Quasi-particle characteristics of the one-dimensional polaron

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Abstract

The main quasi-particle characteristics of the one-dimensional polaron are estimated within and beyond the most general Gaussian approximation at arbitrary electron-phonon coupling. We have derived explicitly the ground-state energy and the effective mass in the weak- and strong-coupling regimes. For arbitrary coupling, the Gaussian leading-order term of the polaron self energy improves the corresponding Feynman estimate and represents the lowest upper bound available. We have calculated the next non-Gaussian corrections. Taking into account systematically higher-order corrections does not perturb considerably the obtained results.

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I. INTRODUCTION

A conducting electron moving slowly in a polar crystal interacts with lattice vibrations and forms a quasi-particle, which is commonly called a polaron. Traditionally, the polaron problem has been considered in three dimensions \([1]-[6]\). In recent years, polaronic effects have been observed in low-dimensional systems \([7]-[9]\) that has stimulated many theoretical enhancements of the conventional theory by lowering the spatial dimension \([10]-[12]\).

The polaron confined in one dimension \((d = 1)\) is usually modeled by the following Hamiltonian \([13,14]\)

\[
H = \frac{p^2}{2} + \sum_k a_k^\dagger a_k + \sqrt{\frac{\alpha}{L}} \sum_k \left( a_k^\dagger e^{-ikr} - a_k e^{ikr} \right),
\]

where \(p\) and \(r\) denote the momentum and position of the electron; \(k, a_k\) and \(a_k^\dagger\) are the wave-vector, annihilation and creation operators of a phonon; \(L\) is the length of lattice crystal and the interaction is characterized by the dimensionless coupling constant \(\alpha \geq 0\). Here we are using appropriate units, such that, \(m_b = \omega_{LO} = \hbar = c = 1\), where \(m_b\) is the electron bare mass, \(\omega_{LO}\) denotes the constant frequency of the longitudinal optical phonons.

Various methods have been devoted to investigate the properties of the system described by (1.1), in particular, the ground-state energy (GSE) and the effective mass (EM). However, strict results for these quantities are known only in the limiting cases of the weak- \((\alpha \to 0)\) and the strong-coupling \((\alpha \to \infty)\) regime \([10,11,14]\).

Among the variety of approaches providing reasonable results for finite \(\alpha\), the Feynman path-integral approach \([4]\) stands out for its flexibility and all-coupling nature. Following this formalism one can integrate out the phonon variables in (1.1) and define the free energy of the polaron \(F_\beta(\alpha)\) as follows:

\[
e^{-\beta F_\beta(\alpha)} = \oint \delta r e^{-S_0[r] + \alpha W[r]}, \quad S_0[r] \overset{\text{def}}{=} \frac{1}{2} \int_0^\beta dt \left( \frac{dr(t)}{dt} \right)^2,
\]

where \(\beta\) is the inverse temperature, \(S_0[r]\) represents the free part of the polaron action while the interaction is described by

\[
\alpha W[r] \overset{\text{def}}{=} \frac{\alpha}{\sqrt{2}} \int_0^\beta dt ds \frac{e^{-|t-s|} + e^{-\beta + |t-s|}}{1 - e^{-\beta}} \delta(|r(t) - r(s)|).
\]

Functional integration symbol \(\oint \delta r\) in (1.2) indicates path integration performed over all closed paths \(r(0) = r(\beta) = x\) followed by ordinary integration over \(x\). Hereby, the free energy of the non-interacting phonons is already subtracted, so the standard normalization condition \(F_\beta(0) = 0\) is obeyed.

Thus, the original many-body model \([14]\) has been transformed into an effective one-particle problem. However, the nonlocality and \(\delta\)-singularity arising in \(W[r]\) prevent any further analytic treatment for finite \(\alpha\). For higher dimensions \((d > 1)\), another Coulomb-like singularity arises in \([3]\). Among the approximate methods, Feynman’s all-coupling variational estimate \([4]\) has been particularly successful (for \(d = 3\)) to interpolate smoothly
between the weak- and the strong-coupling regime of the ground state ($\beta \to \infty$) by introducing the following retarded oscillator

$$\alpha W_F[\mathbf{r}] \overset{\text{def}}{=} -C \int_0^\beta dt ds e^{-\omega|t-s|} (\mathbf{r}(t) - \mathbf{r}(s))^2$$

with adjustable positive parameters $C$ and $\omega$. A combination of the Jensen-Peierls inequality with the variational principle leads to the Feynman upper bound to the exact GSE. A similar scheme has also been suggested by Feynman to estimate the EM. Further improvement of Feynman’s method has been made (for $d=3$) by increasing the number of trial oscillators.

