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Polaron effective mass in d dimensions within and beyond the generalized Gaussian approximation

G Ganbold†§ and G V Efimov‡

† Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstraße 7, D-91058 Erlangen, Germany

‡ Bogolyubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, 141980 Dubna, Russia

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Abstract. The effective mass of the Fröhlich polaron model in d spatial dimensions is obtained within the Gaussian-equivalent representation, that is, within a suitably rearranged perturbative path-integral approach, whose leading order already takes care of all Gaussian fluctuations. In doing so, the authors extend their earlier investigations (*Phys. Rev.* B **50** 3733 (1994)) of the polaron ground-state energy. Analytical expressions for the effective mass are derived in the weak- and strong-coupling limit. In the intermediate-coupling regime, the effective mass is calculated numerically for the cases of two and three dimensions. The new results are compared with previously known data.

1. Introduction

The polaron concept introduced by Landau [1] is devoted to the interaction of an electron placed in a polar or ionic crystal [2, 3]. The resulting interaction with the phonons of longitudinal optical lattice vibrations is typically modelled by a Hamiltonian due to Fröhlich [4], containing a dimensionless coupling constant $\alpha \geqslant 0$. Fröhlich's Hamiltonian has been the subject of a huge number of theoretical investigations, for review-type literature see [5]–[10]. In more recent years the properties of polarons confined to two spatial dimensions ($d = 2$) have also attracted considerable interest [11, 12].

Quantities of interest are the ground-state energy (GSE), the effective mass (EM), and some other quasi-particle characteristics of the Fröhlich polaron. Typically, exact results are available only in the limiting cases of weak coupling ($\alpha \to 0$) and strong coupling ($\alpha \to \infty$). While the weak-coupling results may be obtained by conventional perturbation expansions, rigorous proofs of the strong-coupling behaviour require more advanced techniques [13]–[17], reflecting the qualitative difference between the polaron states in the two limits.

Among the approximations which are believed to describe the polaron characteristics reasonably well for all values of α, Feynman's celebrated path-integral approach [18] stands out in that it smoothly interpolates between the weak- and the strong-coupling regime. It is based on a two-parameter trial action functional representing a retarded harmonic oscillator. Later this variational approach was generalized to two [19], more than two [20, 21], and even to a continuum of such oscillators [22, 23].

§ Permanent address: Institute of Physics and Technology, Mongolian Academy of Sciences, 210651 Ulaanbaatar, Mongolia.

In our previous investigations we estimated the GSE of the Fröhlich polaron in three [24] and $d \geqslant 2$ dimensions [25, 26] within a rearranged perturbative path-integral approach, where the leading order takes into account all Gaussian fluctuations of the polaron in its ground state and higher orders systematically correct for non-Gaussian contributions. In [25, 27] this approach is called the *Gaussian-equivalent representation* (GER). Similar to the treatment of certain models of quantum field theory this approach does not require the smallness of the coupling constant. Not surprisingly, we have found that our leading-order term for $d = 3$ gives the same upper bound to the GSE as was obtained in [23]. The resulting upper bounds to the GSE turned out to improve Feynman's estimate only slightly. Nevertheless, the numerical values of [23, 25] belong to the lowest ones available. Moreover, it has been shown [28] that results based on this action, when suitably extended to d dimensions, become asymptotically exact in the limit $d \to \infty$.

We have also calculated in [25] the next-to-leading non-Gaussian correction to the GSE for both the $d = 3$ and the $d = 2$ case for arbitrary coupling $\alpha > 0$. In the weak- and strong-coupling limits, where exact answers were available for comparison, we have found definite improvements over the Gaussian approximation for the GSE.

Among the unanswered questions in [22]–[25] are the following three. First, what is the quantitative difference between the masses obtained within the Feynman and the general Gaussian approaches? Second, what can be said about the corrections which arise when going beyond the general quadratic action? And third, which results can be obtained when the approach is extended to two dimensions ($d = 2$)?

The purpose of the present paper is to extend our earlier investigations to the EM. In doing so, the general formulation of the GER will be given for arbitrary values of the dimension d. For explicit results we concentrate on the physically relevant cases of $d = 3$ and $d = 2$. In this sense we partially answer all the questions above.

The paper is organized as follows. The basic formalism is developed in section 2. Here we briefly review the path-integral approach to the EM of the Fröhlich polaron (embedded) in d dimensions. In section 3 we derive and discuss the leading-order term of the EM. The next-to-leading order is evaluated in section 4. In section 5 we will compare our analytical and numerical results with previously obtained data for the polaron EM in two and three dimensions.

