Strong-coupling theory for the multidimensional free optical polaron

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A Landau-Pekar variational theory is employed to study the multidimensional free-optical-polaron problem in the strong-coupling regime. The ground-state energy, the effective mass, and the average number of virtual phonons around the electron are obtained in harmonic-oscillator and hydrogenic approximations. It is shown that no simple dimensional scaling relations exist in the hydrogenic approximation.

The multidimensional polaron problem introduced recently by Peeters, Wu, and Devreese[1] (PWD) has generated a great deal of interest. This problem is indeed interesting and holds promise because it serves as a model system for the study of the dimensional dependence of polaronic properties. Several investigations[2-7] have followed since the work of PWD and quantities such as the ground-state (g.s.) energy, the effective mass, the impedance function, the mobility, the average number of virtual phonons around the electron, etc., have been calculated by using different approximate methods. The general consensus is that the polaronic effects are more pronounced in lower dimensions.

In a recent paper[7] we have investigated the multidimensional free-optical-polaron problem in the intermediate-coupling regime by generalizing the Lee-Low-Pines (LLP) canonical transformation method[8] to N dimensions. In the present paper we study the same model problem in the strong-coupling regime. The g.s. energy, the effective mass, and the average number of virtual phonons around the electron in the g.s. are calculated by a variational method in which the phonons are described classically by the coherent state and for the electronic part two trial functions are used, namely, the Gaussian function and the hydrogenic 1s wave function. It turns out that the harmonic oscillator approximation provides a better description for the electron motion. In both cases, however, the polaronic effects appear to diminish with increasing dimensionality. As expected, our harmonic oscillator approximation results for the g.s. energy and the effective mass do follow from the corresponding PWD expressions in the limit $\alpha\rightarrow\infty$. Consequently, the resulting PWD scaling relations for these quantities are obtained. We explicitly show that the strong-coupling expression for the average number of virtual phonons around the electron in the g.s. also satisfies a similar scaling relation in this approximation. (In Ref. 7 the same scaling relation was obtained in the intermediate coupling LLP approximation.) In the hydrogenic approximation, however, the PWD scaling relations are not satisfied by any of the three quantities we have considered.

The multidimensional free-optical polaron may be described by the Fröhlich Hamiltonian[9] generalized to N dimensions (ND):

$$H=-\tfrac{1}{2}\nabla_{\mathbf{r}}^2+\sum_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}}+\sum_{\mathbf{q}}(\xi_{\mathbf{q}}e^{-i\mathbf{q}\cdot\mathbf{r}}b_{\mathbf{q}}^\dagger+\text{H.c.})\ . \tag{1}$$

Here all the vectors are N dimensional and units have been chosen such that $\hbar=m=\omega=1$, m being the Bloch effective mass of the electron and ω the optical-phonon frequency which is assumed to be dispersionless. Following the prescription of PWD the electron-phonon interaction coefficient $\xi_{\mathbf{q}}$ may be written as

$$q=i\left[\frac{\Gamma((N-1)/2)2^{N-3/2}\pi^{(N-1)/2}}{Vq^{N-1}}\alpha\right]^{1/2}, \tag{2}$$

where V is the volume of the N-dimensional polar crystal and α is the dimensionless electron-phonon coupling constant.

We now choose for the trial wave function for the Hamiltonian (1) the Landau-Pekar ansatz

$$|\Psi\rangle=|\Phi(\mathbf{r})\rangle\exp\left[\sum_{\mathbf{q}}(f_{\mathbf{q}}b_{\mathbf{q}}^\dagger-f_{\mathbf{q}}^*b_{\mathbf{q}})\right]|0\rangle\ , \tag{3}$$

where $f_{\mathbf{q}}$ will be treated as a variational function, $|0\rangle$ is the unperturbed zero phonon state satisfying $b_{\mathbf{q}}|0\rangle=0$ for all $\mathbf{q}$, and $\Phi(\mathbf{r})$ is some electronic function to be specified later and extremize the quantity[10]