An essential generalization of the Feynman method has been proposed in [17] and [18] independently. In [17] the Feynman exponential $C \exp(-\omega|t-s|)$ has been changed to an isotropic trial function $f(t-s) \geq 0$ obeying the periodical condition $f(t-\beta) = f(t)$. Appropriate variational optimization has lead to a coupled integral equation for function $f(t)$. By solving it numerically one obtains the best upper bound available for $d=3$ [17]. According to [14] this result can be re-scaled into another spatial dimension.

An improvement over the Feynman estimate in a nonvariational way has been made by applying the Gaussian-equivalent representation method [19,20]. According to this method, the polaron action in arbitrary dimensions $d > 1$ can be identically transformed into an equivalent form

$$S_{\text{GER}}[\mathbf{r}] = \frac{1}{2}(\mathbf{r}, D^{-1}\mathbf{r}) + S_2[\mathbf{r}]:, \quad (\mathbf{r}, D^{-1}\mathbf{r}) \overset{\text{def}}{=} \int_0^\beta dt ds \mathbf{r}(t)D^{-1}(t,s)\mathbf{r}(s),$$

where the Green function of the differential operator $D^{-1}(t,s)$ should be derived from a constraint equation which ensures the normal-ordered form $S_2[\mathbf{r}]:$ of the new interaction functional and the absence of any quadratic path configurations in it. Within this method the entire Gaussian contribution and the next non-Gaussian correction to the GSE have been calculated for arbitrary coupling in two and three dimensions [21,22]. The Gaussian term for the GSE represents an upper bound and in particular, for $d=3$ we observe exact coincidence with the AGL-S result. Appropriate estimate for the EM within and beyond the GER method has been performed in [23].

In the present paper we develop the most general Gaussian approximation for a wide class of path integrals and apply it to the specific case of one-dimensional polaron by estimating its main ground-state characteristics and improving the known results.

### II. POLARON GROUND-STATE PROPERTIES

The main quantities of interest, characterizing the quasi-particle properties of the polaron are the GSE and EM considered at the zero-temperature limit $\beta \to \infty$. The GSE of the system is

$$E(\alpha) = \lim_{\beta \to \infty} \mathcal{F}_\beta(\alpha).$$


The EM of the polaron may be defined in different ways. To define the GSE and EM simultaneously we consider the polaron partition function projected at small fixed momentum $p$ as follows:

$$e^{-\beta F_\beta(p^2,\alpha)} = \frac{1}{\sqrt{2\pi \beta}} \int_{-\infty}^{\infty} dx e^{-ipx} \int_{r(0)=0}^{r(\beta)=\infty} \delta r e^{-S_0[r]+\alpha W[r]} e^{-\beta E_p(\alpha)}. \quad (2.2)$$

Normalization in (2.2) is chosen so that for large $\beta$ we obtain $F_\beta(p^2,0) = \beta p^2 / 2$. By changing the integration variable $r(t) \rightarrow q(t) + r(t)$ with $q(t) = xt/\beta$ one goes to conventional closed paths starting and ending at zero and rewrites (2.2) as follows:

$$e^{-\beta F_\beta(p^2,\alpha)} = \frac{1}{\sqrt{2\pi \beta}} \int_{-\infty}^{\infty} dx e^{-ipx-x^2/2\beta} Z_\beta(\alpha,x), \quad (2.3)$$

$$Z_\beta(\alpha,x) = \int_{r(0)=0}^{r(\beta)=0} \delta r e^{-S_0[r]+\alpha W[r+q]} \equiv \int d\sigma_0[r] e^{\alpha W[r+q]}, \quad \int d\sigma_0[r] \cdot 1 = 1. \quad (2.4)$$

