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Polaron effective masses with extended coherent states

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Abstract. The effective mass of a large polaron is calculated using the extended phonon coherent state proposed in our previous paper. In the weak-coupling limit, the mass expansion obtained can reproduce the fourth-order perturbative result. Moreover, in the intermediate-coupling range, the calculated results are in good agreement with those of other approaches.

1. Introduction

An electron moving slowly in an ionic crystal may cause a distortion of the lattice; the resultant ionic polarization, in turn, acts on the electron and modifies the bare-electron properties. The electron together with its surrounding distortion is known as a polaron and a model for such a system can be investigated using Fröhlich Hamiltonian [1]:

$$H = -\frac{1}{2m}\nabla^2 + \sum_{\boldsymbol{q}} \omega_0 a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}} + \sum_{\boldsymbol{q}} \frac{M_0}{\nu^{1/2}|\boldsymbol{q}|}(a_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{r}} + a_{\boldsymbol{q}}^\dagger e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}) \tag{1}$$

where m is the electron band mass, ω_0 is the frequency of the LO phonons, $a_{\boldsymbol{q}}^\dagger$ and $a_{\boldsymbol{q}}$ are respectively the creation and annihilation operators for the LO phonons with the wave vector $\boldsymbol{q}$, ν is the crystal volume, and $M_0 = [4\pi\alpha\omega_0^{3/2}/(2m)^{1/2}]^{1/2}$ (here α is the electron–phonon coupling constant).

The Fröhlich polaron has been a subject of interest for a very long time due to the many theoretical and practical implications. Various methods in many-body physics have been applied to this problem (see reviews [2]). It is well known that the variational Feynman path integral method [3] is particularly successful in evaluating the polaron ground-state energy and effective mass for all values of the coupling constants. This method is still used to check new approaches and *ansatze*.

The polaron mass is an important quantity which can associate experimental results with theoretical studies where various fundamental assumptions are made. Hence, many investigations have been devoted to this problem to date (an incomplete list is given by [3–10]). In the weak-coupling limit, within the fourth-order perturbation theory [4], Höhler

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and Müllensiefen first calculated the expansion of the polaron effective mass in terms of α; Seljugin and Smondyrev further presented this expansion to greater accuracy:

$$m^* = 1 + \alpha/6 + 0.023\,627\,63\,\alpha^2. \tag{2}$$

This result was also obtained by Röseler [5] and Larsen [6] using different variational approaches and has been accepted as the best result for a long time.

On the other hand, in the intermediate-coupling range, it is in our opinion difficult to decide on which approach has given the best results for the effective mass—unlike the case for the ground-state energy. The reasons for this are twofold. First, it cannot be proved that the variational result for the mass is an upper (or lower) bound for the exact value. Second, there are several definitions of the polaron mass in the literature (one might refer to [10] and [11]). Despite the fact that convincingly good results for the effective mass in the intermediate-coupling range are still lacking, we can judge a new approach by comparison with the often-quoted results, such as those from various path integral approaches [3, 7–9].

As is well known, almost all methods developed in polaron physics can be extended to the calculation of the polaron effective mass. In this paper we will follow our previous method [12] for calculating the polaron effective mass. We had calculated the polaron ground-state energy by a nonvariational method [12] where an extended phonon coherent state was proposed, and the results obtained are in close agreement with the recent Monte Carlo ones. In order to calculate the polaron effective mass, we will keep the total polaron momentum $\boldsymbol{Q}$ in all procedures. Consequently, we derive a self-consistent integral equation from which the energy of a moving polaron can be obtained. In the weak-coupling limit, we analytically calculate the expansion of the effective mass in powers of the coupling constant. Most importantly, we solve the integral equation numerically by an iteration method and evaluate the polaron effective mass for a wide range of the coupling constant. Finally, the present results will be compared with those from other approaches.

2. Integral equation

As before, we first apply the canonical transformation of Lee, Low, and Pines (LLP) [13] to the Hamiltonian (1) and adopt the units $2m = \omega_0 = 1$, which gives

$$H = \left(\boldsymbol{Q} - \sum_{\boldsymbol{q}} \boldsymbol{q} a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}}\right)^2 + \sum_{\boldsymbol{q}} a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}} + \sum_{\boldsymbol{q}} v_{\boldsymbol{q}} (a_{\boldsymbol{q}}^\dagger + a_{\boldsymbol{q}}) \tag{3}$$

where $v_{\boldsymbol{q}} = \sqrt{4\pi\alpha}/\nu^{1/2}|\boldsymbol{q}|$.

