Two- and three-dimensional polarons with extended coherent states

Chen Qinghu
*Chinese Center of Advanced Science and Technology (World Laboratory), P.O. Box 8730, Bejing 100080, People's Republic of China and Department of Physics, Zhejiang University, Hangzhou, Zhejiang 310027, People's Republic of China**

Fang Minghu and Zhang Qirui
Department of Physics, Zhejiang University, Hangzhou, Zhejiang 310027, People's Republic of China

Wang Kelin and Wan Shaolong
Centre for Fundamental Physics, University of Science and Technology of China, Hefei, Anhui 230026, People's Republic of China
(Received 11 August 1995; revised manuscript received 26 December 1995)

The properties of two- and three-dimensional polarons are investigated with the use of extended coherent states. In the weak-coupling limit, the obtained expansions for the ground-state energy and effective mass to the second order in the coupling constant α are the same as the previous exact ones. Moreover, in the intermediate-coupling regime, the numerical results for the ground-state energy and effective mass agree with the results by the Feynman path-integral method, and perhaps closer to the exact results than the Feynman ones. It is suggested that the present approach should be an effective one in polaron physics.

The arbitrary N-dimensional (ND) polaron has been a subject of interest (an incomplete list is given by Refs. 1–10) since the pioneering work by Peeters *et al.*[1] Physically, it is indeed interesting for $N \leqslant 3$, because polaron effects have been observed in low-dimensional systems,[11] certain physical problems have been mapped into a two-dimensional (2D) polaron one,[12] and it has been technologically possible to grow structures in which the electrons are localized in two directions. However, the meaning of the formal extension to higher than three dimensions (3D) is obscure. Therefore it is important to study 2D and 3D polarons.

Recently, a two-polaron bound state (bipolaron) has attracted much attention after the mechanism of the bipolaron Bose-Einstein condensation to explain the high-temperature superconductivity (HTS) was put forward by Emin.[13] It is known that HTS's materials are quasi-two-dimensional, so the bipolaron in 2D should be studied. It is necessary to know the single polaron in 2D for understanding the stability problem of the 2D bipolarons.

In a recent paper,[14] we have proposed a concise approach for calculating the ground-state energy of 3D polarons by means of extended coherent states. The calculated results are in good agreement with the exact Monte Carlo ones.[15] The purpose of this paper is to extend the same method to the calculation of both the ground-state energy and the effective mass of 2D and 3D polarons. Consequently, we derive self-consistent equations by which the energy of a slowly moving polaron can be calculated. Moreover, we analytically calculate the ground-state energy and the effective mass expansions up to the α^2 term in the weak-coupling limit. Alternatively, by solving the self-consistent equation numerically, we calculate the ground-state energy and the effective mass in the intermediate-coupling regime. We also compare our method with the well known ones in the literature.

In order to study the 2D and 3D polaron in a unified way, we begin with the Hamiltonian of arbitrary ND polarons derived by Peeters *et al.*,[1] where the interaction between the electron and the lattice polarization is assumed to be Coulomb-like $(1/r)$ (in units of $2m=\hbar=\omega_0=1$)

$$H=p^2+\sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}+\sum_{\mathbf{k}} v_{\mathbf{k}}(a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}+a_{\mathbf{k}}^\dagger e^{-i\mathbf{k}\cdot\mathbf{r}}), \qquad (1)$$

where all vectors are in ND, $\mathbf{r}$ and $\mathbf{p}$ are the position and the momentum operators of the electron, $a_{\mathbf{k}}^\dagger$ and $a_{\mathbf{k}}$ are respectively the creation and annihilation operators of the LO phonons with the wave vector $\mathbf{k}$,

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

here ν_N is the ND crystal volume and α is the electron-phonon coupling constant.