Note, going to the Fourier transform for $\delta$-function we can rewrite the polaron self-interaction in (1.3) as follows:

$$W[r] = \frac{1}{2\sqrt{2\pi}} \int_0^\beta dt ds e^{-|t-s|} \int_{-\infty}^{\infty} dk e^{ik(r(t)-r(s))} \equiv \int d\Omega_o(t,s,k) e^{ikR(t,s)}. \quad (2.5)$$

Since the polaron action is translationally invariant, $E_p(\alpha)$ is a continuous function of $p$ and one can expand it around small momentum as follows: $E_p(\alpha) = E(\alpha) + p^2/2m^*(\alpha) + O(p^4)$. Therefore, the GSE and EM of the polaron are

$$E(\alpha) = \lim_{\beta \rightarrow \infty} F_\beta(0,\alpha),$$

$$m^*(\alpha) = \left( \lim_{\beta \rightarrow \infty} \frac{\partial^2}{\partial p^2} F_\beta(p^2,\alpha) \right)_{p=0}^{-1}. \quad (2.6)$$

### III. Generalized Gaussian Approximation

As is known, no exact evaluation of (2.4) is available yet. Our strategy is to extract exactly the most general Gaussian contribution out of $Z_\beta(\alpha,x)$. Then, the remaining non-Gaussian correction may be systematically estimated to improve the main approximation and to control the accuracy.

i. First, we demonstrate the basis of our method by evaluating $Z_\beta(\alpha,0)$. This simplification does not harm the GSE and the necessary extension to $x \neq 0$ required for the EM will be given later. In principle, the interaction functional $W[r]$ may be more general than that given in (1.3) and (2.3). So, the aim is to find an optimal representation for
\[ Z_\beta(\alpha) = \langle e^{\alpha \mathcal{W}[r]} \rangle_0, \quad \langle \bullet \rangle_0 \overset{\text{def}}{=} \int d\sigma_0[r] \bullet, \quad \langle 1 \rangle_0 = 1. \] (3.1)

For \( \alpha \ll 1 \), the Gaussian contribution in (3.1) is mainly represented by the functional measure \( d\sigma_0[r] \) and the influence of the quadratic part entering \( \mathcal{W}[r] \) is insignificant. However, as \( \alpha \) increases, the nontrivial Gaussian part of \( \mathcal{W}[r] \) plays considerable role and this drastically diminishes the efficiency of the original representation (3.1). Besides, the first cumulant \( \langle W[r] \rangle_0 \) is nonzero.

To describe the system more efficiently at finite and large \( \alpha \) we go to another functional representation based on the most general Gaussian measure \( d\sigma[r] \) as follows

\[
\int_{r(0)=0}^{r(\beta)=0} \delta r e^{-\frac{1}{2}(r,D_{-1}^{-1})r} \bullet \overset{\text{def}}{=} \int d\sigma[r] \bullet = \langle \bullet \rangle, \quad \langle 1 \rangle = 1, \] (3.2)

A specific restriction imposed on the Green function \( D(t,s) \) of the operator \( D^{-1}(t,s) \) will be given later. Obviously, for \( \beta \to \infty \) we have

\[
\langle r(t) r(s) \rangle = D(t - s), \quad \langle e^{i\mathbf{R}(t,s)} \rangle = e^{-k^2 F(|t-s|)}, \quad F(t) \overset{\text{def}}{=} D(0) - D(t). \] (3.3)

Functional averaging schemes (3.1) and (3.2) are related to each other as follows:

\[
\langle e^{\mathbf{T}[r]} \rangle \equiv \langle e^{\mathbf{T}[r]} \rangle_0 = e^{-C_0} \langle \bullet \rangle_0, \] (3.4)

where

\[
T[r] \overset{\text{def}}{=} \frac{1}{2} \left( r, (D^{-1} - D_0^{-1}) r \right), \quad C_0 \overset{\text{def}}{=} -\ln \sqrt{\frac{\det D_0^{-1}}{\det D^{-1}}}. \] (3.5)

