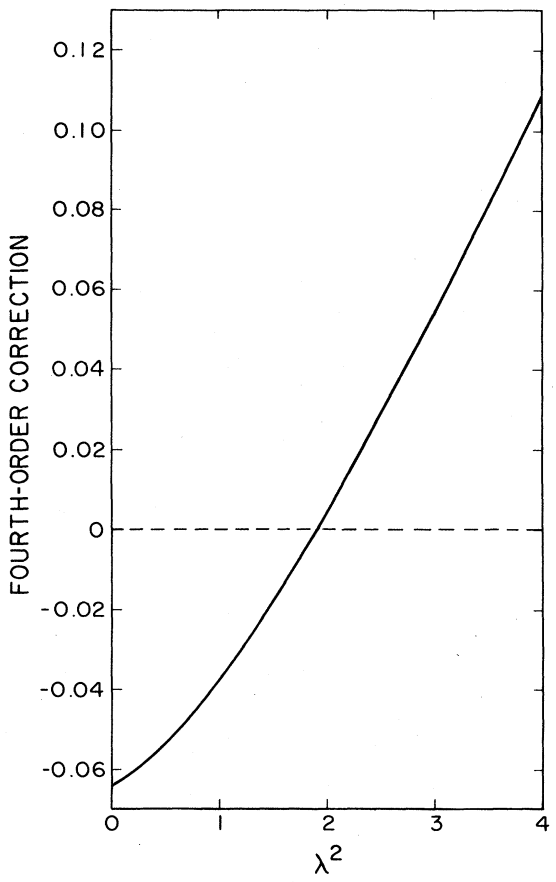

FIG. 1. The fourth-order Rayleigh-Schrödinger perturbation correction to the unperturbed energy of a two-dimensional polaron vs the dimensionless magnetic field strength λ^2. The fourth-order correction is plotted in units of $\alpha^2\hbar\omega_{\rm LO}$. The horizontal dashed line represents $E_{\rm UBF}$ [Eq. (3)] or, equivalently, the second-order perturbation correction.

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