$$J=\langle\Psi|H-\mathbf{u}\cdot\hat{\mathbf{P}}|\Psi\rangle=\langle\Phi(\mathbf{r})|(-\tfrac{1}{2}\nabla_{\mathbf{r}}^2)|\Phi(\mathbf{r})\rangle+\sum_{\mathbf{q}}|f_{\mathbf{q}}|^2+\sum_{\mathbf{q}}(\xi_{\mathbf{q}}f_{\mathbf{q}}^*\rho_{\mathbf{q}}^*+\text{H.c.})-\mathbf{u}\cdot\langle\Phi(\mathbf{r})|-i\nabla_{\mathbf{r}}|\Phi(\mathbf{r})\rangle-\mathbf{u}\cdot\sum_{\mathbf{q}}\mathbf{q}|f_{\mathbf{q}}|^2\ , \tag{4}$$

where $\hat{\mathbf{P}}=\hat{\mathbf{p}}+\sum_{\mathbf{q}}\mathbf{q}b_{\mathbf{q}}^\dagger b_{\mathbf{q}}$ is the total momentum operator, $\hat{\mathbf{p}}$ standing for the electron momentum, $\mathbf{u}$ is the Lagrange multiplier which may be identified as the polaron velocity,[10] and

$$\rho_{\mathbf{q}}=\langle\Phi(r)|e^{i\mathbf{q}\cdot\mathbf{r}}|\Phi(\mathbf{r})\rangle\ . \tag{5}$$

Variation of (4) with respect to $f_{\mathbf{q}}^*$ now yields

$$f_{\mathbf{q}}=-\xi_{\mathbf{q}}\rho_{\mathbf{q}}^*/(1-\mathbf{u}\cdot\mathbf{q})\ , \tag{6}$$

so that (4) becomes

$$J=\langle\Phi(\mathbf{r})|(-\tfrac{1}{2}\nabla_r^2)|\Phi(\mathbf{r})\rangle-\sum_{\mathbf{q}}\frac{|\xi_{\mathbf{q}}|^2|\rho_{\mathbf{q}}|^2}{(1-\mathbf{u}\cdot\mathbf{q})}-\mathbf{u}\cdot\langle\Phi(\mathbf{r})|(-i\nabla_r)|\Phi(\mathbf{r})\rangle\ . \qquad (7)$$

To make further progress we have to choose $\Phi(\mathbf{r})$ for which we take two trial functions. Let us first choose

$$\Phi_{\rm HO}^{\rm ND}(\mathbf{r})=\frac{\lambda^{N/2}}{\pi^{N/4}}e^{-\lambda^2r^2/2}e^{i\mathbf{p}_0\cdot\mathbf{r}}\ , \qquad (8)$$

where λ and $\mathbf{p}_0$ are variational parameters. Equation (7) now reduces to

$$J=\tfrac{1}{2}p_0^2-\mathbf{u}\cdot\mathbf{p}_0+\frac{N}{4}\lambda^2-\frac{\alpha\lambda\Gamma((N-1)/2)}{2\Gamma(N/2)}\left[1+\frac{u^2\lambda^2}{N}\right]\ , \qquad (9)$$

where terms up to quadratic in $\mathbf{u}$ have been retained. Variations with respect to $\mathbf{p}_0$ and λ give

$$p_0=u\ , \qquad (10)$$

$$\lambda\approx\frac{\alpha\Gamma((N-1)/2)}{N\Gamma(N/2)}\left[1+\frac{3\alpha^2}{N^3}\left[\frac{\Gamma((N-1)/2)}{\Gamma(N/2)}\right]^2u^2\right]\ , \qquad (11)$$

and therefore the variational energy takes on the following expression:

$$E_{\rm HO}^{\rm ND}=\langle\Psi|H|\Psi\rangle=-\frac{\alpha^2}{4N}\left[\frac{\Gamma((N-1)/2)}{\Gamma(N/2)}\right]^2+\tfrac{1}{2}u^2\left[1+\left[\frac{\alpha}{N}\frac{\Gamma((N-1)/2)}{\Gamma(N/2)}\right]^4\right]\ , \qquad (12)$$

and the expectation value of the total momentum operator becomes (where av denotes average)

$$\mathbf{P}_{\rm av,HO}^{\rm ND}=\langle\Psi|\hat{P}|\Psi\rangle=\mathbf{u}\left[1+\frac{\alpha^4}{N^4}\left[\frac{\Gamma((N-1)/2)}{\Gamma(N/2)}\right]^4\right]\ . \qquad (13)$$