Applying (3.4) to (3.1) we isolate the most general Gaussian part of the initial PI by performing an identical transformation as follows

\[
\langle e^{\alpha \mathcal{W}[r]} \rangle_0 = e^{C_0} \langle e^{\alpha \mathcal{W}[r]} \rangle = e^{C_0 + \langle T[r] \rangle + \alpha \langle W[r] \rangle} \langle e^{\alpha \mathbf{W}[r]} \rangle \overset{\text{def}}{=} e^{-\beta E_0(\alpha)} \langle e^{\alpha \mathbf{W}[r]} \rangle. \] (3.6)

In particular, for the one-dimensional polaron we have

\[
\alpha \mathbf{W}[r] \overset{\text{def}}{=} \alpha \int d\Omega_0(t,s,k) \left\{ e^{ik\mathbf{R}(t,s)} - e^{-k^2 F(t-s)} \right\} - \langle T[r] \rangle. \] (3.7)

Since all Gaussian parts are concentrated, by definition, in the Gaussian measure, the new interaction (3.7) should not contain any quadratic path configurations. This requirement leads to the following equality

\[
0 = \langle T[r] \rangle - \frac{\alpha}{2} \int d\Omega_0(t,s,k) e^{-k^2 F(t-s)} k^2 \langle \left( R(t,s) \right)^2 \rangle
= \frac{1}{2} \left( (D^{-1} - D_0^{-1}), D \right) - \alpha \int d\Omega_0(t,s,k) e^{-k^2 F(t-s)} k^2 F(|t-s|). \] (3.8)

Therefore, the adjustable function \( F(t) \) playing a key role in the new representation should be derived from the constraint equations:
\(F(t) = \frac{1}{\pi} \int_0^\infty dk \left[1 - \cos(kt)\right] \tilde{D}(k),\)
\[
\tilde{D}(k) = \left(k^2 + \frac{\alpha}{\sqrt{2\pi}} \int_0^\infty dt e^{-t} \left[1 - \cos(kt)\right] F^{-3/2}(t)\right)^{-1},
\]
(3.9)

where \(\tilde{D}(k)\) is the Fourier transform of \(D(t)\).

Exact analytic solutions to (3.9) are available in the weak- and strong-coupling limit:
\[
\tilde{D}(k) = \begin{cases} 
\{k^2 + \alpha \gamma(k) + \alpha^2 \chi(k)\}^{-1} + O(\alpha^3), & \alpha \to 0, \\
\{k^2 + \nu^2\}^{-1} + O(1), & \nu = 4\alpha^2 / \pi, \quad \alpha \to \infty,
\end{cases}
\]
(3.10)

where
\[
\gamma(k) \overset{\text{def}}{=} 2\sqrt{2} \left(\sqrt{1 + \sqrt{1 + k^2}} - \sqrt{2}\right), \quad \chi(k) \overset{\text{def}}{=} \frac{k^2}{2\pi} \int_0^\infty dz \frac{(1 + z)^3 + |1 - z|^3 - 2z^3 - 2}{z^{3/2}(1 + z)(k^2 + (1 + z)^2)}.
\]

Note, function \(\chi(k)\) can be further simplified, but the result is a long expression consisting of rational and trigonometric functions.

Substituting (3.8) into (3.7) we rewrite the new interaction functional as follows
\[
W_2[r] = \int d\Omega_0(t, s, k) \ e^{-k^2 F(t-s)} \left\{e^{ik[r(t) - r(s)]} + k^2 F(t-s) - 1 + \frac{k^2}{2} [r(t) - r(s)]^2 \right\}.
\]
(3.11)

Note again that \(W_2[r]\) does not contain any quadratic path configurations. Besides, the first cumulant is trivial \(\langle W_2[r]\rangle = 0\).

Finally, we write
\[
e^{-\beta E(\alpha)} = \langle e^{\alpha W[r]} \rangle_0 = e^{-\beta E_o(\alpha)} \langle e^{\alpha W_2[r]} \rangle,
\]
(3.12)

where \(E_o(\alpha)\) is the general Gaussian contribution to the one-dimensional polaron GSE.