2. Polaron path integral within the GER method

The Hamiltonian operator of the Fröhlich polaron model is:

$$H = \frac{\boldsymbol{p}^2}{2} + \sum_{\boldsymbol{k}} a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + \frac{1}{\sqrt{\Omega}} \sum_{\boldsymbol{k}} g_{\boldsymbol{k}} \left(a_{\boldsymbol{k}}^\dagger \mathrm{e}^{-\mathrm{i}\boldsymbol{kr}} - a_{\boldsymbol{k}} \mathrm{e}^{\mathrm{i}\boldsymbol{kr}} \right) \tag{1}$$

where, $\boldsymbol{p}$ and $\boldsymbol{r}$ denote the momentum and position operators of the electron, Ω is the quantization volume, and $\boldsymbol{k}$, $a_{\boldsymbol{k}}$ and $a_{\boldsymbol{k}}^\dagger$ are the wavevector, annihilation and creation operators of a phonon. Here we are using appropriate units, such that $m_B = \omega = \hbar = c = 1$, where m_B is the electron bare mass, ω denotes the frequency of the LO-mode of lattice vibrations. The electron–phonon coupling factor $g_{\boldsymbol{k}} = \mathrm{i}(4\pi\alpha)^{1/2}/|\boldsymbol{k}|$ is characterized by the dimensionless coupling constant α. All the vectors in (1) are three dimensional.

To extend the consideration to arbitrary spatial dimensions ($d \geqslant 2$) we redefine the coupling factor as follows [25] (see also [29]):

$$|g_{\boldsymbol{k}}|^2 := (2\pi)^d \Lambda_d \, \alpha / \, |\boldsymbol{k}|^{d-1} \qquad \Lambda_d := \Gamma[(d-1)/2]/\sqrt{8}\pi^{(d+1)/2}. \tag{2}$$

The linear character of the electron–phonon coupling in (1) allows one to integrate over the phonons in the path-integral (PI) formulation. The free energy $F(\alpha,\beta)$ of the polaron at temperature $(1/k_B\beta)$ may then be found in the following way

$$\mathrm{e}^{-\beta F(\alpha,\beta)} = \int\limits_{\boldsymbol{r}(0)=0} \mathcal{D}\boldsymbol{r}\,\delta(\boldsymbol{r}(\beta))\,\mathrm{e}^{\alpha\,\Phi_\beta(\boldsymbol{r})}$$
$$\Phi_\beta(\boldsymbol{r}) := \frac{1}{\sqrt{8}}\iint\limits_0^\beta \mathrm{d}t\,\mathrm{d}s\,\frac{\mathrm{e}^{|t-s|}+\mathrm{e}^{\beta-|t-s|}}{(\mathrm{e}^\beta-1)|\boldsymbol{r}(t)-\boldsymbol{r}(s)|} \tag{3}$$

where Wiener's functional path measure is heuristically given as follows:

$$\mathcal{D}\boldsymbol{r} \propto \delta\boldsymbol{r}\exp\left\{-\frac{1}{2}\int\limits_0^\beta \mathrm{d}t\,\dot{\boldsymbol{r}}^2(t)\right\} \qquad \int\limits_{\boldsymbol{r}(0)=0}\mathcal{D}\boldsymbol{r}\cdot 1 = 1. \tag{4}$$

The GSE of the system is the zero-temperature limit: $F(\alpha,\beta) \underset{\beta\to\infty}{\longrightarrow} E(\alpha)$.

The advantage of the PI formulation is obvious: the original many-body problem has been transformed into an effective one-particle model, with just the electron coordinate $\boldsymbol{r}(t)$. On the other hand, one obtains in (3) an effective action which is nonlocal in time and has a Coulomb-like singularity that—up to now—has prevented any further exact analytic treatment except in the limits $\alpha\to 0$ and $\alpha\to\infty$.

The EM of the polaron may be defined in different ways. We follow the standard definition by using an expansion of the real part of the self-energy with respect to small momentum (see, e.g., [30]). For this purpose, we introduce the polaron partition function projected at small fixed momentum $\boldsymbol{p}$ as follows:

$$\mathrm{e}^{-\beta\widetilde{\mathcal{F}}(\boldsymbol{p},\alpha,\beta)} := \int\limits_{\boldsymbol{r}(0)=0}\mathcal{D}\boldsymbol{r}\,\mathrm{e}^{-\mathrm{i}\boldsymbol{p}\boldsymbol{r}(\beta)}\,\mathrm{e}^{\alpha\,\Phi_\beta(\boldsymbol{r})} = \int \mathrm{d}\boldsymbol{x}\,\mathrm{e}^{-\mathrm{i}\boldsymbol{p}\boldsymbol{x}}\,\mathrm{e}^{-\beta\mathcal{F}(\boldsymbol{x},\alpha,\beta)}$$
$$\mathrm{e}^{-\beta\mathcal{F}(\boldsymbol{x},\alpha,\beta)} := \int\limits_{\boldsymbol{r}(0)=0}\mathcal{D}\boldsymbol{r}\,\delta(\boldsymbol{x}-\boldsymbol{r}(\beta))\,\mathrm{e}^{\alpha\,\Phi_\beta(\boldsymbol{r})}. \tag{5}$$

For zero coupling it becomes

$$\mathrm{e}^{-\beta\widetilde{\mathcal{F}}(\boldsymbol{p},0,\beta)} = \mathrm{e}^{-\frac{\beta}{2}\boldsymbol{p}^2} \tag{6}$$

which can inspire one to find the effective mass of the polaron as follows:

$$m^*(\alpha) := d\left(\frac{\partial^2 \lim_{\beta\to\infty}\widetilde{\mathcal{F}}(\boldsymbol{p},\alpha,\beta)}{\partial\boldsymbol{p}^2}\bigg|_{|\boldsymbol{p}|=0}\right)^{-1}. \tag{7}$$

This definition obeys the conventional normalization condition $m^*(0) = 1$ and is in agreement with (6). Furthermore, it is convenient to change the variables of integration to $\boldsymbol{r}(t)\mapsto\boldsymbol{r}(t)+\boldsymbol{x}t/\beta$ in (5).