Then, we take the phonon state as the following coherent state:

$$|\ \rangle_0 = \prod_{\boldsymbol{q}'} \mathrm{e}^{\alpha(\boldsymbol{q}')a_{\boldsymbol{q}'}^\dagger}|0\rangle \qquad a_{\boldsymbol{q}}|\ \rangle_0 = \alpha(\boldsymbol{q})|\ \rangle_0. \tag{4}$$

The Schrödinger equation for $|\ \rangle_0$ is

$$E|\ \rangle_0 = Q^2 + \sum_{\boldsymbol{q}} (1 - 2\boldsymbol{Q}\cdot\boldsymbol{q} + q^2)\alpha(\boldsymbol{q}) a_{\boldsymbol{q}}^\dagger|\ \rangle_0 + \sum_{\boldsymbol{q}} v_{\boldsymbol{q}}\alpha(\boldsymbol{q})|\ \rangle_0 + \sum_{\boldsymbol{q}} v_{\boldsymbol{q}} a_{\boldsymbol{q}}^\dagger|\ \rangle_0 \tag{5}$$

where we have neglected the $(a^\dagger)^2$-term. Equating the coefficients of $(a^\dagger)^0$ and $(a^\dagger)^1$ yields

$$\alpha(\boldsymbol{q}) = -\frac{v_{\boldsymbol{q}}}{1 - 2\boldsymbol{Q}\cdot\boldsymbol{q} + q^2} \tag{6}$$

$$E = Q^2 + \sum_{\boldsymbol{q}} v_{\boldsymbol{q}}\alpha(\boldsymbol{q}). \tag{7}$$

By inserting equation (6) into equation (7) and replacing the discrete summation by a continuous integral, the energy of moving polaron $E(Q)$ can be obtained as

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

If we set the polaron momentum $\boldsymbol{Q}$ equal to zero, we get $E_0 = -\alpha$. This is just the well known result for the ground-state energy in second-order perturbation theory.

In this paper, the effective mass of a slowly moving polaron is defined as

$$m^* = \frac{1}{\frac{1}{2}(\partial^2/\partial Q^2)E(Q)|_{Q=0}} \qquad (2m = 1). \tag{9}$$

This is one of several definitions given in [11], and has usually been employed in approaches developed on the basis of the LLP transformation [13].

After substituting (8) into (9) we obtain the effective mass of polarons easily:

$$m^* = 1 + \alpha/6. \tag{10}$$

This is identical to the second-order perturbative result for the effective mass [4].

To calculate the polaron effective mass more accurately, we will follow our previous approach as fully discussed in [12]. It is straightforward to improve the phonon state (4) to the following extended coherent-state form:

$$|\,\rangle = |\,\rangle_0 + \sum_{\boldsymbol{q}_1, \boldsymbol{q}_2} b(\boldsymbol{q}_1, \boldsymbol{q}_2) a^\dagger_{\boldsymbol{q}_1} a^\dagger_{\boldsymbol{q}_2} |\,\rangle_0 \tag{11}$$

where $b(\boldsymbol{q}_1, \boldsymbol{q}_2)$ is the interchanging symmetrical function of $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$, and will be determined below. Physically, it is implied in equation (11) that correlations between wave vectors of pairs of emitted phonons in the field are under consideration.

We will omit the detailed procedures, which are the same as in [12], and present the following three identities directly:

$$E = Q^2 + \sum_{\boldsymbol{q}} v_{\boldsymbol{q}} \alpha(\boldsymbol{q}) \tag{12}$$

$$v_{\boldsymbol{q}} + (1 - 2\boldsymbol{Q}\cdot\boldsymbol{q} + q^2)\alpha(\boldsymbol{q}) + 2\sum_{\boldsymbol{q}'} v_{\boldsymbol{q}'} b(\boldsymbol{q}', \boldsymbol{q}) = 0 \tag{13}$$

$$\left\{ \sum_{\boldsymbol{q}} v_{\boldsymbol{q}} \alpha(\boldsymbol{q}) - E + Q^2 + [2 - 2\boldsymbol{Q}\cdot(\boldsymbol{q}_1 + \boldsymbol{q}_2) + q_1^2 + q_2^2] + 2\boldsymbol{q}_1\cdot\boldsymbol{q}_2 \right\} b(\boldsymbol{q}_1, \boldsymbol{q}_2) = -\boldsymbol{q}_1\cdot\boldsymbol{q}_2\, \alpha(\boldsymbol{q}_1)\alpha(\boldsymbol{q}_2). \tag{14}$$

