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An extensive calculation of the properties of a one-dimensional polaron

Chen Qinghu, Wang Kelin and Wan Shaolong

Centre for Fundamental Physics, University of Science and Technology of China, Hefei, Anhui 230026, People's Republic of China

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Abstract. A refined approach where the wave function is gradually improved is developed in the one-dimensional (1D) large-Fröhlich-polaron problem. The results for the ground-state energy, the effective mass, and the average number of virtual phonons are obtained for a wide range of the coupling constant α, and are in agreement with those of the Feynman path-integral formalism. In addition, in the weak-coupling limit, the expansions of these observables in powers of the coupling constant are exactly calculated up to the α^3-term. They are $E = -\alpha - 0.060\,66\alpha^2 - 0.008\,44\alpha^3$, $m^* = 1 + 0.5\alpha + 0.191\,94\alpha^2 + 0.069\,12\alpha^3$, and $N = 0.5\alpha + 0.121\,32\alpha^2 + 0.029\,54\alpha^3$, which agree with the known results of the fourth-order perturbation theory.

1. Introduction

The problem of the one-dimensional (1D) polaron has attracted much attention in the last decade. The reason is threefold. First, it has been technologically possible to produce well characterized quasi-1D structures (i.e. quantum wires). Second, the polaron effect is theoretically enhanced with the lowering of the dimension [1–3]. Third, owing to the simplicity of the mathematics, it provides a subject of interest where a new *ansatz* can be developed extensively.

There are two types of model employed for the 1D polaron. They are the small- and the large-polaron model. The former describes the 1D polaron which emerges from the linear conjugative organic polymers conductors *cis-* and *trans*-polyacetylene ($(CH)_x$) [4]. Both the kink soliton solution [4] and the non-linear soliton-type polaron solution [5] were found in the same theoretical model. The latter is the standard polaron model, i.e. the 1D large-Fröhlich-polaron one [3, 6, 7], where the electrons interact with the lattice vibration through the deformation potential in one dimension. Campbell *et al* [8] have shown that these two models are almost identical in the weak-coupling range.

In this paper we will focus on the 1D large Fröhlich polaron. The Hamiltonian is given by [3, 6, 7]

$$H = \frac{1}{2m}p^2 + \sum_q \hbar\omega_0 a_q^\dagger a_q + \sum_q v\left(a_q e^{iqx} + a_q^\dagger e^{-iqx}\right) \tag{1}$$

$$v = \hbar\omega_0\left(\frac{\hbar}{2m\omega_0}\right)^{1/2}\left(\frac{2\alpha}{L}\right)^{1/2}$$

where m is the electron band mass, ω_0 is the frequency of the LO phonons, $a_q^\dagger$ and a_q are respectively the creation and annihilation operators of the LO phonons with the wave vector

q, and L is the length of the crystal lattice. In this paper the coupling constant α is identical to α' in [7] and $2\pi\alpha_{op}$ in [6].

Degani *et al* [6] had calculated the ground-state energy and effective mass for all values of the coupling constant by using the Feynman path-integral formalism. Recently, with the fourth-order perturbation theory, Peeters *et al* [7] found the expansions of the ground-state energy, the effective mass, and the number of virtual phonons in powers of the coupling constant as $E = -\alpha - 0.060\,66\alpha^2$, $m^* = 1 + 0.5\alpha + 0.191\,94\alpha^2$, and $N = 0.5\alpha + 0.121\,32\alpha^2$. To the best of our knowledge, no exact result for the 1D polaron has been found up to now.

The present paper is intended to develop a new approach to calculate the properties of the 1D polaron. We first apply the canonical transformation of Lee, Low and Pines (LLP) [9] to the Hamiltonian (1) and get a Hamiltonian which no longer contains the electron coordinates. Then, on the basis of the zero-order approximate wave function, taking into account correlations of the wave vectors of the emitted virtual phonons, we gradually improve the wave function to diagonalize the Hamiltonian. As a result, we obtain not only the results for the ground-state energy, the effective mass, and the number of virtual phonons for a wide range of the coupling constant, but the expansions of those observables in the weak-coupling limit as well. Finally, we compare our results with the well known previous ones.