Equations (3.6)-(3.12) serve as the basis of the new representation which we call the generalized Gaussian approximation. The remaining non-Gaussian corrections should be evaluated by considering the following new PI
\[
J_\beta(\alpha) = \langle e^{\alpha W_2[r]} \rangle.
\]
(3.13)

Note, by applying the Jensen-Peierls inequality to (3.13) one obtains
\[
J_\beta(\alpha) \geq e^{\alpha \langle W_2[r]\rangle} = 1.
\]
(3.14)

Therefore, \(E_o(\alpha)\) represents a upper bound to the GSE of the one-dimensional polaron:
\[
E_o(\alpha) \geq E(\alpha).
\]
(3.15)

ii. The described above scheme can be easily generalized to the case \(x \neq 0\) that is necessary to evaluate the EM of the polaron. Omitting details of the extension we write the final result as follows
\[ Z_\beta(\alpha, x) = e^{-\beta \mathcal{E}_G(x, \alpha, \beta)} \cdot \langle e^{\alpha \mathcal{W}_2[r, x]} \rangle, \]  

where the leading-order Gaussian approximation is:

\[
e^{-\beta \mathcal{E}_G(x, \alpha, \beta)} = \exp \left\{ \frac{\beta}{2\pi} \int_0^\infty dk \ln(k^2 \widetilde{D}(k)) + \frac{1}{2} (D^{-1} - D_o^{-1}, D) \right\} + \alpha \int d\Omega_o(t, s, k) e^{-k^2 F(t-s)} e^{ikx(t-s)/\beta} \]  

and the non-Gaussian correction is described by

\[
\langle e^{\alpha \mathcal{W}_2[r, x]} \rangle = \langle \exp \left\{ \alpha \int d\Omega_0(t, s, k) e^{-k^2 F(t-s)+ikx(t-s)/\beta} \right\} \cdot \left[ e^{ik[r(t)-r(s)]+k^2 F(t-s)} - 1 + \frac{k^2}{2} [r(t) - r(s)]^2 \right] \rangle.
\] 

iii. Now we consider the pure Gaussian approximation to \( Z_\beta(\alpha, x) \) as follows

\[ Z^{G}_\beta(\alpha, x) = e^{-\beta \mathcal{E}_G(x, \alpha, \beta)}. \] 

Substituting (3.17) and (3.19) into (2.6) we obtain the leading-order Gaussian approximations to the GSE and EM as follows:

\[
E_o(\alpha) = -\frac{1}{2\pi} \int_0^\infty dk \left[ \ln(k^2 \widetilde{D}(k)) - k^2 \widetilde{D}(k) + 1 \right] + \frac{\alpha}{\sqrt{2\pi}} \int_0^\infty dt \ e^{-t} F^{-1/2}(t),
\]

\[
m^*_o(\alpha) = 1 + \frac{\alpha}{2\sqrt{2\pi}} \int_0^\infty dt \ t^2 \ e^{-t} F^{-3/2}(t).
\] 

Taking into account (3.10) we obtain the following analytic solutions

\[
E_o(\alpha) = \begin{cases} -\alpha - (1/4 - 2/3\pi) \alpha^2 - O(\alpha^3), & \alpha \to 0, \\ -\alpha^2/\pi - O(1), & \alpha \to \infty, \end{cases}
\]

\[
m^*_o(\alpha) = \begin{cases} 1 + \alpha/2 + (3/2 - 4/\pi) \alpha^2 + O(\alpha^3), & \alpha \to 0, \\ (16/\pi^2) \alpha^4 + O(\alpha^2), & \alpha \to \infty. \end{cases}
\] 

iv. The Feynman estimate can be reproduced, if one builds a convex combination of the two known asymptotical solutions (3.10) as follows

\[ \widetilde{D}_F(k) = w/k^2 + (1 - w)/(k^2 + v^2). \] 

Substituting (3.22) into (3.20) and optimizing the obtained energy with respect to parameters \( \{w, v\} \) one is able to reproduce a Feynman-type upper bound \( E_F(\alpha) \) for the one-dimensional polaron. It is inferior to the general Gaussian result for finite \( \alpha \), i.e. \( E_F(\alpha) > E_0(\alpha) \). Accordingly, \( m^*_F(\alpha) \) deviates slightly from \( m^*_0(\alpha) \). Note, however, that (3.22) is not the exact solution to (3.3).
IV. NON-GAUSSIAN CORRECTION