Thus the g.s. energy and the effective mass of an N-dimensional polaron are given in the harmonic oscillator approximation by

$$E_{\rm g.s.,HO}^{\rm ND}=-\frac{\alpha^2}{4N}\left[\frac{\Gamma((N-1)/2)}{\Gamma(N/2)}\right]^2\ , \qquad (14)$$

$$m_{\rm HO}^{\rm ND*}=\frac{\alpha^4}{N^4}[\Gamma((N-1)/2)/\Gamma(N/2)]^4\ , \qquad (15)$$

which follow immediately from the $\alpha\to\infty$ limits of the general expressions obtained by PWD and Peeter and Devreese.[5] We can also calculate the average number of virtual phonons around the electron in the g.s. which is given by

$$\mathcal{N}^{\rm ND}=\langle\Psi|b_{\mathbf{q}}^\dagger b_{\mathbf{q}}|\Psi\rangle=\sum_{\mathbf{q}}|f_{\mathbf{q}}|^2\ . \qquad (16)$$

In the harmonic oscillator approximation we get

$$\mathcal{N}_{\rm g.s.,HO}^{\rm ND}=\frac{\alpha^2}{2N}\left[\frac{\Gamma((N-1)/2)}{\Gamma(N/2)}\right]^2\ . \qquad (17)$$

Though (17) can be shown to follow from (14) and (15) it has not been reported earlier, to our knowledge, in its explicit form. It is apparent from (14), (15), and (17) that polaronic effects diminish with increasing dimensionality and for $N=3$ we get back the Landau-Pekar results with the Gaussian function. Comparison of (14), (15), and (17) with the corresponding three-dimensional (3D) expressions leads to the PWD scaling relations

$$E_{\rm g.s.,HO}^{\rm ND}=\frac{N}{3}E_{\rm HO}^{\rm 3D}\left[\frac{\Gamma((N-1)/2)}{\Gamma(N/2)}\frac{3\sqrt{\pi}}{2N}\alpha\right]\ , \qquad (18)$$

$$m_{\rm HO}^{\rm ND*}=\frac{N}{3}m_{\rm HO}^{\rm 3D*}\left[\frac{\Gamma((N-1)/2)}{\Gamma(N/2)}\frac{3\sqrt{\pi}}{2N}\alpha\right]\ . \qquad (19)$$

Also for the average number of virtual phonons in the cloud around the electron in the g.s. there exists a similar scalar relation

$$\mathcal{N}_{\rm g.s.,HO}^{\rm ND}=\frac{N}{3}\mathcal{N}_{\rm HO}^{\rm 3D}\left[\frac{\Gamma((N-1)/2)}{\Gamma(N/2)}\frac{3\sqrt{\pi}}{2N}\alpha\right]\ . \qquad (20)$$

For the electronic function we next take the ND Coulomb g.s. wave function

$$\Phi_C^{\rm ND}(\mathbf{r})=2^{N-1/2}\left[\frac{\gamma}{\sqrt{\pi}(N-1)}\right]^{N/2}\left[\frac{\Gamma(N/2)}{\Gamma(N)}\right]^{1/2}\times e^{-[(2\gamma/N-1)r]}e^{i\mathbf{p}_0\cdot\mathbf{r}} \qquad (21)$$

with γ and $\mathbf{p}_0$ as the variational parameters. The results are

$$E_{{\rm g.s.},C}^{\rm ND}=-\frac{\alpha^2}{4}\left[\frac{\Gamma((N-1)/2)\Gamma(N+\frac{1}{2})}{\Gamma(N/2)\Gamma(N+1)}\right]^2\ , \qquad (22)$$

$$m_C^{\rm ND*}=\frac{\alpha^4}{N(N-\frac{1}{2})}\left[\frac{\Gamma(N+\frac{1}{2})\Gamma((N-1)/2)}{\Gamma(N/2)\Gamma(N+1)}\right]^4\ , \qquad (23)$$

$$N_{C,{\rm g.s.}}^{\rm ND}=\frac{\alpha^2}{2}\left[\frac{\Gamma((N-1)/2)\Gamma(N+\frac{1}{2})}{\Gamma(N/2)\Gamma(N+1)}\right]^2\ , \qquad (24)$$

which again show that the polaronic effects become weaker in higher dimensions. But now we do not have any simple scaling relations like (18)–(20). Thus, as has been rightly pointed out by Peeters and Devreese,[5] the existence of the scaling relations depends crucially on the approximation one invokes.

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