This paper is arranged as follows. In section 2 we describe in detail the basic process involved in our method for the 1D polaron, when considering correlations between the wave vectors of pairs of virtual phonons in the field. Moreover, we calculate the results for some observables for a wide range of the coupling constant and in the weak-coupling limit. In section 3, the method in section 2 is directly extended to take account of correlations among the wave vectors of three phonons, and analogous calculations are performed. We compare our results with the Feynman and the fourth-order perturbative ones and present some discussions and conclusions in the last section.

2. Two-phonon correlation

First of all,we apply the transformation of LLP [9] to the Hamiltonian (1) and adopt the units of $2m = \hbar = \omega_0 = 1$, which results in

$$H = \left(Q - \sum_q q a_q^\dagger a_q\right)^2 + \sum_q a_q^\dagger a_q + \sum_q v(a_q^\dagger + a_q) \tag{2}$$

$$v = \sqrt{\frac{2\alpha}{L}}.$$

The total momentum Q is conserved and regarded as a c-number, since the Hamiltonian is translationally invariant. For convenience we rewrite the Hamiltonian (2) in the following form:

$$H = Q^2 + \sum_q (1 - 2Qq + q^2) a_q^\dagger a_q + \sum_q v(a_q^\dagger + a_q) + \sum_{q_1, q_2} q_1 q_2 a_{q_1}^\dagger a_{q_2}^\dagger a_{q_1} a_{q_2} \tag{3}$$

where the last term in the right-hand side is referred to as the recoil term.

The next step is to find a wave function $|\rangle$ which satisfies the Schrödinger equation

$$H\,|\rangle = E\,|\rangle. \tag{4}$$

Ivic and Brown [10] dealt with the problem of the small polaron in a 1D crystal lattice with the phonon coherent state proposed by Davydov *et al* [11]. In this paper, it is not far-fetched to suggest preliminarily the following coherent state:

$$|\rangle_0 = \prod_{q'} e^{\alpha(q')a^\dagger_{q'}} \mid 0\rangle \qquad (5)$$

$$a_q \; |\rangle_0 = \alpha(q) \; |\rangle_0$$

as the wave-function solution of the Hamiltonian (3). Substituting equation (5) into equation (4), followed by collecting together the terms in $(a^\dagger)^0 \; |\rangle_0$, $(a^\dagger)^1 \; |\rangle_0$, and $(a^\dagger)^2 \; |\rangle_0$, neglecting the $(a^\dagger)^2 \; |\rangle_0$-term, and equating the coefficients of the terms of $(a^\dagger)^0 \; |\rangle_0$ and $(a^\dagger)^1 \; |\rangle_0$ yields

$$\alpha(q) = -\frac{v}{1 - 2Qq + q^2} \qquad (6)$$

$$E = Q^2 + \sum_q v \; \alpha(q). \qquad (7)$$

Inserting equation (6) into equation (7) we obtain the energy of a moving polaron

$$E = Q^2 - \frac{\alpha}{\pi}\int_0^\infty \frac{\mathrm{d}q}{1 - 2Qq + q^2}. \qquad (8)$$

Setting the polaron momentum $Q = 0$, we have the 1D polaron ground-state energy

$$E = -\alpha. \qquad (9)$$

In order to study the dynamics properties of the 1D polaron, it is fundamental to evaluate the effective mass. The relation between the effective mass and the energy at small momentum is generally expressed as

$$m^* = \frac{1}{\frac{1}{2}(\partial^2 E/\partial Q^2)\mid_{Q=0}} \; (2m = 1). \qquad (10)$$