The path integral (5) is the central quantity of the present paper. To evaluate it we use the GER method which has previously been applied successfully to the polaron GSE [25, 26] and to other problems in quantum physics [27]. The key idea of our approach is a representation which isolates the most general Gaussian part in PIs, including (5). Within this approach one is able to describe the ground state of the system more precisely by introducing a new Gaussian measure $\mathrm{d}\sigma(\boldsymbol{r})$ instead of the original measure $\mathcal{D}\boldsymbol{r}$. This goal is achieved through a canonical transformation which is constrained by the requirements that the interaction part of the polaron action should be rewritten in normal-ordered form and must not contain linear and quadratic path configurations (we call this form *correct*). These requirements lead to the equations governing the possible form of the Gaussian measure $\mathrm{d}\sigma$.

As a result the PI (5) may be rewritten as

$$\mathrm{e}^{-\beta\mathcal{F}(\boldsymbol{x},\alpha,\beta)} = \mathrm{e}^{-\beta\mathcal{F}_G(\boldsymbol{x},\alpha,\beta)} J_\beta(\alpha,\boldsymbol{x}) \tag{8}$$

where the *leading-order Gaussian approximation* is defined as follows:

$$\begin{aligned}\mathrm{e}^{-\beta\mathcal{F}_G(\boldsymbol{x},\alpha,\beta)} := \exp\bigg\{ & -\frac{\boldsymbol{x}^2}{2\beta} + \frac{1}{2}\ln\det(D_o^{-1}, D) \\ & - \frac{1}{2}([D_o^{-1} - D^{-1}], D) + \frac{\alpha}{2}\int \mathrm{d}\Omega\, \exp\left(\mathrm{i}\boldsymbol{k}\boldsymbol{x}\frac{t-s}{\beta}\right)\bigg\}.\end{aligned} \tag{9}$$

Here and in the following we use the notation

$$\int \mathrm{d}\Omega\,(\ldots) := \Lambda_d \iint\limits_0^\beta \mathrm{d}t\,\mathrm{d}s\,\exp(-|t-s|)\int \frac{\mathrm{d}\boldsymbol{k}}{|\boldsymbol{k}|^{d-1}}\exp\left\{-\boldsymbol{k}^2 F(t-s)\right\}(\ldots)$$

$$(A,B) := \int\limits_0^\beta \mathrm{d}t\, A(t)\,B(t) \qquad \mathrm{e}_2^x := \mathrm{e}^x - 1 - x - x^2/2 \qquad \alpha_d := \alpha\frac{3\sqrt{\pi}\,\Gamma[(d-1)/2]}{2\,d\,\Gamma[d/2]} \tag{10}$$

where α_d plays the role of a *re-scaled* coupling constant depending on the spatial dimension number d. The relation between the re-scaled and physical coupling constants are $\alpha_2 = 3\pi\alpha/4$ and $\alpha_3 = \alpha$ in two and three dimensions, respectively.

The *non-Gaussian corrections* to (9) should be obtained by evaluating the following new PI

$$J_\beta(\alpha,\boldsymbol{x}) := \int \mathrm{d}\sigma\,\exp\left\{\frac{\alpha}{2}\int \mathrm{d}\Omega\,\exp\left(\mathrm{i}\boldsymbol{k}\boldsymbol{x}\frac{t-s}{\beta}\right)\, :\mathrm{e}_2^{\mathrm{i}\boldsymbol{k}(\boldsymbol{r}(t)-\boldsymbol{r}(s))}:\right\} \tag{11}$$

$$\mathrm{d}\sigma \propto \delta\boldsymbol{r}\,\exp\left\{-\frac{1}{2}\iint\limits_0^\beta \mathrm{d}t\,\mathrm{d}s\,\boldsymbol{r}(t)D^{-1}(t,s)\boldsymbol{r}(s)\right\} \qquad \int \mathrm{d}\sigma\cdot 1 = 1$$

where the symbol : : denotes 'normal-ordering' with respect to the general Gaussian measure $\mathrm{d}\sigma$ defined on paths which start and end at the origin: $\boldsymbol{r}(0) = \boldsymbol{r}(\beta) = \boldsymbol{0}$. For $\beta\to\infty$, the adjustable function $F(t) = D(0) - D(t)$ has to be derived from the following set of integral equations:

$$\begin{aligned}\tilde{\Sigma}(k) &= \frac{1}{3\sqrt{2\pi}}\int\limits_0^\infty \mathrm{d}t\,\exp(-t)\,\frac{1-\cos(kt)}{F^{3/2}(t)} \\ F(t) &= \frac{1}{\pi}\int\limits_0^\infty \mathrm{d}k\,\frac{1-\cos(kt)}{k^2+\alpha_d\tilde{\Sigma}(k)}.\end{aligned} \tag{12}$$

The Fourier transform of $D(t)$ is given by

$$\tilde{D}(k) = \frac{1}{k^2+\alpha_d\tilde{\Sigma}(k)}. \tag{13}$$

One should note that $\tilde{D}(k)$ has the typical form of the propagator of a scalar particle, but with a k-dependent mass equal to $\mu = [\alpha_d\tilde{\Sigma}(k)]^{1/2}$.

