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A new variational calculation for N-dimensional polarons in the strong-coupling limit

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Abstract. A novel variational approach is presented for the calculation of the ground-state energy of the polaron in arbitrary N dimensions in the strong-coupling limit. By using the phonon coherent state to represent the wavefunction of phonons, a self-consistent integro-differential equation for the electron wavefunction is derived. The calculated results of the ground-state energy for $N = 1$, 2 and 3 agree well with the best results in the literature. It is also found that, for arbitrary N, the present results are less than the Feynman path integral ones by small percentages. It is proposed that this approach should be universal for systems involving polarons in the strong-coupling regime.

1. Introduction

The problem of arbitrary N-dimensional polarons has attracted much attention (an incomplete list of studies is given in [1–6]) since the pioneering work by Peeters *et al* [1]. It is indeed interesting and holds promise. In recent years, polaron effects have been observed in low-dimensional systems [7], some physical problems have been mapped in two-dimensional polarons [8] and it has been technologically possible to confine the electrons in one direction [9] (quantum wires) and in two directions [10] (such as GaAs–$Al_xGa_{1-x}As$ heterostructures).

On the other hand, the stability problem of a two-polaron bound state (bipolaron) has become of interest since the mechanism of bipolaron Bose–Einstein condensation was proposed by Emin [11] to explain high-temperature superconductivity (HTSC). In fact, the HTSC materials are not restricted to three dimensions only and bipolarons are known to exist in the strong-coupling regime [12, 13]. Therefore, it is important to investigate the single polaron in arbitrary N dimensions in the strong-coupling limit.

The main purpose of this paper is to present a new variational approach for calculations of the ground-state energy of N-dimensional polarons in the strong-coupling limit. We select the wavefunction of the phonon part to be the coherent state form and derive a self-consistent integro-differential equation satisfied by the electron wavefunction. Furthermore, we obtain the ground-state energy by solving this equation numerically, rather than by choosing any trial electron wavefunctions. We also compare our results with those available in the literature.

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2. Integro-differential equations

We start with the Hamiltonian of polarons in N dimensions derived by Peeters *et al* [1] (in units of $2m = \hbar = \omega_0 = 1$)

$$H = \boldsymbol{p}^2 + \sum_{\boldsymbol{k}} a_{\boldsymbol{k}}^{\dagger} a_{\boldsymbol{k}} + \sum_{\boldsymbol{k}} v_{\boldsymbol{k}} \left(a_{\boldsymbol{k}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + a_{\boldsymbol{k}}^{\dagger} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} \right) \tag{1}$$

where all vectors are N dimensional, $\boldsymbol{r}$ and $\boldsymbol{p}$ are the position and the momentum operators of the electron, $a_{\boldsymbol{k}}^{\dagger}$ and $a_{\boldsymbol{k}}$ are respectively the creation and annihilation operators of the LO phonons with the wavevector $\boldsymbol{k}$ and

$$v_{\boldsymbol{k}}^2 = \frac{\Gamma\left(\frac{N-1}{2}\right) 2^{N-1} \pi^{(N-1)/2} \alpha}{v_N \boldsymbol{k}^{N-1}} \tag{2}$$

with v_N being the N-dimensional crystal volume and α being the electron–phonon coupling constant.

The solution to this Hamiltonian is assumed to take the following form:

$$|\ldots\rangle = \varphi(\boldsymbol{r})|A\rangle \tag{3}$$

where $\varphi(\boldsymbol{r})$ is the electron wavefunction to be determined and $|A\rangle$ is the coherent state

$$|A\rangle = \exp\left(\sum_{k} \left[\alpha(\boldsymbol{k}) a_{\boldsymbol{k}}^{\dagger} - \alpha^*(\boldsymbol{k}) a_{\boldsymbol{k}} \right] \right) |0\rangle. \tag{4}$$

Here $\alpha(\boldsymbol{k})$ will be treated as a variational function, $|0\rangle$ is the unperturbed zero-phonon state satisfying $a_{\boldsymbol{k}}|0\rangle = 0$ for all $\boldsymbol{k}$.

It should be mentioned that equations (3) and (4) have also been employed to deal with N-dimensional polarons in the strong-coupling regime by Chatterjee [5]. For further progress, he chose two trial wavefunctions, namely, the Gaussian function and the hydrogenic 1s wavefunction, for the electronic part. However, in this paper it is unnecessary to use any trial electron wavefunction, as will be shown below.