As usual, applying the canonical transformation of Lee, Low, and Pines (LLP) (Ref. 16) to the Hamiltonian (1) leads to

$$H=\left(Q-\sum_{\mathbf{k}} \mathbf{k}a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\right)^2+\sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}+\sum_{\mathbf{k}} v_{\mathbf{k}}(a_{\mathbf{k}}^\dagger+a_{\mathbf{k}}), \quad (3)$$

where $\mathbf{Q}$ is the total momentum of the polaron. It should be kept in mind that the momentum Q remains throughout this paper, so that both the ground-state energy and the effective mass can be evaluated simultaneously.

To solve the Hamiltonian (1) with a high accuracy, we will follow our previous approach as fully discussed in Ref. 14. In this paper, it is straightforward to take the phonon wave function as the following extended coherent state form:

$$|\rangle=|\rangle_0+\sum_{\mathbf{k}_1,\mathbf{k}_2} b(\mathbf{k}_1,\mathbf{k}_2)a_{\mathbf{k}_1}^\dagger a_{\mathbf{k}_2}^\dagger|\rangle_0, \qquad (4)$$

where $|\rangle_0$ is the coherent state

$$|\rangle_0=\prod_{\mathbf{q}'} e^{f(\mathbf{q}')a^\dagger_{\mathbf{q}'}}|0\rangle,\quad a_{\mathbf{q}}|\rangle_0=f(q)|\rangle_0, \tag{5}$$

and $b(\mathbf{k}_1,\mathbf{k}_2)$ is the interchanging symmetrical function of $\mathbf{k}_1$ and $\mathbf{k}_2$ to be determined. The physics behind Eq. (4) hints that correlation between wave vectors of pairs of emitted phonons in the field are under consideration.

Inserting Eq. (4) into the Schrödinger equation $H|\rangle=E|\rangle$, neglecting $(a^\dagger)^3|\rangle_0$ and $(a^\dagger)^4|\rangle_0$ terms, and equating the coefficients of the terms of $|\rangle_0$, $(a^\dagger)|\rangle_0$, and $(a^\dagger)^2|\rangle_0$ on both sides of the Schrödinger equation, we have the following three coupled equations:

$$E=\mathbf{Q}^2+\sum_{\mathbf{k}} v_{\mathbf{k}}f(\mathbf{k}), \tag{6}$$

$$v_{\mathbf{k}}+(1-2\mathbf{Q}\cdot\mathbf{k}+\mathbf{k}^2)f(\mathbf{k})+2\sum_{\mathbf{k}'} v_{\mathbf{k}'}b(\mathbf{k}',\mathbf{k})=0, \tag{7}$$

$$\left\{\sum_{\mathbf{k}} v_{\mathbf{k}}f(\mathbf{k})-E+\mathbf{Q}^2+[2-2\mathbf{Q}\cdot(\mathbf{k}_1+\mathbf{k}_2)+\mathbf{k}_1^2+\mathbf{k}_2^2] +2\mathbf{k}_1\cdot\mathbf{k}_2\right\}b(\mathbf{k}_1,\mathbf{k}_2)=-\mathbf{k}_1\cdot\mathbf{k}_2f(\mathbf{k}_1)f(\mathbf{k}_2). \tag{8}$$

If the three equations are simultaneously satisfied, the wave function (4) will be a approximate solution to the Hamiltonian (1) and approximate results for the energy will then be obtained.

Next, according to Eqs. (6) and (8), we find $b(\mathbf{k}_1,\mathbf{k}_2)$ satisfies

$$b(\mathbf{k}_1,\mathbf{k}_2)=-\frac{\mathbf{k}_1\cdot\mathbf{k}_2f(\mathbf{k}_1)f(\mathbf{k}_2)}{2-2\mathbf{Q}\cdot(\mathbf{k}_1+\mathbf{k}_2)+(\mathbf{k}_1+\mathbf{k}_2)^2}. \tag{9}$$

Substituting Eq. (9) into Eq. (7) we get the self-consistent equation obeyed by $f(\mathbf{k})$

$$f(\mathbf{k})=-\frac{v_{\mathbf{k}}}{1-2\mathbf{Q}\cdot\mathbf{k}+\mathbf{k}^2}+\frac{2}{1-2\mathbf{Q}\cdot\mathbf{k}+\mathbf{k}^2}\times\sum_{\mathbf{k}'} v_{\mathbf{k}'}\frac{\mathbf{k}\cdot\mathbf{k}'f(\mathbf{k})f(\mathbf{k}')}{2-2\mathbf{Q}\cdot(\mathbf{k}+\mathbf{k}')+(\mathbf{k}+\mathbf{k}')^2}. \tag{10}$$