After substituting equation (8) into equation (10) we get the effective mass of the 1D polaron

$$m^* = 1 + \tfrac{1}{2}\alpha. \qquad (11)$$

The average number of virtual phonons can also be directly obtained from the energy

$$N(Q) = \left(1 - \frac{3}{2}\alpha\frac{\partial}{\partial\alpha} - \frac{1}{2}Q\frac{\partial}{\partial Q}\right)E(Q). \qquad (12)$$

This has been proved exactly in [12]. According to equations (8) and (12), when the polaron is in the ground state the average number of virtual phonons is given by

$$N = \tfrac{12}{\alpha}. \qquad (13)$$

It is noteworthy that equations (9), (11), and (13) are just the results of the weak-coupling approximation of the Feynman path-integral formalism [6] and the second-order perturbation theory [7].

We now return to the Hamiltonian (3) and the coherent state determined by equations (5) and (6). It is not difficult to find that this coherent state is a exact solution to the Hamiltonian (3) in the absence of the recoil term. We refer to it as the zero-order wave-function solution. It is a good approximation when the virtual phonon number is very small, but as the number of virtual phonons increases with increasing α, the recoil term should be taken into account.

In order to further diagonalize the Hamiltonian (3), we should revise the form of the coherent state (5). It is instructive to apply the Hamiltonian (3) to this zero-order wave function

$$H\,|\rangle_0 = E\,|\rangle_0 + \sum_{q_1,q_2} q_1 q_2 \alpha(q_1)\alpha(q_2) a^\dagger_{q_1} a^\dagger_{q_2}. \tag{14}$$

We find that a $(a^\dagger)^2\,|\rangle_0$-term is superfluous when $H\,|\rangle_0$ gives $E\,|\rangle_0$. It is apparent that there is, at least, a $(a^\dagger)^2\,|\rangle_0$-term in the exact solution of the Hamiltonian (3). Therefore we improve the coherent state (5) as the following extended form:

$$|\rangle_2 = |\rangle_0 + \sum_{q_1,q_2} b_2(q_1,q_2) a^\dagger_{q_1} a^\dagger_{q_2}\,|\rangle_0 \tag{15}$$

where $b_2(q_1, q_2)$ is the interchanging symmetrical function of q_1 and q_2. It is implied in equation (15) that correlations between wave vectors of pairs of emitted phonons in the field are under consideration.

In a similar manner, substituting equation (15) into equation (4), neglecting $(a^\dagger)^3\,|\rangle_0$- and $(a^\dagger)^4\,|\rangle_0$-terms, and equating the coefficients of the terms of $(a^\dagger)^0\,|\rangle_0$, $(a^\dagger)^1\,|\rangle_0$, and $(a^\dagger)^2\,|\rangle_0$ in both sides of the Schrödinger equation supplies

$$E = \sum_q v\alpha(q) + Q^2 \tag{16}$$

$$v + (1 - 2Qq + q^2)\alpha(q) + 2\sum_{q'} v b_2(q', q) = 0 \tag{17}$$

$$\left\{\sum_q v\alpha(q) - E + Q^2 + [2 - 2Q(q_1 + q_2) + q_1^2 + q_2^2] + 2q_1 q_2\right\} b_2(q_1, q_2)$$
$$= -q_1 q_2 \alpha(q_1)\alpha(q_2). \tag{18}$$

In terms of the above three equations we get the self-consistent equation satisfied by $\alpha(q)$

$$\alpha(q) = -\frac{v}{1 - 2Qq + q^2} + \frac{2}{1 - 2Qq + q^2}\sum_{q'} v' \frac{qq'\alpha(q)\alpha(q')}{2 - 2Q(q + q') + (q + q')^2}. \tag{19}$$