For the next step, averaging the Hamiltonian (1) over the wavefunction (3), we have the following energy expectation:

$$E = \left\langle P^2 \right\rangle + \sum_{\boldsymbol{k}} \alpha^*(\boldsymbol{k}) \alpha(\boldsymbol{k}) + \sum_{\boldsymbol{k}} v_{\boldsymbol{k}} [\alpha(\boldsymbol{k}) \langle \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) \rangle + \alpha^*(\boldsymbol{k}) \langle \exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) \rangle] \tag{5}$$

where $\langle \ldots \rangle$ denotes averaging over the wavefunction $\varphi(\boldsymbol{r})$. Minimizing the energy expectation with respect to $\alpha(\boldsymbol{k})$ and $\alpha^*(\boldsymbol{k})$ results in

$$\alpha(\boldsymbol{k}) = -v_{\boldsymbol{k}} \langle \exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) \rangle \tag{6}$$

$$\alpha^*(\boldsymbol{k}) = -v_{\boldsymbol{k}} \langle \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) \rangle. \tag{7}$$

It is easily found that $\alpha(\boldsymbol{k}) = \alpha^*(\boldsymbol{k})$, both depending on the modulus of the vector $\boldsymbol{k}$ only. In the averaging, the volume element in N-dimensional $\boldsymbol{r}$-space can be reduced to

$$\mathrm{d}\boldsymbol{r} = \frac{2\pi^{\frac{N-1}{2}}}{\Gamma\left(\frac{N-1}{2}\right)} r^{N-1} \mathrm{d}r \sin^{N-2}\theta \, \mathrm{d}\theta \tag{8}$$

where θ is the angle between $\boldsymbol{k}$ and $\boldsymbol{r}$. So $\alpha(\boldsymbol{k})$ can be expressed as

$$\alpha(\boldsymbol{k}) = -v_{\boldsymbol{k}} \frac{(2\pi)^{\frac{N}{2}}}{k^{\frac{N}{2}-1}} \int J_{\frac{N}{2}-1} r^{\frac{N}{2}} \varphi(r)^2 \, \mathrm{d}r \tag{9}$$

where $J_m(x)$ is the mth-order Bessel function.

Eliminating the phonon coordinates by averaging the Hamiltonian (1) over the phonon coherent state $|A\rangle$, we derive the following effective Hamiltonian in the representation of the electron coordinate:

$$H_{eff} = -\nabla^2 + \sum_{\boldsymbol{k}} \alpha^*(\boldsymbol{k})\alpha(\boldsymbol{k}) + \sum_{\boldsymbol{k}} v_k[\alpha(\boldsymbol{k}) \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) + \alpha^*(\boldsymbol{k}) \exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})]. \tag{10}$$

It is of some interest to note from equation (9) that the effective Hamiltonian (10) contains the wavefunction of the electron $\varphi(r)$. Substituting equation (9) into equation (10), transforming the summation $\sum_{\boldsymbol{k}}$ into an integral $v_N/(2\pi)^N \int \mathrm{d}\boldsymbol{k}$, integrating over all angles analytically, followed by using the variable transformation $\varphi(r) = \alpha^{\frac{N}{2}}\psi(\alpha r)$, $x = \alpha r$ and $E = E_0\alpha^2$, the Schrödinger equation for the reduced electron wavefunction $\psi(x)$ is finally obtained as follows:

$$\begin{aligned} E_0\psi(x) = &-\frac{1}{x^{N-1}}\frac{\mathrm{d}}{\mathrm{d}x}\left(x^{N-1}\frac{\mathrm{d}}{\mathrm{d}x}\psi(x)\right) + \left\{\frac{8\pi^N}{[\Gamma(\frac{N}{2})]^2}\right. \\ &\times \int_0^\infty \mathrm{d}x_1\,\psi^2(x_1)x_1^{N-2}\int_0^{x_1}\mathrm{d}x_2\,\psi^2(x_2)x_2^{N-1}F\left(\frac{1}{2},\ \frac{3-N}{2};\ \frac{N}{2};\ \left(\frac{x_2}{x_1}\right)^2\right) \\ &-\frac{4\pi^{\frac{N}{2}}}{\Gamma(\frac{N}{2})}\left[\int_0^x \mathrm{d}x_1\,\psi^2(x_1)\frac{x_1^{N-1}}{x}F\left(\frac{1}{2},\ \frac{3-N}{2};\ \frac{N}{2};\ \left(\frac{x_1}{x}\right)^2\right)\right. \\ &\left.\left.+\int_x^\infty \mathrm{d}x_1\,\psi^2(x_1)x_1^{N-2}F\left(\frac{1}{2},\ \frac{3-N}{2};\ \frac{N}{2};\ \left(\frac{x}{x_1}\right)^2\right)\right]\right\}\psi(x) \end{aligned} \tag{11}$$

where $F(a,\ b;\ c;\ z)$ is the hypergeometric function and use has been made of the following definite integral of special functions:

$$\int_0^\infty \frac{J_m(\mu t)J_m(\nu t)}{t^{2m}}\,\mathrm{d}t = \frac{\mu^m\nu^{m-1}\sqrt{\pi}}{4^m\Gamma(\frac{2m+1}{2})\Gamma(m+1)}F\left(\frac{1}{2},\ \frac{1-2m}{2};\ m+1;\ \left(\frac{\mu}{\nu}\right)^2\right) \tag{12}$$

which is valid for $\mathrm{Re}(2m) > -1$ and $0 < \mu < \nu$.