A generalization of equations (12) has been obtained previously by the authors [31] for a quantum-field model with a general action $W[\varphi]$. In [24] it is shown that this generalization indeed turns into (12), when specialized to the three-dimensional polaron. To our knowledge, an equivalent form of these integral equations, extracting the complete quadratic part of the polaron ground-state, has been obtained previously, e.g. in [23] for $d = 3$, by considering the stationarity condition for an extension of Feynman's variational approach to general quadratic trial actions. This idea was proposed independently also in [22]. Note also that the same equations govern the leading term of a $1/d$-expansion scheme applied to the polaron model [28].

3. Gaussian approximation to the polaron mass

Up to now the PI (5) has not been evaluated explicitly. Various approximation methods have therefore been developed. We first consider the zero-temperature limit of (5) in the Gaussian (leading-order) approximation of the GER method, that is

$$\mathrm{e}^{-\beta\mathcal{F}_G(\boldsymbol{x},\alpha,\beta)} \xrightarrow[\beta\to\infty]{} \exp\left\{-\beta E_o(\alpha) - \frac{\boldsymbol{x}^2}{2\beta}\left[1 + M_o(\alpha)\right]\right\} \tag{14}$$

$$M_o(\alpha) := \lim_{\beta\to\infty} \frac{\alpha}{2\beta d}\int \mathrm{d}\Omega\, \boldsymbol{k}^2\,(t-s)^2 = \frac{\alpha_d}{2}\frac{\partial^2\tilde{\Sigma}(p)}{\partial p^2}\bigg|_{p=0}.$$

The Gaussian approximation $E_o(\alpha)$ to the GSE has been obtained previously in [25]. It gives an upper bound to the exact polaron GSE, which slightly improves Feynman's celebrated estimate. Using the right-hand side of (14) as an approximation in (5) and (7), we obtain the Gaussian leading-order EM of the polaron in d dimensions as follows:

$$m_o^*(\alpha) = 1 + M_o(\alpha) = 1 + \frac{\alpha_d}{6\sqrt{2\pi}}\int_0^\infty \mathrm{d}t\, t^2\,\frac{\exp(-t)}{F^{3/2}(t)}. \tag{15}$$

Again, the adjustable function $F(t)$ in (15) is the solution of equations (12). The following four remarks are in order.

i. Exact analytic solutions to (12) are available in the weak- and strong-coupling limits:

$$F(t) = \begin{cases} t/2 - O(\alpha_d) & \alpha\to 0 \\ \left[1-\exp(-v_\infty t)\right]/2v_\infty \qquad v_\infty := 4\alpha_d^2/9\pi & \alpha\to\infty. \end{cases} \tag{16}$$

Note that these solutions correspond to the propagator (13), but with fixed masses $\mu = 0$ and $\mu = v_\infty$, respectively. Corresponding solutions for the EM are given in section 5.

ii. For intermediate-coupling ($\alpha \approx 1$), equations (12) seem to admit no analytic solutions. Nevertheless, any strictly positive function can be used instead of $F(t)$ to derive an approximation to the GSE and the EM following the lines of the Gaussian approximation. The result, however, will in general be inferior to the one corresponding to $F(t)$. For example, Feynman's celebrated variational model can be recovered, if one chooses a convex combination

$$F_1(t) := w_o\frac{t}{2} + (1-w_o)\frac{1-\exp(-vt)}{2v} \tag{17}$$

of the two known asymptotical solutions (16) instead of $F(t)$. The stronger the interaction, the smaller the weight factor $w_o := (w/v)^2 \leqslant 1$ should be. Optimizing the two parameters $\{w, v\}$ reproduces Feynman's upper bound $E_F(\alpha)$ to the GSE. Corresponding substitution of the optimal $F_1(t)$ into (15) results in Feynman's mass $m_F^*(\alpha)$. Note, however, that (17) is *not* a solution of equations (12).

iii. An obvious improvement of the Feynman approximation can be obtained by convex combining more strong-coupling components to (17)

$$F_N(t) = w_o \frac{t}{2} + \sum_{i=1}^{N} w_i \frac{1-\exp(-v_i t)}{2v_i} \qquad N \geqslant 2. \tag{18}$$

Optimization with $N = 2$, $N = 3$ and $N = 8$ reproduces the data obtained in [19], [20] and [21], respectively. The limiting case $N \to \infty$ leads, obviously, to the results of the general quadratic action [23].

iv. Due to certain features of the functions $F(t)$ and $\tilde{\Sigma}(k)$ shown in [25], it is possible to obtain the Gaussian leading-order mass for two dimensions in terms of that for three dimensions by rescaling the coupling constant. More precisely,

$$m_o^{*(2)}(\alpha) = m_o^{*(3)}\,(3\pi\alpha/4)\,. \tag{19}$$

For the special case of Feynman's approximation this has been observed previously [12].