The Gaussian leading-order terms \( E_0(\alpha) \) and \( m_0^*(\alpha) \) approximate well the exact GSE and EM of the polaron. To estimate the influence of the non-Gaussian correction we evaluate (3.18) by using the following expansion:

\[
J_\beta(\alpha, x) = \langle e^{\alpha W_2[r,x]} \rangle = \exp \left\{ \alpha \langle W_2[r,x] \rangle + \frac{\alpha^2}{2} \left[ \langle (W_2[r,x])^2 \rangle - \langle W_2[r,x] \rangle^2 \right] + \ldots \right\} .
\]  

(4.1)

We stress that this is not a conventional perturbation series on the coupling constant \( \alpha \), each term of the exponent in the r.h.s. of (4.1) contains \( \alpha \) in more complicated way and the result is a rapidly converging series even for large \( \alpha \).

In doing so we restrict ourselves by estimating only up to the second cumulant in (4.1). Appropriate analysis performed in the weak- and strong-coupling regimes for the third cumulant indicates that taking into account higher-order cumulants results in only tiny improvement over the obtained estimate (see, e.g. (5.3) and (5.9)). We suppose that this picture remains generally valid in the intermediate region of \( \alpha \). We obtain

\[
J_\beta(\alpha, x) = \exp \left\{ -\beta \Delta E_2(\alpha) - \frac{x^2}{2\beta} \Delta M_2(\alpha) - \ldots \right\} ,
\]  

(4.2)

where

\[
\Delta E_2(\alpha) = \lim_{\beta \to \infty} \frac{\alpha^2}{4\beta} \int_0^\beta dt \int_0^\beta ds \int_{-\infty}^\infty dx \int_{-\infty}^\infty dy \rho(t, s, x, y) ,
\]

\[
\Delta M_2(\alpha) = \lim_{\beta \to \infty} \frac{\alpha^2}{4\beta} \int_0^\beta dt \int_0^\beta ds \int_{-\infty}^\infty dx \int_{-\infty}^\infty dy \int_{-\infty}^\infty dk \int_{-\infty}^\infty dp \rho(t, s, x, y) (k|t - s| + p|x - y|)^2 .
\]  

(4.3)

Above, we have introduced the following correlation functions:

\[
\Xi(t, s, x, y) \overset{\text{def}}{=} F(t - x) + F(s - y) - F(s - x) - F(t - y) ,
\]

\[
\rho(t, s, x, y) \overset{\text{def}}{=} e^{-|t-s|-|x-y|} \exp \left\{ -k^2 F(t - s) - p^2 F(x - y) + kp \Xi(t, s, x, y) \right\} .
\]  

(4.4)

The second-order non-Gaussian contributions in (4.3) may be derived analytically for the weak- and strong-coupling limit. For finite \( \alpha \) we integrate out (4.3) explicitly over variables \( k, p, x \) and \( y \) and the remaining double integrals are calculated numerically.

Finally, taking into account both the leading-order Gaussian and the second-order non-Gaussian contribution we estimate the one-dimensional polaron GSE and EM as follows:

\[
E_2(\alpha) = E_0(\alpha) + \Delta E_2(\alpha) ,
\]

\[
m_2^*(\alpha) = m_0^*(\alpha) + \Delta M_2(\alpha) .
\]  

(4.5)
V. EXACT AND NUMERICAL RESULTS

We have calculated analytically the GSE and EM of the one-dimensional polaron explicitly with accuracy $O(\alpha^4)$ and $O(1)$ in the weak- and strong-coupling limit, respectively.