Note that if $f(\mathbf{k})$ from this self-consistent equation is really solved, by means of Eq. (6), we will get the polaron energy of the moving polaron. Further, we can calculate its important observables such as the ground-state energy and the effective mass. Thus it remains to solve Eq. (10) for $f(\mathbf{k})$.

For the first approximation, neglecting the second term in the right-hand side of Eq. (10), we then have

$$f(\mathbf{k})=\frac{v_{\mathbf{k}}}{1-2\mathbf{Q}\cdot\mathbf{k}+\mathbf{k}^2}. \tag{11}$$

Inserting Eq. (11) into Eq. (6), replacing the discrete summation by a continuous integral, and integrating out all angles except θ, the angle between $\mathbf{Q}$ and $\mathbf{k}$, the energy of the moving polaron $E(Q)$ can be obtained as

$$E(Q)=Q^2-\int_0^\infty dk\int_{-1}^1 dx\,\frac{\alpha}{\pi}\,\frac{(1-x^2)^{(N-3)/2}}{1-2Qkx+k^2}, \tag{12}$$

where the variable $x=\cos\theta$. By means of Eq. (12), we easily obtain the ground-state energy and effective mass as

$$E=-\frac{\sqrt{\pi}}{2}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\alpha, \tag{13}$$

$$m^*=1+\frac{\sqrt{\pi}}{4N}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\alpha, \tag{14}$$

which are just the well known results obtained by many authors with different approximate schemes.[1–10,17] For later use, we also present the average number of virtual phonons to order α

$$n^p=\frac{\sqrt{\pi}}{4}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\alpha. \tag{15}$$

For the second iteration, inserting Eq. (11) into the right-hand side of Eq. (10) gives

$$f(\mathbf{k})=-\frac{v_{\mathbf{k}}}{1-2\mathbf{Q}\cdot\mathbf{k}+\mathbf{k}^2}+\frac{2}{1-2\mathbf{Q}\cdot\mathbf{k}+\mathbf{k}^2}\times\sum_{\mathbf{k}'} v_{\mathbf{k}'}\frac{\mathbf{k}\cdot\mathbf{k}'}{2-2\mathbf{Q}\cdot(\mathbf{k}+\mathbf{k}')+(\mathbf{k}+\mathbf{k}')^2}\times\frac{v_{\mathbf{k}}}{1-2\mathbf{Q}\cdot\mathbf{k}+\mathbf{k}^2}\;\frac{v_{\mathbf{k}'}}{1-2\mathbf{Q}\cdot\mathbf{k}'+\mathbf{k}'^2}. \tag{16}$$

According to Eq. (6), we have the energy of the moving polaron

$$E=Q^2-\sum_{\mathbf{k}}\frac{v_{\mathbf{k}}^2}{1-2\mathbf{Q}\cdot\mathbf{k}+\mathbf{k}^2}+\sum_{\mathbf{k},\mathbf{k}'} v_{\mathbf{k}}^2v_{\mathbf{k}'}^2\frac{2\mathbf{k}\cdot\mathbf{k}'}{2-2\mathbf{Q}\cdot(\mathbf{k}+\mathbf{k}')+(\mathbf{k}+\mathbf{k}')^2}\times\frac{1}{(1-2\mathbf{Q}\cdot\mathbf{k}+\mathbf{k}^2)^2}\;\frac{1}{1-2\mathbf{Q}\cdot\mathbf{k}'+\mathbf{k}'^2}. \tag{17}$$

We easily find that this energy is truncated to order α^2, for v_k^2 is proportional to α as shown in Eq. (2). It is very interesting to note that Eq. (17) is just equal to the sum of Eqs. (6)–(9) in Ref. 5 derived with the fourth-order perturbation theory. Thus, a simple form (17) contains the overall information of the fourth-order perturbation theory. In other words, only the second iteration in our approach can supply the fourth-order perturbative results.