Analytical and numerical derivations to $m_o^*(\alpha)$ obtained for $d = 2$ and $d = 3$ are discussed in section 5.

Unfortunately, in contrast to the case of the GSE, where a simple minimum criterion for the optimal solution exists for general α, there is no such criterion for the sign of the sum of all non-Gaussian corrections to the Gaussian leading-order EM. For example, the Gaussian approximation $E_o(\alpha)$ gives an upper bound to the true GSE, but this is not true for $m_o^*(\alpha)$.

4. Non-Gaussian corrections to the polaron mass

The exact mass of the polaron differs from the Gaussian leading-order approximation $m_o^*(\alpha)$ because $J_\beta(\alpha, \boldsymbol{x}) \neq 1$ in (8). This difference disappears only in nonphysical high dimensions $J_\beta(\alpha, \boldsymbol{x}) \underset{d\to\infty}{\longrightarrow} 1$ due to the weakening of the re-scaled coupling $\alpha_d \underset{d\to\infty}{\longrightarrow} 0$. For physically meaningful cases, $d \leqslant 3$, a more precise estimate for (11) is required.

In this section we restrict ourselves to the *second-order* non-Gaussian corrections to the EM. In doing so, we derive the following expression:

$$\begin{aligned} J_\beta(\alpha, \boldsymbol{x}) &= 1 - \beta\Delta E_2(\alpha) - \frac{\boldsymbol{x}^2}{2\beta}\Delta M_2(\alpha) \\ &= 1 + \frac{\alpha^2\Lambda_d^2}{8} \iint_0^\beta \mathrm{d}t\,\mathrm{d}s \iint_0^\beta \mathrm{d}x\,\mathrm{d}y\,\mathrm{e}^{-|t-s|-|x-y|} \\ &\quad\times \int \frac{\mathrm{d}\boldsymbol{k}}{|\boldsymbol{k}|^{d-1}} \int \frac{\mathrm{d}\boldsymbol{p}}{|\boldsymbol{p}|^{d-1}} \exp\left[-\boldsymbol{k}^2 F(t-s) - \boldsymbol{p}^2 F(x-y)\right] \\ &\quad\times \exp\left(\mathrm{i}\boldsymbol{k}\boldsymbol{x}\frac{t-s}{\beta} + \mathrm{i}\boldsymbol{p}\boldsymbol{x}\frac{x-y}{\beta}\right) \mathrm{e}_2^{\boldsymbol{k}\boldsymbol{p}\cdot\Xi(t,s,x,y)} \end{aligned} \tag{20}$$

where a four-point correlation function Ξ has been introduced:

$$\Xi(t,s,x,y) := F(t-x) + F(s-y) - F(s-x) - F(t-y). \tag{21}$$

Omitting the details of the calculations we write the final result for the non-Gaussian correction to the leading-order mass as follows:

$$\Delta M_2(\alpha) = \frac{4\alpha_d^2\, d\, \Gamma[d/2]}{9\pi^{3/2}\Gamma[(d-1)/2]} \int_0^1 \mathrm{d}\xi (1-\xi^2)^{\frac{d-3}{2}} \int_0^\infty \mathrm{d}z_1 \int_{z_1}^\infty \mathrm{d}z_2 \int_{z_2}^\infty \mathrm{d}z_3 \Bigg\{ \mathrm{e}^{-z_3-|z_1-z_2|}$$
$$\times \Bigg[[F(z_2-z_3)z_1^2 + F(z_1)(z_2-z_3)^2] \left(\frac{1}{[4F(z_1)F(z_2-z_3) - \xi^2 \Xi^2]^{3/2}} \right.$$
$$\left. - \frac{1}{[4F(z_1)F(z_2-z_3)]^{3/2}} - \frac{3\xi^2}{2} \frac{\Xi^2(z_1,z_2,z_3,0)}{[4F(z_1)F(z_2-z_3)]^{5/2}} \right)$$
$$+ \xi^2\, z_1\, (z_2-z_3)\, \Xi(z_1,z_2,z_3,0) \left(\frac{1}{[4F(z_1)F(z_2-z_3) - \xi^2 \Xi^2]^{3/2}} \right.$$
$$\left. - \frac{1}{[4F(z_1)F(z_2-z_3)]^{3/2}} \right) \Bigg] + (z_1 \leftrightarrow z_2) + (z_1 \leftrightarrow z_3) \Bigg\}. \qquad (22)$$

In particular, for $d = 3$ the integration over ξ in (22) can be performed explicitly.