Weak-coupling solutions

In the weak-coupling limit, various perturbation methods give convergent series in powers of $\alpha$. For example, analytic results up to the second order in $\alpha$ read

$$E_{PS}(\alpha) = -\alpha - \left(\frac{3}{2}\sqrt{2} - 1\right) \alpha^2 - O(\alpha^3),$$

$$m_{PS}^*(\alpha) = 1 + \alpha/2 + \left(\frac{5}{8}\sqrt{2} - 1/4\right) \alpha^2 + O(\alpha^3).$$

A Lee-Low-Pines type method taking into account three-phonon correction to the Davydov phonon coherent state results in the following numerical results

$$E_{CWW}(\alpha) = -\alpha - 0.06066 \alpha^2 - 0.00844 \alpha^3 + O(\alpha^4),$$

$$m_{CWW}^*(\alpha) = 1 + \alpha/2 + 0.19194 \alpha^2 - 0.06912 \alpha^3 + O(\alpha^4).$$

By using the GGA method we calculate exactly the GSE and EM of the one-dimensional polaron up to the $\alpha^3$ terms. Knowing explicitly the weak-coupling solution (3.10) we calculate the second and third-order non-Gaussian corrections to the GSE and EM. Adding them to the leading-order Gaussian contributions we obtain

$$E_0(\alpha) + \Delta E_2(\alpha) + \Delta E_3(\alpha)$$

$$= -\alpha - (3/\sqrt{8} - 1) \alpha^2 - (5 - 63\sqrt{2}/16 + 19\sqrt{3}/16 - 29\sqrt{6}/48) \alpha^3 - O(\alpha^4),$$

$$m_0^*(\alpha) + \Delta m_2^*(\alpha) + \Delta m_3^*(\alpha)$$

$$= 1 + (1/2) \alpha + (5/8\sqrt{2} - 1/4) \alpha^2 + 0.0691096281 \alpha^3 + O(\alpha^4).$$

Strong-coupling solutions

According to the Pekar “Produkt-Ansatz”, the polaron ground-state wave function $|\psi\rangle$ in the strong-coupling regime ($d = 3$) is written as a direct product of the electron $|\Psi\rangle$ and field $|\varphi\rangle$ wave functions, besides, $|\varphi\rangle$ depends parametrically on $|\Psi\rangle$. Further development of this method can be found, in particular, in [24,25]. A reliable numerical computation of the minimal value of the corresponding Hartree-type functional for $d = 3$ was performed in [26]. The most rigorous investigations for the strong-coupling limit for $d = 1$ have been reported in [11,27,10]. Following the Pekar Ansatz the GSE of the one-dimensional polaron may be found by solving the following variational task

$$- \lim_{\alpha \to \infty} \frac{E(\alpha)}{\alpha^2} = \sup_{\langle\Psi|\Psi\rangle = 1} \int dx \left\{ \Psi(x) \Delta \Psi(x) + 2|\Psi(x)|^4 \right\}.$$  

The EM is obtained as follows:
\[
\lim_{\alpha \to \infty} \frac{m^*(\alpha)}{\alpha^4} = \frac{4}{\pi} \int_{-\infty}^{\infty} dk \, k^2 \, |\langle \Psi | e^{ikx} | \Psi \rangle|^2.
\]  

(5.5)

The corresponding optimized wave function obeying appropriate boundary conditions is the nontrivial solution of the following constrained differential equation:

\[
\Psi''(x) + 4 \Psi^3(x) - \Psi(x) = 0, \quad \int_{-\infty}^{\infty} dx |\Psi(x)|^2 = 1.
\]  

(5.6)

It admits an explicit analytic solution

\[
\Psi(x) = \sqrt{2}/(e^x + e^{-x}) = \left[\sqrt{2} \cosh(x)\right]^{-1}
\]  

(5.7)

that results in

\[
E(\alpha) = -\frac{1}{3} \alpha^2 - O(1),
\]

\[
m^*(\alpha) = \frac{32}{15} \alpha^4 + O(1).
\]  

(5.8)

These solutions coincide (after the appropriate re-scaling) with the exact results reported first in \[10\].