According to equations (12) and (14) it can be seen that $b(\boldsymbol{q}_1, \boldsymbol{q}_2)$ satisfies

$$b(\boldsymbol{q}_1, \boldsymbol{q}_2) = -\frac{\boldsymbol{q}_1\cdot\boldsymbol{q}_2\, \alpha(\boldsymbol{q}_1)\alpha(\boldsymbol{q}_2)}{2 - 2\boldsymbol{Q}\cdot(\boldsymbol{q}_1 + \boldsymbol{q}_2) + (\boldsymbol{q}_1 + \boldsymbol{q}_2)^2}. \tag{15}$$

Inserting equation (15) into equation (13) we get the self-consistent equation obeyed by $\alpha(\boldsymbol{q})$:

$$\alpha(\boldsymbol{q}) = -\frac{v_{\boldsymbol{q}}}{1 - 2\boldsymbol{Q}\cdot\boldsymbol{q} + q^2} + \frac{2}{1 - 2\boldsymbol{Q}\cdot\boldsymbol{q} + q^2} \sum_{\boldsymbol{q}'} v_{\boldsymbol{q}'} \frac{\boldsymbol{q}\cdot\boldsymbol{q}'\, \alpha(\boldsymbol{q})\alpha(\boldsymbol{q}')}{2 - 2\boldsymbol{Q}\cdot(\boldsymbol{q}_1 + \boldsymbol{q}_2) + (\boldsymbol{q} + \boldsymbol{q}')^2}. \tag{16}$$

It remains to obtain $E(Q)$ from equations (12) and (16). Obviously, it is more difficult to solve these equations than in the previous calculation of the ground-state energy, due to the presence of the vector $\boldsymbol{Q}$. Note that the expression for $\alpha(\boldsymbol{q})$ should include the angle θ between the vectors $\boldsymbol{Q}$ and $\boldsymbol{q}$. Without loss of generality, we select $\boldsymbol{Q}$ to be along the z-axis, and suppose that $\boldsymbol{Q}$ and $\boldsymbol{q}$ are in the y–z plane; therefore the coordinates of the vectors $\boldsymbol{Q}$, $\boldsymbol{q}$, and $\boldsymbol{q}'$ can be expressed as $(0, 0, Q)$, $(0, q\sin\theta, q\cos\theta)$, and $(q'\sin\theta'\cos\varphi', q'\sin\theta'\sin\varphi', q'\cos\theta')$. The relevant scalar products of these vectors are given by

$$\begin{aligned}\boldsymbol{Q}\cdot\boldsymbol{q} &= Qq\cos\theta\\ \boldsymbol{Q}\cdot\boldsymbol{q}' &= Qq'\cos\theta'\\ \boldsymbol{q}\cdot\boldsymbol{q}' &= qq'(\sin\theta\sin\theta'\cos\varphi' + \cos\theta\cos\theta').\end{aligned} \tag{17}$$

Next, converting the summation $\sum_{\boldsymbol{q}'}$ in equation (16) into an integration

$$(\nu/(2\pi)^3)\int \mathrm{d}\boldsymbol{q}'$$

and performing the φ'-dependent integration over the interval $[0, 2\pi]$ analytically gives

$$\begin{aligned}\alpha(q,\theta) = &-\frac{v_q}{1-2Qq\cos\theta+q^2} + \frac{\nu}{4\pi^2(1-2Qq\cos\theta+q^2)}\\ &\times\int_0^\infty \mathrm{d}q'\int_0^\pi \mathrm{d}\theta'\; q'^2\sin\theta' v_{q'}\alpha(q,\theta)\alpha(q',\theta')\\ &\times\left\{1-\frac{A}{\sqrt{[A+2qq'\cos(\theta+\theta')][A+2qq'\cos(\theta-\theta')]}}\right\}\end{aligned} \tag{18}$$

where $A = 2-2Q(q\cos\theta+q'\cos\theta')+q^2+q'^2$. Here we have used the definite integral formula

$$\int_0^\pi \frac{\mathrm{d}x}{a+b\sin x} = \frac{\pi}{\sqrt{a^2-b^2}} \qquad (\text{if } a^2 \geqslant b^2).$$