Finally, taking into account both the Gaussian leading-order and the second-order non-Gaussian contribution we estimate the polaron effective mass as follows:

$$m^*(\alpha) = m_o^*(\alpha) + \Delta M_2(\alpha). \qquad (23)$$

5. Analytic and numerical results

Both the Gaussian leading-order mass and the second-order non-Gaussian correction may be derived analytically for the weak- and strong-coupling limits. For intermediate coupling, equations (12), and hence, the masses $m_o^*(\alpha)$ and $\Delta M_2(\alpha)$ will be evaluated numerically.

5.1. The weak-coupling limit

The exact results using fourth-order perturbation theory [12, 32, 33, 34] for the polaron EM are:

$$m^*(\alpha) = \begin{cases} 1 + (\pi/8)\,\alpha + 0.1272348\,\alpha^2 + O(\alpha^3) & d = 2 \\ 1 + (1/6)\,\alpha + 0.02362763\,\alpha^2 + O(\alpha^3) & d = 3. \end{cases} \qquad (24)$$

The coefficient of the α^2 term of the Feynman polaron mass overestimates the exact value by 7.8% and 4.5% for $d = 2$ and $d = 3$. The second-order correction to the Feynman result [30] for $d = 3$ fits the correct behaviour in (24).

Knowing explicitly the weak-coupling behaviour of $F(t)$ (see [25]) we derive the leading-order Gaussian contribution to the polaron mass:

$$m_o^*(\alpha) = \begin{cases} 1 + (\pi/8)\,\alpha + \left(3\pi^2/32 - \pi/4\right)\,\alpha^2 + O(\alpha^3) & d = 2 \\ 1 + (1/6)\,\alpha + (1/6 - 4/9\pi)\,\alpha^2 + O(\alpha^3) & d = 3. \end{cases} \qquad (25)$$

Considering the second-order non-Gaussian correction, it is sufficient to use the asymptotic solution $F(t) = t/2$ because the neglected term $O(\alpha_d)$ will generate a mass correction proportional to $O(\alpha_d^3)$. Thus we obtain

$$\Delta M_2(\alpha) = \begin{cases} (1/8)\left[-5 + 9\pi^2\,(19/6\pi - 1)\,/8 + 4\,C_1\right]\alpha^2 + O(\alpha^3) & d = 2 \\ (1/36 - 5/4\sqrt{2} + 4/9\pi + 4\ln(1+1/\sqrt{2})/3)\,\alpha^2 + O(\alpha^3) & d = 3 \end{cases} \qquad (26)$$

where

$$C_1 := \int_0^1 \mathrm{d}x \, \frac{1+6x^2-6x^4+4x^6}{\sqrt{1-x^2}\,(1+x^2)^{7/2}} \arctan\left(\sqrt{\frac{1+x^2}{1-x^2}}\right) = 1.202560452\ldots.$$

Adding (26) to (25) we obtain

$$m^*(\alpha) = \begin{cases} 1 + (\pi/8)\,\alpha + 0.127234835\,\alpha^2 + O(\alpha^3) & d = 2 \\ 1 + (1/6)\,\alpha + 0.0236276301\,\alpha^2 + O(\alpha^3) & d = 3. \end{cases} \tag{27}$$

Our final results (27) for the weak-coupling polaron mass are in complete agreement with previously known data obtained within perturbation [12, 33, 34] and $1/d$-expansion [35] methods.

5.2. *The strong-coupling limit*

For $\alpha \to \infty$, exact results for the polaron EM are available within Pekar's adiabatic approximation [15, 17, 36, 37]:

$$m^*(\alpha) = \begin{cases} 0.7328\,\alpha^4 + O(1) & d = 2 \\ 0.022702\,\alpha^4 + O(1) & d = 3. \end{cases} \tag{28}$$

As α becomes very large, $F(t)$ behaves as in (16). By using this asymptotical solution, we derive

$$m_o^*(\alpha) = \begin{cases} (\pi^2/16)\,\alpha^4 + O(1) & d = 2 \\ (16/81\pi^2)\,\alpha^4 + O(1) & d = 3. \end{cases} \tag{29}$$

One can see that the leading-order Gaussian mass $m_o^*(\alpha)$ for $\alpha \to \infty$ behaves similarly to corresponding results due to Feynman's and the $1/d$-expansion methods. These results underestimate the corresponding exact ones [36, 37]. This is probably due to the fact that for increasing α the nonlocal Coulomb-like polaron self-interaction is less well approximated by an oscillator-type term used for our leading-order mass.

The second-order non-Gaussian corrections become:

$$\Delta M_2^*(\alpha) = \begin{cases} 0.065027\,\alpha^4 & d = 2 \\ (64\{\ln[4(2-\sqrt{3})] - 1/16\}/27\pi^2)\,\alpha^4 & d = 3. \end{cases} \tag{30}$$

Finally we get:

$$m^*(\alpha) = \begin{cases} 0.681878\,\alpha^4 + O(1) & d = 2 \\ 0.021656\,\alpha^4 + O(1) & d = 3. \end{cases} \tag{31}$$

This underestimates Pekar's adiabatic solutions by 6.9% and 4.6% in two and three dimensions, respectively. Hence, higher-order non-Gaussian corrections are required to fill this gap.