Introducing the distribution function

$$F(q) = \left(\frac{\alpha L}{2\pi^2}\right)^{1/2} \alpha(q) \tag{20}$$

and transforming the summation $\sum_q$ into a integral $(L/2\pi)\int \mathrm{d}q$, then equations (16) and (19) can be respectively reduced to

$$E = \int_{-\infty}^{\infty} F(q)\mathrm{d}q + Q^2 \tag{21}$$

$$F(q) = -\frac{\alpha}{\pi(1 - 2Qq + q^2)} + \frac{2}{1 - 2Qq + q^2}\int_{-\infty}^{\infty} \mathrm{d}q' \frac{qq'F(q)F(q')}{2 - 2Q(q + q') + (q + q')^2}. \tag{22}$$

It can be noticed from equations (21) and (22) that $F(q)$ is the distribution function of the 1D polaron ground-state energy in terms of q and equation (22) is its self-consistent integral equation.

If we only take the first term in the right-hand side of equation (22), we will obtain

$$F(q) = -\frac{\alpha}{\pi(1-2Qq+q^2)}. \tag{23}$$

Inserting equation (23) into equation (22) we obtain $E = -\alpha$, which is just the zero-order approximate result equation (9) mentioned above. For further iteration, substituting equation (23) into the right-hand side of equation (22) gives

$$F(q) = -\frac{\alpha}{\pi(1-2Qq+q^2)} + \frac{2\alpha^2}{\pi^2(1-2Qq+q^2)^2} \times \int_{-\infty}^{\infty} \mathrm{d}q' \frac{qq'}{(1-2Qq'+q'^2)[2-2Q(q+q')+(q+q')^2]}. \tag{24}$$

Inserting equation (24) into equation (21), the ground-state energy reads

$$E = -\alpha - 0.060\,66\alpha^2. \tag{25}$$

In addition, the expansions of the effective mass and the number of virtual phonons are calculated as follows:

$$m^* = 1 + 0.5\alpha + 0.191\,94\alpha^2 \tag{26}$$

$$N = 0.5\alpha + 0.121\,32\alpha^2 \tag{27}$$

where use has been made of equations (10) and (12). These are none other than the previous fourth-order perturbative result as given in [7].

Repeating the same procedure step by step, we will get the expansions of the observables including α^3 and its subsequent terms. It is nonsense to write down these terms in the expansions, because they are incompletely calculated due to the fact that the $(a^\dagger)^3\ |\rangle_0$ and $(a^\dagger)^4\ |\rangle_0$ term are neglected in deriving the coupled integral equations. However the coefficient of the α^2-terms is exactly calculated, as will be shown in the next section.

On the other hand, the infinite-iteration technique can be used to solve the self-consistent integral equation (22) satisfied by $F(q)$ numerically. Solving for $F(q)$,with the help of equation (2) we numerically calculate the 1D polaron ground-state energy for a wide range of coupling constant up to $\alpha = 2.0$. In addition, by means of equations (10) and (12) we can obtain the effective mass up to $\alpha = 1.5$, and the average number of virtual phonons up to $\alpha = 2.0$. The results are shown in figures 1–3 with dashed lines.

3. Three-phonon correlation

In order to solve for the 1D polaron more accurately, we can straightforwardly extend the method described in section 2 to take account of correlations among the wave vectors of three virtual phonons in this section.