Our leading-order Gaussian contributions in \((3.21)\) differ from the adiabatic ones in \((5.8)\). The reason is that as \(\alpha\) increases the polaron self-interaction is less well approximated by a general Gaussian functional. Hence, non-Gaussian corrections are required to fill this gap. Taking into account higher-order corrections \((4.1)\) we obtain a series converging rapidly to the exact value in \((5.8)\) as follows:

\[
E_o(\alpha) = -0.318310 \alpha^2,
\]

\[
E_o(\alpha) + \Delta E_2(\alpha) = -0.327014 \alpha^2,
\]

\[
E_o(\alpha) + \Delta E_2(\alpha) + \Delta E_3(\alpha) = -0.330205 \alpha^2.
\]  

(5.9)

Appropriate series for the EM reads

\[
m^*_o(\alpha) = 1.621139 \alpha^4,
\]

\[
m^*_o(\alpha) + \Delta M_2(\alpha) = 1.858065 \alpha^4,
\]

\[
m^*_o(\alpha) + \Delta M_2(\alpha) + \Delta M_3(\alpha) = 1.966430 \alpha^4.
\]  

(5.10)

**Intermediate-coupling results**

For finite \(\alpha\) we have solved equations \((3.9)\) numerically by means of an iteration accepting \((3.22)\) as the first approximation. After the sixth iteration step the numerical results do not change within the given accuracy. The obtained intermediate-coupling results for the Gaussian leading-order contributions and the second-order non-Gaussian corrections are presented in Tables 1, 2; and depicted in Figure 1 in comparison with several known data.
In conclusion, we have evaluated the ground-state energy and effective mass of the one-dimensional polaron by developing the generalized Gaussian approximation method. We have obtained exact analytic solutions to these quantities in the weak-coupling limit including the $\alpha^3$ term. For the strong coupling, we have derived the exact GSE and EM by adapting the Pekar adiabatic theory, then have estimated the same quantities within the GGA method by developing a systematic iterative scheme to approach rapidly the exact results.

We have shown that for intermediate coupling the leading-order Gaussian contribution to the self-energy slightly improves the Feynman estimate and represents the lowest upper bound available. Considering the non-Gaussian corrections, we have calculated the second-order terms for the GSE and EM. Appropriate analysis performed for the weak- and strong-coupling regimes indicates that taking into account higher-order corrections results in tiny improvement over the obtained estimate. We deduct that this picture changes inconsiderably in the intermediate region of $\alpha$. Our method works well in the entire range of $\alpha$, does not require extensive numerical calculations and provides reliable results rather quickly.

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FIGURES

FIG. 1. The ground-state energy and effective mass of the one-dimensional polaron as functions of the electron-phonon coupling constant $\alpha$. All curves are normalized to the corresponding Feynman estimates so that the horizontal dotted lines show the Feynman approximations. Dashed lines depict the leading-order Gaussian contributions and solid curves correspond to the corrected results taking into account the second-order non-Gaussian corrections.
TABLES

TABLE I. The ground-state energy of the one-dimensional polaron in the intermediate-coupling range.

| α  | $E_{os}$ | $E_F$   | $E_o$   | $E_2$   |
|----|---------|---------|---------|---------|
| 0.5| -0.5000 | -0.51006| -0.51027| -0.51589|
| 1.0| -1.0000 | -1.04444| -1.04532| -1.06710|
| 1.5| -1.5000 | -1.61314| -1.61522| -1.66119|
| 2.0| -2.0086 | -2.23696| -2.24044| -2.31150|
| 2.5| -2.7043 | -2.95968| -2.96352| -3.05052|
| 4.0| -5.7934 | -6.04779| -6.04964| -6.20592|
| 6.0| -12.155 | -12.4074 | -12.4083| -12.7345|
| 8.0| -21.067 | -21.3178 | -21.3183| -21.8871|

TABLE II. The effective mass of the one-dimensional polaron in the intermediate-coupling range.

| α  | $m_{os}^*$ | $m_F^*$ | $m_o^*$ | $m_2^*$ |
|----|------------|---------|---------|---------|
| 0.5| 1.25000    | 1.32084 | 1.32246 | 1.31091 |
| 1.0| 1.50000    | 1.88895 | 1.89862 | 1.83258 |
| 1.5| 1.75000    | 3.11732 | 3.15094 | 2.91361 |
| 2.0| 5.85933    | 6.83836 | 6.90814 | 6.13458 |
| 2.5| 31.6793    | 21.4723 | 21.4372 | 19.4943 |
| 4.0| 331.719    | 281.622 | 281.474 | 295.800 |
| 6.0| 1911.78    | 1784.90 | 1784.82 | 1973.85 |
| 8.0| 6302.70    | 6068.77 | 6068.73 | 6821.14 |