5.3. *The intermediate-coupling range*

For intermediate coupling we have solved equations (12) numerically by means of an iterative procedure starting from (17) as the first approximation. We have checked that different numbers of iteration steps and cutoff points for numerical integration do not influence the final results within the given accuracy.

The intermediate-coupling results obtained for the Gaussian leading-order mass $m_o^*(\alpha)$ and the corrected mass $m^*(\alpha)$ for $d = 2$ and $d = 3$ are presented in tables 1 and 2, respectively, compared with known data.

Table 1. The present results for the two-dimensional polaron effective mass in the intermediate-coupling range of α compared with the data obtained within the Feynman model.

α	m_F^*	m_o^*	m^*
0.5	1.23762	1.23854	1.23456
1.0	1.59971	1.60469	1.58370
2.0	3.40873	3.44773	3.26923
3.0	15.2066	15.2215	14.1534
4.0	81.1692	81.0063	80.3848
5.0	257.453	257.302	266.300
7.0	1217.64	1217.55	1304.18
9.0	3603.70	3603.65	3910.61
11.0	8362.91	8362.87	9132.64
15.0	29974.8	29974.8	32921.9

Table 2. The present results for the three-dimensional polaron effective mass in the intermediate-coupling range of α compared with known data.

α	m_F^*	m_{LR}^* [30]	m_{GLS}^* [38]	m_{AR}^* [39]	m_{Lar}^* [40]	m_o^*	m^*
0.5	1.08999	—	—	—	—	1.09013	1.08970
1.0	1.19551	1.19408	1.196	1.1942	1.19146	1.19615	1.19423
3.0	1.88895	1.86818	1.900	1.824	1.7229	1.89862	1.87007
5.0	3.88562	3.76384	3.940	3.30	2.3543	3.93259	3.76961
6.0	6.83836	—	—	—	—	6.90814	6.53710
7.0	14.3941	13.7277	—	10.3	—	14.4162	13.6535
9.0	62.7515	62.0588	—	—	—	62.5987	61.7556
11.0	183.125	186.724	—	—	—	182.964	186.453
15.0	797.499	837.039	—	820.0	—	797.391	837.073
20.0	2809.14	2990.02	—	—	—	2809.07	2990.18
30.0	15311.8	16451.8	—	—	—	15311.7	16451.5
40.0	49627.5	—	—	—	—	49627.5	53488.7

The scaling feature (19) for $m_o^*(\alpha)$ allows us to depict both two- and three-dimensional Gaussian leading-order masses by only one curve in figure 1. Actually, this is true for any $d \geqslant 2$. In doing so, we plot our two-dimensional results scaled by a factor of $\alpha_d/\alpha = 3\pi/4$ in the horizontal (α-axis) direction. Data cited as Feynman's in tables 1 and 2 have been re-obtained by us to cover more data sets. To show the deviation of all results from Feynman's more clearly, we have plotted them only after first dividing by Feynman's values. The results of the fourth-order perturbation theory and the adiabatic strong-coupling model extrapolated to the intermediate-coupling region $1 < \alpha_d < 10$ have not been plotted due to their relative large deviations from Feynman's result.

The difference between Gaussian and Feynman's masses reaches 1.2% at $\alpha_d \approx 5$ for any $d \geqslant 2$, vanishing for very small and very large α_d. Note that for $\alpha_d \approx 7$ the leading-order Gaussian mass $m_o^*(\alpha)$ converges to $m_F^*(\alpha)$. For $\alpha_d < 7$ $m_o^*(\alpha)$ is larger than $m_F^*(\alpha)$, and vice verse for $\alpha_d > 7$.

Taking into account non-Gaussian corrections to the EM breaks the scaling feature (19) and the deviation of the corrected mass from Feynman's result (and from Gaussian, too) for $d = 2$ is larger than for $d = 3$. This is because α_d decreases as $d \to \infty$. The smaller the spatial dimension, the more important are non-Gaussian corrections. One can observe that near $\alpha_d \approx 10$ the second-order non-Gaussian correction vanishes because this correction