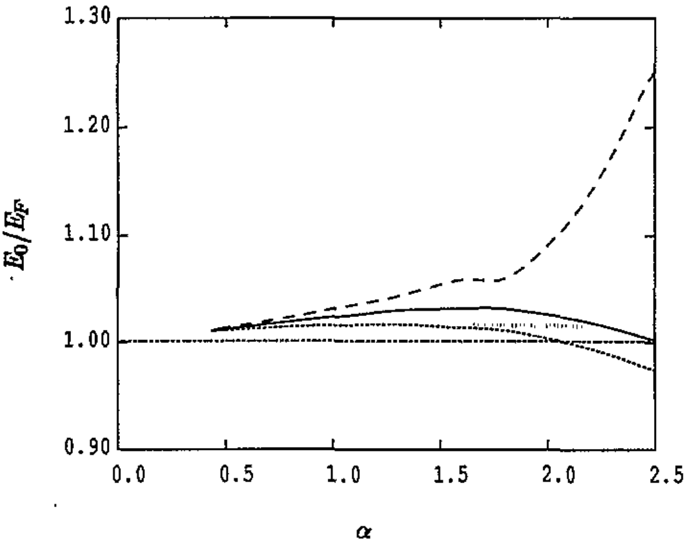

Figure 1. The ground-state energy of the 1D polaron normalized to the Feynman energy E_0/E_F as a function of the coupling constant α up to $\alpha = 2.5$. The solid line and the dashed line, respectively, represent the results calculated in sections 3 and 2. The dotted line denotes the fourth-order perturbative results.

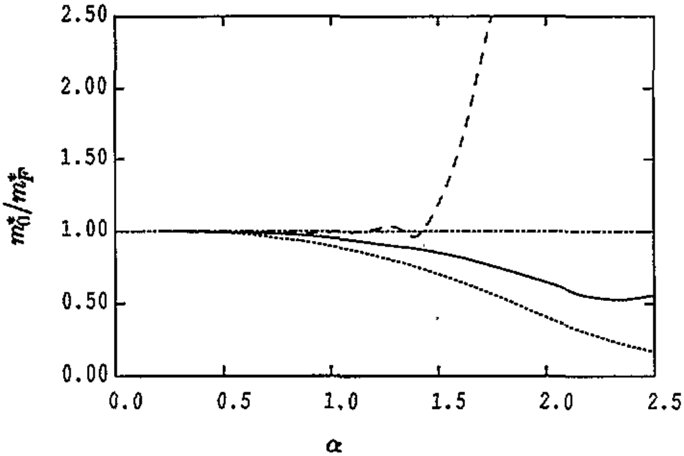

Figure 2. The effective mass of the 1D polaron normalized to the Feynman mass m_0^*/m_F^* as a function of the coupling constant α up to $\alpha = 2.5$. The notation is the same as in figure 1.

According to the analogous discussion in section 2, the improved wave function should take the form

$$|\rangle_3 = |\rangle_0 + \sum_{q_1,q_2} b_2(q_1,q_2) a_{q_1}^\dagger a_{q_2}^\dagger |\rangle_0 + \sum_{q_1,q_2,q_3} b_3(q_1,q_2,q_3) a_{q_1}^\dagger a_{q_2}^\dagger a_{q_3}^\dagger |\rangle_0 \tag{28}$$

where $b_3(q_1, q_2, q_3)$ is the interchanging symmetrical function of q_1, q_2, and q_3. The

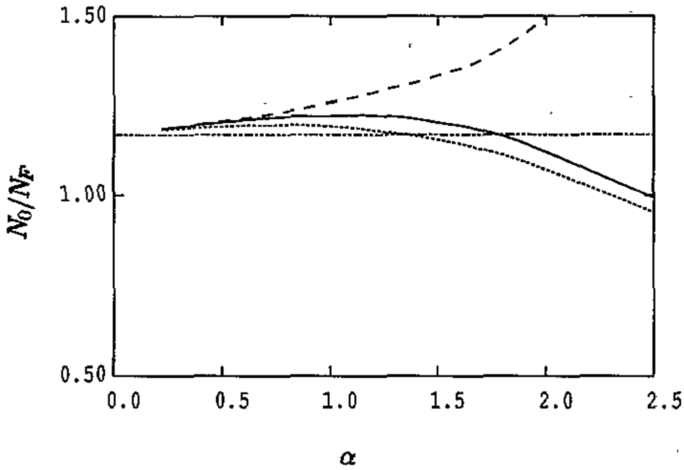

Figure 3. The average number of virtual phonons of the 1D polaron normalized to the Feynman phonon number N_0/N_F as a function of the coupling constant α up to $\alpha = 2.5$. The notation is the same as in figure 1.

physics behind equation (32) hints that correlations among wave vectors of three emitted phonons in the field are taken into consideration.