It should be mentioned that the inequality condition in the brackets is met automatically for small Q in the treatment of the effective mass, so this formula can be used straightforwardly.

For simplicity, we introduce the following function:

$$F(q,\theta) = \frac{\nu}{(2\pi)^2}q^2\sin\theta\, v_q\alpha(q,\theta). \tag{19}$$

Thus, equations (12) and (16) can be respectively reduced to

$$E = Q^2 + \int_0^\infty \mathrm{d}q\int_0^\pi \mathrm{d}\theta\; F(q,\theta) \tag{20}$$

$$\begin{aligned}F(q,\theta) = &-\frac{\alpha\sin\theta}{\pi(1-2Qq\cos\theta+q^2)} + \frac{1}{1-2Qq\cos\theta+q^2}\\ &\times\int_0^\infty \mathrm{d}q'\int_0^\pi \mathrm{d}\theta'\; F(q,\theta)F(q',\theta')\\ &\times\left\{1-\frac{A}{\sqrt{[A+2qq'\cos(\theta+\theta')][A+2qq'\cos(\theta-\theta')]}}\right\}.\end{aligned} \tag{21}$$

It is seen that equation (21) is the self-consistent integral equation obeyed by $F(q,\theta)$, and equation (20) can be used to calculate the energy of a moving polaron $E(Q)$ if we actually solve for $F(q,\theta)$. Some analytical and numerical results are presented in the next section.

3. Results and discussion

It can be seen that, if the second term in the right-hand side of equation (21) is disregarded, we have

$$F(q,\theta) = -\frac{\alpha\sin\theta}{\pi(1-2Qq\cos\theta+q^2)}. \tag{22}$$

Inserting equation (22) into equation (20), equation (8) is then recovered. For further iteration, substituting equation (22) into the right-hand side of equation (21), followed by insertion of the resultant new expression for $F(q,\theta)$ into equation (20) and performing of the multiple integrations, leads to the energy with a small momentum $\boldsymbol{Q}$ given as follows:

$$E(Q) = -(\alpha + 0.015\,9196\,\alpha^2) + (1 - \alpha/6 + 0.004\,150\,15\,\alpha^2)Q^2 + \mathrm{O}(Q^4). \tag{23}$$

It is interesting to note that the previous expansions of the ground-state energy up to the α^2-term emerge in their entirety in the first brackets in the right-hand side of equation (23), which is just the fourth-order perturbative ground-state energy [4]. Consequently, on inserting equation (23) into equation (9), we get the polaron effective mass as follows:

$$m^* = 1 + \alpha/6 + 0.023\,627\,63\,\alpha^2. \tag{24}$$

This is simply the previous fourth-order perturbative result for the effective mass of equation (2) mentioned above. For the next iteration, we would have the polaron effective mass expansion up to the α^3-term. To the best of our knowledge, the effective mass in sixth-order perturbation theory has not been calculated to date. On the other hand, the α^3-term in the mass expansion in this paper is not completely calculated either, because we used an approximate wave function (11). Hence it is pointless to write this term down. Note that such a procedure can be performed step by step; generally speaking, we could obtain the following expansion of the effective mass in powers of α analytically:

$$m^* = 1 + \alpha/6 + 0.023\,627\,63\,\alpha^2 + \sum_{k=3}^{\infty} C_k\alpha^k. \tag{25}$$

It is clear that the infinite-iteration technique can be used to solve the self-consistent integral equation (21) numerically. Solving for $F(q,\theta)$, with the help of equations (20) and (9), we can calculate the polaron effective mass for a wide range of coupling constant, not merely in the weak-coupling limit. By the way, on setting the polaron momentum to $Q = 0$, our previous results for the ground-state energy would be obtained naturally.