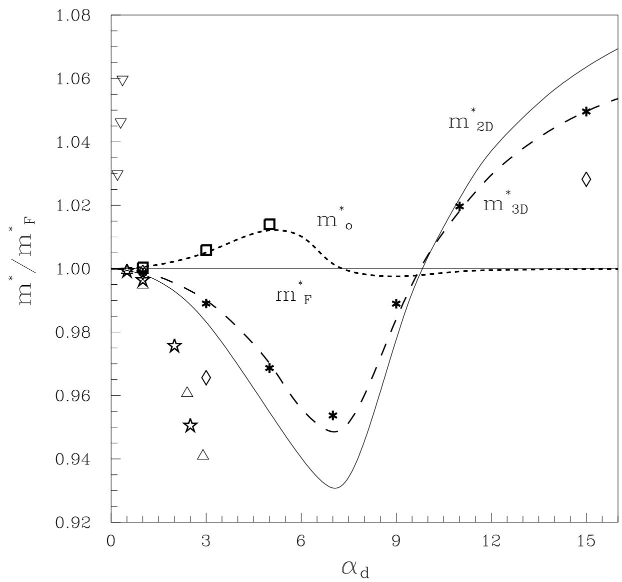

Figure 1. Effective mass of the two- and three-dimensional polaron normalized to the Feynman variational result as a function of the re-scaled electron–phonon coupling constant α_d. The short-dashed curve represents our leading-order Gaussian mass $m_o^*(\alpha_d)$ obtained for spatial dimension $d \geqslant 2$. The solid and long-dashed curves depict our corrected mass $m^*(\alpha)$ for $d = 2$ and $d = 3$, respectively. For comparison, some three-dimensional results are shown: rhomba and squares denote Monte Carlo data from [39] and [38]; stars correspond to results from [40]; asterisks show the corrected Feynman result from [30]; and up and down triangles depict lower and upper bounds due to the Páde scheme [43].

was negative for small α_d and positive for large α_d.

Clearly, the corrected mass $m^*(\alpha_d)$ does not converge to the Feynman result for $\alpha_d \to \infty$. In this limit $m^*(\alpha)$ differs from the exact (adiabatic) result by 7.4% (or, 4.8%) for $d = 2$ ($d = 3$), while Feynman's mass $m_F(\alpha)$ differs by 18.8% (13.4%). From the analyses of weak- and strong-coupling results it can be deduced that the exact EM of the polaron must be below m_F^* for small coupling, and above $m_F(\alpha)$ for large coupling. Our leading-order Gaussian mass $m_o^*(\alpha)$ does not exhibit such a behaviour, but the corrected result $m_o^*(\alpha)$ is in agreement with this result.

Comparing our results in the intermediate-coupling range to that of other approaches we note that our method works well in a unique way in the whole range of α and for both two and three dimensions. It does not require extensive numerical calculations on supercomputers, but is able to give reliable and consistent results rather quickly. Our results are more accurate than those obtained in [41] only for $\alpha < 3$. A Monte Carlo method based on partial averaging of the high-order Fourier coefficients [39] improves the Feynman variational mass for a restricted region $\alpha < 7$ but has a large systematic error and has required several thousand hours of super-computer time. The reported inaccuracy due to the treatment of the Coulomb singularity [42] or due to the considerable accumulation of statistical errors [41] does not appear in our approach. Moreover, since the ground-state characteristics only follow for $\beta \to \infty$, the simulation results obtained for finite $\beta < \infty$ have to be extrapolated accurately. There exists another type of approach to construct interpolation algorithms based on the known asymptotical ($\alpha \to 0$ and $\alpha \to \infty$) behaviours of the EM. Various attempts have been made in this direction [43, 44], although they definitely need more expansion coefficients to achieve acceptable reliability.

However, we would like to point out that our present results should also be improved. First, in the weak-coupling limit, our Gaussian leading-order mass $m_o^*(\alpha)$ overestimates slightly the result of the fourth-order perturbation method and the Feynman result. Although the last difference is very small, about 2% in the coefficient of α^2, our $m_o^*(\alpha)$ surprisingly deviates from the exact perturbative result more than Feynman's two-parameter approach; consider that our leading-order Gaussian approximation for the GSE [25] surpassed the Feynman approach in the same region. However, the next non-Gaussian correction $\Delta M_2^*(\alpha)$ compensates exactly this gap and we obtain for the final mass $m^*(\alpha)$ complete agreement with conventional higher-order perturbation theory [33, 34, 22] in both two and three dimensions. The observation is that the GER method describes the EM worse than the GSE to leading order for $\alpha \ll 1$.

On the other hand, for $\alpha \gg 1$, we see that there is still a need for higher-order corrections beyond $\Delta M_2^*(\alpha)$. A similar picture has been noticed earlier [24] for the GSE.

6. Conclusion

To summarize, we have evaluated the effective mass of the polaron in $d > 1$ dimensions within and beyond the general Gaussian approximation in the weak-, strong- and intermediate-coupling regimes. For this purpose, we have utilized the GER method, that is, a rearranged perturbative path-integral approach, where the leading order takes into account all Gaussian fluctuations of the polaron in its ground state and higher orders correct systematically for non-Gaussian contributions. Actually, we have shown that the Gaussian leading order can serve as a source of various approximations, including, in particular, Feynman's early variational approach. We have found that the Gaussian leading-order approximation to the mass lies not too far from that of Feynman, being within 1.3% for any spatial dimension $d \geqslant 2$. The second-order non-Gaussian correction changes the previous result for different values d of the spatial dimension parameter. For $d = 2$ and $d = 3$ these changes are about 7% and 5%, respectively, for intermediate α. The corrected mass for $d = 3$ lies close to the analogously corrected Feynman result [30], but differs considerably from some Monte Carlo results [38, 39]. The present data for intermediate α (shown in table 1) obtained for $d = 2$ are new and may serve as a standard of reference for the two-dimensional polaron mass. It can be expected that the totality of all non-Gaussian corrections beyond second order will not dramatically change the obtained results.

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