Note that this self-consistent integro-differential equation is independent of α. Based on the transformation $E = E_0\alpha^2$, it is found that the ground-state energy of the N-dimensional polaron in the strong-coupling limit is proportional to α^2.

3. Numerical results and discussion

It is possible to solve equation (11) numerically and to obtain the electron wavefunction and the polaron ground-state energy for arbitrary N-dimensional polarons except the one-dimensional polaron. A brief description of the numerical procedures is needed here. First, choosing an initial wavefunction, say, the trial wavefunction in the literature, and inserting it into the curly brackets $\{\ldots\}$ in the second term on the right-hand side of equation (11), the numerical problem is then reduced to the standard two-point boundary value problem with the boundary condition $\psi'(0) = 0$ and $\psi(\infty) = 0$. For each iteration, we can get a new solution for the wavefunction by the shooting method. Generally, it is not the true solution to the Schrödinger equation (11), because it is different from that in curly brackets. However, it is predicted that after sufficient time iterations the obtained solution can be brought into excellent agreement with the true ones. If the electron wavefunction is actually found, the polaron ground-state energy can be obtained simultaneously. In the following calculations, on the basis of extensive tests, we believe that the polaron ground-state energies are accurate for the given digits.

For one-dimensional polarons, all polaron characteristics diverge due to the Coulomb nature of this problem. However, upon introducing

$$\alpha' = \frac{\sqrt{\pi}}{2}\frac{\Gamma(\frac{N-1}{2})}{\Gamma(\frac{N}{2})}\alpha \tag{13}$$

by using α' instead of α, we can get the finite polaron ground-state energy for finite α' in one-dimensional polarons with the same approach. Equation (13) has been used to treat one-dimensional polarons in [14, 15].

After tedious calculations, the numerical results for the ground-state energies for $N = 1$, 2 and 3 are obtained as follows:

$$E^{1D} = -0.333\,12\alpha'^2 \tag{14}$$

$$E^{2D} = -0.404\,74\alpha^2 \tag{15}$$

$$E^{3D} = -0.108\,51\alpha^2. \tag{16}$$

For comparison, in tables 1–3, we list the present results with the known results of the ground-state energies of one-, two- and three-dimensional polarons in the strong-coupling limit. It is interesting to note that the present results are in good agreement with the former best results, which are $-0.333\,088\alpha'^2$ for one-dimensional polarons by Peeters *et al* [14], $-0.4047\alpha^2$ for two-dimensional polarons by Wu Xiaoguang *et al* [17] and $-0.108\,513\alpha^2$ for three-dimensional polarons by Miyake [20]. It should be recalled from [14, 17] that the authors obtained the best results for the one- and two-dimensional polaron ground-state energies by selecting an improved Pekar wavefunction into which far more variational parameters and higher-order terms in r are incorporated. However, in this paper, we obtain the energy and the electron wavefunction by numerically solving the derived self-consistent integro-differential equation, rather than by selecting a trial one. In principle, if the equation is actually solved, the present results are no larger than their results. Fortunately, it is to be noted that our results are really less than their results by very small percentages. It follows that we have indeed developed a good variational approach for N-dimensional polarons in the strong-coupling limit.

Table 1. The comparison of some results for the ground-state energies of one-dimensional polarons in the strong-coupling limit.

Authors	E^{1D}/α'^2
Peeters *et al* [14]	$-0.333\,088$
Degani *et al* [16]	$-1/\pi$
Smondyrev [3]	$-0.346\,233$
Present	$-0.333\,12$

We will also compare the present results with the elegant Feynman path-integral ones. It is useful to list the general formalism for the calculation of the N-dimensional polaron ground-state energy [1] in the Feynman path integral *ansatz*:

$$E = \frac{N}{4}\frac{(v-w)^2}{v} - \frac{\Gamma(\frac{N-1}{2})}{\Gamma(\frac{N}{2})}\frac{\alpha v}{2}\int_0^\infty \mathrm{d}s\,\frac{\mathrm{e}^{-s}}{f(s)^{\frac{1}{2}}} \tag{17}$$

$$f(s) = \frac{v^2-w^2}{v}\left(1-\mathrm{e}^{-vs}\right) + w^2 s \tag{18}$$

Table 2. The comparison of some results for the ground-state energies of two-dimensional polarons in the strong-coupling limit.