We skip the details of the derivation and directly present the coupled integral equations as follows:

$$E = \int_{-\infty}^{\infty} F(q)\mathrm{d}q + Q^2 \tag{29}$$

$$F(q) = -\frac{\alpha}{\pi(1-2Qq+q^2)} - \int_{-\infty}^{\infty} \mathrm{d}q' \frac{G(q,q')}{1-2Qq+q^2} \tag{30}$$

$$G(q_1,q_2) = -\frac{2q_1q_2F(q_1)F(q_2)}{2-2Q(q_1+q_2)+(q_1+q_2)^2} + \int_{-\infty}^{\infty} \frac{A\ \mathrm{d}q}{[3-2Q(q_1+q_2+q)+(q_1+q_2+q)^2][2-2Q(q_1+q_2)+(q_1+q_2)^2]} \tag{31}$$

where

$$F(q) = \left(\frac{\alpha L}{2\pi^2}\right)^{1/2} \alpha(q) \qquad G(q_1,q_2) = \frac{\alpha L}{\pi^2} b_2(q_1,q_2) \tag{32}$$

$$\begin{aligned} A = &\left[\frac{\alpha}{\pi} + (1-2Qq+q^2)F(q) + 2(q_1+q_2)qF(q)\right]G(q_1,q_2) \\ &+ \left[\frac{\alpha}{\pi} + (1-2Qq_1+q_1^2)F(q_1) + 2(q_2+q)q_1F(q_1)\right]G(q_2,q) \\ &+ \left[\frac{\alpha}{\pi} + (1-2Qq_2+q_2^2)F(q_2) + 2(q_1+q)q_2F(q_2)\right]G(q,q_1). \end{aligned} \tag{33}$$

Without regard to the second term in equation (31), all the results in section 2 will be recovered. It is evident from the next iteration that the contribution of the second term in equation (31) to the energy begins with the α^3-term. Choosing $F_0(q)$ in equation (23) and

$$G_0(q_1,q_2) = -\frac{2q_1q_2F_0(q_1)F_0(q_2)}{2-2Q(q_1+q_2)+(q_1+q_2)^2} \tag{34}$$

as the initial values for iteration and inserting them into the second term of the right-hand side of equation (31), with the help of equations (29) and (30) we obtain an α^3-term first, so the coefficient of the α^2-term is unchanged. In other words, the coefficient of the α^2-term in the expansion of the energy is exactly calculated in section 2. Furthermore, we can say that the coefficient of the α^3-term in the energy expansion is exactly calculated in this section for the reason that the next improvement of the wave function will not lead to modification of the coefficient of the α^3-term. Similar statements also hold true for the effective mass and the average number of virtual phonons. Consequently, collecting all the α^3-terms, we arrive at the expansions of the three observables up to α^3-terms

$$\begin{aligned} E &= -\alpha - 0.060\,66\alpha^2 - 0.008\,44\alpha^3 \\ m^* &= 1 + 0.5\alpha + 0.191\,94\alpha^2 + 0.069\,12\alpha^3 \\ N &= 0.5\alpha + 0.121\,32\alpha^2 + 0.029\,54\alpha^3. \end{aligned} \tag{35}$$

Alternatively, proceeding as outlined in section 2, we can also numerically solve the coupled self-consistent equations (30) and (31) simultaneously, and obtain the ground-state energy, the effective mass, and the number of virtual phonons for $\alpha < 2.5$ in the light of equations (29), (10), and (12). The results are presented in figures 1–3 with solid lines.

4. Comparison and discussions

It can be seen that, in the weak-coupling limit, we have obtained the expansions of the ground-state energy, the effective mass, and the average number of virtual phonons up to the α^2-term in section 2; these are the same as the known fourth-order perturbative results [7]. Furthermore we have exactly calculated the expansions of those observables up to the α^3-term in section 3. It is predicted that the results in equation (35) are identical to those of the sixth-order perturbation theory which are unknown. To the best of our knowledge, the present paper is the first one to give the coefficients of the α^3-term in the expansions of some observables for the 1D polaron in the weak-coupling limit.