Table 1. The comparison of some results for the polaron effective mass as a function of the coupling constant up to $\alpha = 4$. (The notation is defined in the text.)

α	m^*	m^*_F	m^*_{LR}	m^*_{AFR}	m^*_{GLS}	m^*_{SQZ}	m^*_{PT4}
1	1.195	1.196	1.194	1.196	1.196	1.194	1.190
2	1.476	1.472	1.465	—	1.476	1.442	1.428
3	1.909	1.889	1.868	1.824	1.900	1.744	1.713
4	2.725	2.579	2.526	—	2.606	2.102	2.045

In this paper, we calculate the polaron effective mass for a wide range of the coupling constant numerically up to $\alpha = 4$. In order to test our method, we compare the present results with often-quoted ones. In table 1, in addition to the present results, various path integral results are also collected together. The Feynman effective mass (m^*_F) calculated by Schultz (see [3]) is listed in the third column, and the second-order correction to the

Feynman effective mass given by Lu and Rosenfelder [9] (m^*_{LR}) and the recent Monte Carlo results obtained by Alexandrou *et al* [8] (m^*_{AFR}) are displayed in the fourth and fifth columns respectively. In the sixth column, we list the results of Gerlach *et al* [7] (m^*_{GLS}), which were calculated from the ground-state energy by means of a different definition in the framework of the path integral *ansatz*. We also present the effective mass calculated with a two-mode squeeze state by Kandemir and Altanhan [10] (m^*_{SQZ}) and using the fourth-order perturbation theory (m^*_{PT4}) in the last two columns.

It is demonstrated in table 1 that our results are very close to the results of Gerlach *et al* [7], and agree with the Feynman ones (see [3]) and their second-order corrections [9] for $\alpha \leqslant 4$. Even at $\alpha = 4$, our results are only higher than these results by about 5%. We have also calculated the effective mass for $\alpha > 4$ and find that our results deviate more and more from the well known results. This is to say, our approach to the calculation of the effective mass is not valid for $\alpha > 4$ and its validity range is slightly smaller than that in the calculation of the ground-state energy. It is indicated that the effective mass is a more sensitive quantity than the energy as regards evaluation by our approach.

It is interesting to note that, in the intermediate-coupling range, our results are a little higher than those obtained by various path integral approaches except the Monte Carlo ones. In our opinion, this may be partly attributed to the fact that the definition of the effective mass is not well founded in the path integral *ansatz*, unlike that of the ground-state energy. By the way, the results for the mass obtained with the two-mode squeeze state and in the fourth-order perturbation theory depart from the common behaviour of the well known results more drastically with the increasing of the coupling constant, as is also shown in table 1.

We would like to add a few remarks about the results from various path integral methods and the present ones. Recently, Lu *et al* have made second-order corrections to the Feynman effective mass. But the corrections stay very small over the whole coupling range, from which it follows that the Feynman effective mass remains an elegant one against which to check the results obtained by other approaches. Fortunately, our results for the mass are in agreement with the Feynman ones for a wide coupling range. As regards the large-scale Monte Carlo calculations [2, 8], in our opinion the exact results obtained for the effective mass should be restricted to the weak-coupling range due to the insufficient convergence in the intermediate-coupling range. It is likely that the effective mass is also a much more sensitive quantity than the ground-state energy as regards stochastic Monte Carlo calculation.

It is very important to link the average number of virtual phonons to the validity range of our method in the calculation of the effective mass. For $\alpha = 4$, the average number of virtual phonons is roughly estimated to be two by means of the simple approximate relation $N = \alpha/2$, which is the well known LLP result [13]. Physically, if the average number of particles in the field is less than two, it is sufficient to consider correlations of the vectors of pairs of virtual phonons. Fortunately, from the above discussions, this is exactly the case—at least for the effective mass. It can be predicted that if the correlations of the wave vectors of more than two phonons are taken into account, the validity range will be enlarged further. By the way, the difference between the present and the unknown exact results in the intermediate-coupling range may be attributed to an inadequacy of the present approach.

Finally, on the basis of the above discussions, it can be concluded that our previous approach is also suited to the calculation of the polaron effective mass, which again underlines the effectiveness of our approach in polaron physics. It should be pointed out that this well developed approach could also be useful in other polaron-like problems.

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