Authors	E^{2D}/α^2
Wu Xiaoguang *et al* [17]	−0.404 7
Das Sarma *et al* [18]	−0.392 699
Feynman's theory [17]	−0.392 699
Hipolito [19]	−0.392 699
Smondyrev [3]	−0.409 9
Ganbold *et al* [6]	−0.400 538
Present	−0.404 74

Table 3. The comparison of some results for the ground-state energies of three-dimensional polarons in the strong-coupling limit.

Authors	E^{3D}/α^2
Miyake [20]	−0.108 513
Schultz [21]	−0.106 1
Pekar (quoted by Miyake [20])	−0.108 504
Luttinger *et al* [22]	−0.106 6
Marshall *et al* [23]	−0.107 8
Seng *et al* [24]	−0.106 5
Smondyrev [3]	−0.109 206
Adamowski *et al* [25]	−0.108 512 8
Feranchuk *et al* [26]	−0.107 8
Efimov *et al* [27]	−0.108 43
Ganbold *et al* [6]	−0.107 766
Present	−0.108 51

where v and w are variational parameters which are determined by minimizing the energy (17). By expansion of equation (17) for large α, we obtain the N-dimensional polaron ground-state energy in the strong-coupling limit

$$E_F = -\frac{1}{4N}\left(\frac{\Gamma(\frac{N-1}{2})}{\Gamma(\frac{N}{2})}\alpha\right)^2. \tag{19}$$

Note that, for the one-dimensional polaron, the energy diverges. However, with the help of equation (13), we have $E_F^{1D} = -(1/\pi)\alpha'^2$.

In figure 1, we plot the relative difference between our results and the Feynman ones for the polaron ground-state energy $(E - E_F)/E_F$, which is independent of α (or α'), as a function of the dimension N. It is shown that our variational approach supplies a lower ground-state energy of the N-dimensional polaron than does the Feynman approach in the strong-coupling limit, which again emphasizes the effectiveness of our approach in polaron physics. It is also interesting to note that, as the dimension increases, our results become closer and closer to the Feynman ones. It is well known that polaron effects are weakened with increases in the dimension. So it is natural that the larger the value of the dimension N the better the Feynman path-integral approximation.

Finally, we would like to point out that the present approach is universal for the problems involving polarons in the strong-coupling regime. It is possible to map the Hamiltonian of such systems as strongly coupled bound polarons, polarons in a quantum well, bipolarons

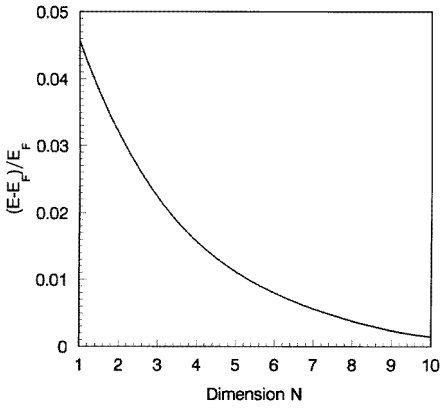

Figure 1. The relative difference between the present and the Feynman polaron ground-state energy in the strong-coupling limit as a function of the dimension N.

and excitonic polarons into the following more general form:

$$H = \frac{\boldsymbol{p}^2}{2\boldsymbol{m}} + V(\boldsymbol{r}) + \sum_{\boldsymbol{k}} \omega_{\boldsymbol{k}} a_{\boldsymbol{k}}^{\dagger} a_{\boldsymbol{k}} + \sum_{\boldsymbol{k}} \left[F_{\boldsymbol{k}}(\boldsymbol{r}) a_{\boldsymbol{k}} \, \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + F_{\boldsymbol{k}}^{*}(\boldsymbol{r}) a_{\boldsymbol{k}}^{\dagger} \, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} \right]. \quad (20)$$

By means of equation (3), we can eliminate the phonon degrees of freedom and get an effective Hamiltonian including the wavefunction of the electron. Then the wavefunction can be numerically calculated and the energy of the system can be obtained. The key difference between our approach and some other variational ones is that we need not select any trial variational wavefunction. Therefore, the artificial errors can be removed and only the intrinsic errors of the approach itself are left. By the way, this approach has been applied successfully to bipolarons [13] and excitonic polarons [28] by us.

4. Conclusions

We have presented a new variational approach to the calculation of the ground-state energy of N-dimensional polarons in the strong-coupling limit. The calculated results are as good as the best ones in the literature, if not better. It is also shown that this proposed approach is a universal one in problems involving polarons in the strong-coupling regime. Applications and extensions to other systems are in progress.

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