On the other hand, we have calculated the ground-state energy, the effective mass, and the average number of virtual phonons for a wide coupling range, by solving the coupled integral equations numerically. As is well known, among various approaches applied to the polaron problem, the variational path-integral method of Feynman is a particularly elegant one for the whole coupling range and can be used to check a variety of approaches and new ideas, so it is natural in the present paper that we compare our results obtained in sections 2 and 3 with the Feynman ones [6] for a range of the coupling constant.

Here we digress briefly to analyse qualitatively the relation between the exact results and the Feynman ones for some observables in the whole coupling range, by comparing their corresponding results in the weak- and strong-coupling limits. Recently, through the scaling law, Peeters *et al* [7] have presented the Feynman results for some observables in the weak-coupling limit

$$E = -\alpha - \tfrac{1}{27}\alpha^2 \qquad m^* = 1 + \tfrac{1}{2}\alpha + \tfrac{2}{9}\alpha^2 \qquad N = \tfrac{1}{2}\alpha + \tfrac{2}{27}\alpha^2 \tag{36}$$

and in the strong-coupling limit

$$E = -\frac{1}{\pi}\alpha^2 \qquad m^* = \frac{16}{\pi^2}\alpha^4 \qquad N = \frac{1}{2\pi}\alpha^2. \tag{37}$$

Alternatively, the exact results in the strong-coupling limit have also been obtained in [7] with a systematic adiabatic strong-coupling approximation

$$E = -0.333\,088\alpha^2 \qquad m^* = 2.1254\alpha^4 \qquad N = 0.666\,176\alpha^2. \tag{38}$$

Usually, the known fourth-order perturbative results [7] can be referred to as the exact ones in the weak-coupling limit. Comparing these exact results with the Feynman ones equations (36) and (37) in the two limits, we first deduce that the Feynman results for the ground-state energy are a little higher than the exact ones for all coupling constants. This point is confirmed by the fact that the Feynman approach is a variational one. For the effective mass, it is then inferred that the Feynman results are higher than the exact ones in the weak-coupling range and lower in the strong-coupling range. It is also learned from the comparison that the Feynman results for the average number of virtual phonons are a little less than the exact ones in the whole coupling range.

In figure 1 we have displayed the ground-state energy normalized to the Feynman energy E_0/E_F versus the coupling constant. It is of some interest to note that the results for the energy calculated in section 2 (3) are about 4% (2%) less than the Feynman ones when $\alpha < 2$ (2.5).

It should be pointed out that the present approach is not a variational one, so the obtained ground-state energy is not a upper bound to the exact one. In the 3D polaron Alexandrou and Rosenfelder [13] found the exact energy to be about 2% less than 3D Feynman one. Therefore it is possible that the exact ground-state energy is less than the Feynman one by the same percentage in the 1D polaron. Based on this analysis we can say that the present results for the ground-state energy obtained in sections 2 and 3 are closer to the exact ones than the Feynman ones. More importantly, with the coupling constant increasing, the results obtained in section 3 seem to be better than those in section 2 as also indicated in figure 1.

It is very interesting to link the average number of virtual phonons in the field with the valid range of our method in sections 2 and 3. We can easily check that the Feynman results for the average number of phonons are $N_F = 1.745$ for $\alpha = 2$ and $N_F = 2.971$ for $\alpha = 2.5$. The exact values of the average number of virtual phonons, which are little higher than the Feynman ones as stated before, are estimated as $N_{ex} \simeq 2$ for $\alpha = 2$ and $N_{ex} \simeq 3$ for $\alpha = 2.5$. On the other hand, physically, if the average number of particles in the field is less than two (three) it is sufficient to consider two- (three-) particle correlations. So it is predicted theoretically that the valid range of our method described in section 2 (3) should be $\alpha \leqslant 2$ (2.5). Fortunately, from figure 1 we can see that this is exactly that case. It may not be superfluous to stress that the validity of our approach is self-consistent with the average number of virtual phonons and its reliability is beyond doubt.