By the third iteration, we can also calculate the coefficients of the α^3 term in the expansions. Up to now, only the ground-state energy expansions of the 3D and 2D polaron up to the α^3 term have been exactly calculated by Seljugin *et al.*[18] and Larsen[19] with the sixth-order perturbation theory.

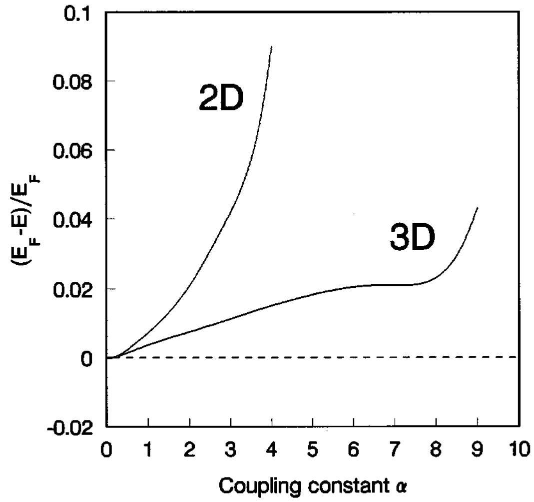

FIG. 1. The relative difference between the present and Feynman polaron ground-state energy as a function of the coupling constant α for the dimensions $N=2,3$.

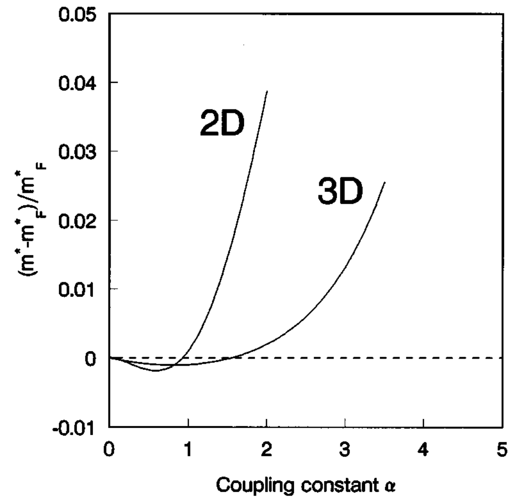

FIG. 2. The relative difference between the present and Feynman polaron effective mass as a function of the coupling constant α for the dimension $N=2,3$.

The coefficients of the α^3 term are 0.000 806 07 and 0.0074, respectively. For comparison, in this paper, the corresponding coefficients are computed to be 0.000 759 09 and 0.007 611 92, which are very close to the exact sixth-order perturbative ones. It is clear that the differences are due to the approximate wave function (4).

Generally speaking, above procedures can be carried out step by step and we could analytically obtain the polaron ground-state energy and effective mass expansions in higher powers of α. However, analytically calculations are obviously rather complicated for further iterations.

On the other hand, it is possible to solve the self-consistent Eq. (10) accurately by the numerical method, because above iteration procedures are easily performed on a computer for sufficient times. Therefore, we can numerically obtain these polaron observables as a function of α in the intermediate-coupling regime. The numerical results for the ground-state energy and effective mass of 2D and 3D polarons are displayed in Figs. 1 and 2.

To test the validity and effectiveness of our approach in this regime, we will compare the present results with the elegant Feynman path-integral ones.[20–22]

In Fig. 1, we plot the relative difference between our results and the Feynman ones for the polaron ground-state energy $(E-E_F)/E_F$ as a function of the coupling constant. It is shown that, for 3D (2D) polarons, our results are lower than the Feynman ones by around 2% (4%) for α interval $[0,6]$ ($[0,3]$). As the coupling constant increases further, our results deviate from the Feynman ones more and more. It seems that the relative difference between our results and Feynman ones is a bit larger in 2D than in 3D.

We would like to point out that our approach is not a variational one, so the obtained ground-state energy is not the upper bound to the exact result. Fortunately, for 3D polarons, it is recalled from Ref. 14 that our results for the ground-state energy are in excellent agreement with the recent exact Monte Carlo calculations up to $\alpha=6$. As for 2D polarons, we do not know the magnitude of the relative difference between the exact and Feynman results in the intermediate-coupling regime, since the corresponding exact calculations are still lacking. But we can estimate it qualitatively by comparing the weak-coupling approximation. It is convenient to collect the ground-state energy expansions to order α^2 in the Feynman path-integral and fourth-order perturbation theory:

$$E_F^{2D} = -\frac{\pi}{2}\alpha - 0.04569\alpha^2; \;\; E_{PT4}^{2D} = -\frac{\pi}{2}\alpha - 0.06397\alpha^2, \tag{18}$$

for 2D polarons[21] and

$$E_F^{3D} = -\alpha - 0.012347\alpha^2; \;\; E_{PT4}^{3D} = -\alpha - 0.0159196\alpha^2, \tag{19}$$

for 3D polarons.[10,23] Usually, the known fourth-order perturbative results are referred to as the exact ones in the weak-coupling limit. According to Eqs. (24) and (25), it is easily found that the difference between the exact and Feynman energy is $0.0183\alpha^2(0.00357\alpha^2)$ for 2D(3D) polarons. It is clear that, in the intermediate-coupling regime, the relative difference between the exact and Feynman ones in 2D is larger than in 3D. Therefore, although our results for the ground-state energy in 2D polarons are less than Feynman ones by a larger percentage, it is still possible that our results for the ground-state energy are closer to the unknown exact results than Feynman ones, like in 3D polarons.

The relative difference between our results and Feynman ones for the effective mass $(m^*-m_F^*)/m_F^*$ as the coupling constant is displayed in Fig. 2. We see that, for both 3D and 2D polarons, our results in the weak-coupling regime are lower than the Feynman ones by the very small percentage. As the coupling constant increases, the present results become larger than the Feynman ones.

It is found that in the weak-coupling regime the exact results are really lower than the Feynman ones, as proven in the following weak-coupling expansions in the Feynman and fourth-order perturbation theory:

$$m_F^{*2D} = 1 + \frac{\pi}{8}\alpha + 0.1371\alpha^2;\quad m_{PT4}^{*2D} = 1 + \frac{\pi}{8}\alpha + 0.1272\alpha^2, \tag{20}$$

for 2D polarons[22] and

$$m_F^{*3D} = 1 + \tfrac{1}{6}\alpha + 0.024691\alpha^2;$$

$$m_{PT4}^{*3D} = 1 + \tfrac{1}{6}\alpha + 0.0236276\alpha^2, \tag{21}$$

for 3D polarons.[24] It follows that our results in the weak-coupling regime are perhaps closer to the exact ones. We would mention that the present results for the effective mass in 3D do not agree with the Monte Carlo results[15] so well as for the ground-state energy in the intermediate-coupling regime. In our opinion, the obtained exact results for the effective mass in the Monte Carlo calculation[15] should be restricted to the weak-coupling regime due to the insufficient convergence in the intermediate-coupling regime. It is likely that the effective mass is a sensitive quantity to calculated stochastically in the Monte Carlo calculation, contrary to the ground-state energy. Alternatively, the convincing exact results for 2D polarons are also lacking up to now. So it is difficult to say that which approach can supply the better results for the effective mass, unlike for the ground-state energy. Anyway, in both 3D and 2D polarons, our results for the effective mass agree with the Feynman ones to some degree for a finite coupling range, as indicated in Fig. 2.

Finally, as expected from Figs. 1 and 2, the valid range of our approach for the 3D polaron is wider than for the 2D polaron. According to Eq. (15), we can see that the average number of virtual phonons of the 2D polaron is larger than that of the 3D polaron for a fixed coupling constant α. Physically, our approach, where only correlations between wave vectors of pairs of emitted phonons in the field are taken into account, is not suited to the polaron problem with a very large phonon number. Qualitatively, this is just that case as shown in Figs. 1 and 2.