The curves of the effective mass normalized to the Feynman result m_0^*/m_F^* against the coupling constant are plotted in figure 2. It can be seen that, when $\alpha < 1.5$, the results obtained in section 2 are in agreement with the Feynman ones, and the results in section 3 are less than the Feynman ones and higher than the fourth-order perturbative ones when $\alpha < 2.5$.

It should be recalled from previous discussions that the exact results for the effective mass are less than the Feynman results in the weak-coupling range. In addition, the fourth-order perturbative results are less than the exact ones since the higher-order terms are neglected in the expansion. Therefore we can say that the exact results for the effective mass in the weak-coupling range are just between the results of the Feynman and the perturbation theory. Thus, it can be inferred from figure 2 that the results for the effective mass obtained in section 3 are the closest to the exact ones, and the results in section 2 which agree with the Feynman ones are a little higher than the exact ones in a wide coupling range. What is more, the valid range of our method in section 3 is much wider than that in section 2, as also shown in figure 2.

Figure 3 presents the number of virtual phonons normalized to the Feynman result N_0/N_F versus the coupling constant. With increasing coupling constant, the results for the phonon number in the field calculated in section 3 are much closer to the Feynman ones than those in section 2 when $\alpha < 2.5$. It is believed by similar discussion that the results calculated in section 3 are better than the results in section 2 and the Feynman ones when $\alpha < 1.8$.

Finally, it is tedious but straightforward to extend our approach to consider correlations of the wave vectors of any n phonons. Without loss of generality, the wave function should take the following more general form:

$$|\rangle_n = \Big[1 + \sum_{q_1,q_2} b_2(q_1,q_2)a^\dagger_{q_1}a^\dagger_{q_2} + \sum_{q_1,q_2,q_3} b_3(q_1,q_2,q_3)a^\dagger_{q_1}a^\dagger_{q_2}a^\dagger_{q_3} + \cdots \sum_{q_1,q_2,\ldots,q_n} b_n(q_1,q_2,\ldots,q_n)a^\dagger_{q_1}a^\dagger_{q_2}\ldots a^\dagger_{q_n}\Big]|\rangle_0. \tag{39}$$

By means of analogous procedures, we could exactly obtain the expansions of some observables up to α^n, because the next extension would not modify the α^n-term, which could be induced from the context. When n approaches infinity the results are exact and the wave function $\lim_{n\to\infty}|\rangle_n$is the exact solution.

It is to be expected that the valid range of our approach will be enlarged with larger n, but it should be pointed out that, even if n is extended to infinity, the results for all values of the coupling constant cannot be obtained. The reason is that in the strong-coupling limit some observables of the Fröhilch optical polaron are expanded in powers of $1/\alpha^2$ instead of α [14].

Most importantly, it can be concluded (at least for the large polaron) that our extended approach considering correlations of n phonons is superior to the corresponding $2n$th-order perturbation theory, because we can explicitly and directly calculate the expansions of the observables up to the α^n-term in a strict mathematical sense, but in the $2n$th-order perturbation theory, it is very difficult to calculate all the contributions from the complicated nth-order Feynman diagrams for large n.

In summary, we have presented a novel approach to deal with the 1D polaron system. For a wide range of the coupling constant, the results of the ground-state energy, the effective mass, and the average number of virtual phonons have been calculated; these agree with the Feynman ones and are perhaps closer to the exact ones. In the weak-coupling limit, we reobtain the results for some observables known in the fourth-order perturbation theory. In addition, we evaluate the coefficients of the α^3-term in the expansions for some observables for the first time.

The present approach considering two-phonon correlations has been applied to the 3D polaron [15]. We would like to point out that this new idea may also be suited to the treatment of other polaron-like problems.

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