In summary, we have studied 2D and 3D polarons with extended coherent states. In the weak-coupling limit, the obtained expansions of some observables are very close to the sixth-order perturbative ones and cover the fourth-order perturbative ones. It is implied that we have completely calculated the contributions from all Feynman diagrams in the fourth-order perturbation theory by the second iteration, and evaluated for the most part the contributions from the Feynman diagrams in the sixth-order perturbation theory by the third iteration. Moreover, the numerical results for the ground-state energy and effective mass as a function of α agree with the well known Feynman path-integral results, and perhaps are closer to the exact results in the intermediate-coupling regime, which again underlines the effectiveness of our approach in polaron physics. Finally, we would like to point out that our approach is perhaps helpful to other polaronlike problems.

This work was partially supported by the Centre for Research and Development on Superconductivity of China under Contract No. J-A-5222. One of the authors (C.Q.) gratefully acknowledges the support from the Postdoctoral Science Foundation of China.

---

*Mailing address.

[1] F. M. Peeters, Wu Xiaoguang, and J. T. Devreese, Phys. Rev. B **33**, 3926 (1986).
[2] F. M. Peeters and J. T. Devreese, Phys. Rev. B **36**, 4442 (1987).
[3] V. V. Paranjape and P. V. Panat, Phys. Rev. B **35**, 2942 (1987).
[4] B. E. Sernelius, Phys. Rev. B **36**, 9059 (1987).
[5] O. V. Seljugin and M. A. Smondyrev, Physica A **142**, 555 (1987).
[6] M. A. Smondyrev, Physica A **171**, 191 (1991).
[7] S. Sil and A. Chatterjee, Phys. Lett. A **140**, 59 (1989).
[8] A. Chatterjee, Phys. Rev. B **41**, 1668 (1990).
[9] Shiliang Ban, Ruisheng Zheng, Xianmei Meng, and Liyun Zhao, J. Phys. Condens. Matter **5**, 6055 (1993).
[10] G. Ganbold and G. V. Efimov, Phys. Rev. B **50**, 3733 (1994).
[11] M. Horst, U. Merkt, and J. P. Kotthaus, Phys. Lett. **50**, 754 (1983).
[12] S. A. Jackson and P. M. Platzman, Phys. Rev. B **24**, 499 (1981).
[13] D. Emin, Phys. Rev. Lett. **62**, 1544 (1989); Phys. Rev. B **45**, 5525 (1992).
[14] Kelin Wang, Qinghu Chen, and Shaolong Wan, Phys. Lett. A **185**, 216 (1994).
[15] C. Alexandrou and R. Rosenfelder, Phys. Rep. **215**, 1 (1992); C. Alexandrou, W. Fleischer, and R. Rosenfelder, Phys. Rev. Lett. **65**, 2615 (1992); C. Alexandrou, W. Fleischer, and R. Rosenfelder, Mod. Phys. Lett. B **5**, 613 (1991).
[16] T. D. Lee, F. E. Low, and D. Pines, Phys. Rev. **90**, 297 (1953).
[17] F. M. Peeters and J. T. Devreese, Phys. Rev. B **36**, 4442 (1987).
[18] O. V. Seljugin and M. A. Smondyrev, Physica A **142**, 155 (1989).
[19] D. M. Larsen, Phys. Rev. B **35**, 4435 (1987).
[20] R. P. Feynman, Phys. Rev. **97**, 660 (1955); T. D. Schultz, *ibid.* **116**, 526 (1959).
[21] Wu Xiaoguang, F. M. Peeters, and J. T. Devreese, Phys. Rev. B **31**, 3420 (1985).
[22] F. M. Peeters, Wu Xiaoguang, and J. T. Devreese, Phys. Rev. B **37**, 933 (1988).
[23] J. Röseler, Phys. Status Solidi **25**, 311 (1958).
[24] Yang Lu and R. Rosenfelder, Phys. Rev. B **46**, 5211 (1992).