The polaron confined in one dimension

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Abstract

The ground-state energy, the effective mass and the number of virtual phonons of the optical large polaron confined strictly in one dimension have been estimated by using the generalized Gaussian approximation. The leading-order terms take care of all Gaussian fluctuations in the system and improve the conventional variational estimates at finite coupling. Particularly, the lowest upper bound to the polaron ground-state energy has been obtained. The non-Gaussian contributions systematically correct the leading-order approximations. We have obtained exact analytical solutions in the weak- and strong-coupling limit and reasonable numerical data for intermediate coupling. Our result for the number of excited phonons limits the validity region of the few-phonon approximation methods.

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1 Introduction

A conducting electron in a polar crystal polarizes the surrounding lattice and, by interacting with the quanta of lattice vibration, phonons, forms a quasi-particle, the polaron.

The polaron problem traditionally has been investigated in three dimensions \[1, 2\], although the electron motions may be localized in reduced dimensionality \[3\]. Many theoretical investigations have been made to study the polaronic properties in lower dimensions (see, e.g. \[4, 5\]). A considerable research attention has been devoted to the study of the polaron confined in one dimension \[6, 7, 8, 9\]. In particular, recent studies on the electron-phonon interaction in quasi one-dimensional systems have explored a polaronic effect pronounced stronger than in two-dimensional structures \[10\]. There are two distinct models employed for the one-dimensional polaron: the small and the large polaron. Small polarons are more strictly bounded and observed in linear conjugative organic polymer conductors \[11\] while the latter model describes electrons confined in one-direction in polar semiconductors \[12\]. The phonons have been considered in the optical and acoustic modes, depending on the specific dispersion rule \[8\]. Regardless of the extremely confined structure of the system, polar optical phonons are treated in the spirit of bulk theory.

The resulting interaction of an electron confined in one dimension with the phonons of longitudinal optical lattice vibrations can be modelled by the following Hamiltonian \[6, 7, 8\]

\[
H = \frac{p^2}{2m} + \hbar \omega_0 \sum_k a_k^\dagger a_k + g \sum_k \left( a_k e^{ikr} + a_k^\dagger e^{-ikr} \right), \quad g = \hbar \omega_0 (\hbar \alpha/m \omega_0 L)^{1/2}, \tag{1}
\]
where \( m, p \) and \( r \) denote the electron bare mass, the momentum and position of the electron, \( L \) is the length of lattice crystal, whereas \( k, a_k \) and \( a_k^\dagger \) are wave vector, annihilation and creation operators of a phonon. The optical polaron model imposes the phonon frequency \( \omega_0 \) independent on \( k \). Further we will use appropriate units, such that, \( m = \omega_0 = \hbar = 1 \). The electron-phonon coupling factor \( g \) behaves \( g \propto \sqrt{\alpha/\Omega}/|k|^{(d-1)/2} \) in \( d \) dimensions \[13, 14\]. Therefore, \( g \) does not depend on \( k \) in one dimension \[6, 8\]. The Fröhlich dimensionless coupling constant \( \alpha \) takes values ranging from 0.02 to 4 for most actual crystals. In this paper the coupling constant \( \alpha \) is identical to \( 2\pi\alpha_{op} \) in \[6\], \( \alpha' \) in \[7\] and \( \alpha \) in \[8\].

Many approaches have been developed to investigate the quasi-particle properties of the system (1) in the ground state \[6, 7\]. Strict results for these quantities are available only in the weak- (\( \alpha \to 0 \)) and strong-coupling (\( \alpha \to \infty \)) limit (see, e.g. \[4, 8\]). In the present paper we have made a systematic investigations of the large optical polaron confined strictly in one dimension within a path-integral (PI) method. We have obtained exact analytical solutions of the self-energy, the effective mass and the number of virtual phonons in the weak- and strong-coupling limit as well as reasonable numerical data improving known results \[6, 7, 8\] at finite \( \alpha \). Particularly, our result for the number of excited phonons limits the validity region of the few-phonon approximations \[8\] and shows that as \( \alpha \) grows, the efficiency of the general Gaussian approximation drops faster than in higher dimensions.

## 2 Polaron Ground-state Properties

1. The phonon variables in (1) may be exactly eliminated by using the Feynman PI technique \[4\]. The partition function for a resting polaron reads

\[
Z_\beta(\alpha) = e^{-\beta F(\alpha, \beta)} = \langle e^{\alpha W[r]} \rangle_0, \quad \langle (\ldots) \rangle_0 = \int_0^{r(\beta)=0} \delta r e^{-S_0[r](\ldots)},
\]

\[
S_0[r] = \frac{1}{2} \int_0^\beta dt ds \ r(t) \ D_0^{-1}(t,s) \ r(s), \quad D_0^{-1}(t,s) = -\delta(t-s) \frac{d^2}{dt^2},
\]

where the inverse temperature \( \beta = 1/k_B T \) is infinite in the ground state: \( \beta \to \infty \). Therefore, \( E(\alpha) = F(\alpha, \infty) \) represents the polaron ground-state energy (GSE). The polaron retarded self-interaction is given by

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

2. For a slow polaron the partition function projected at small fixed momentum \( p \) is

\[
Z_\beta(\alpha, p) = e^{-\beta E(\alpha, p)} = \frac{1}{\sqrt{2\pi\beta}} \int dx \ e^{-ipx} \int_0^{\beta} k_{\alpha p} \ e^{-k R(t,s)} \ e^{-S_0[r(\rho) + \alpha W[p]]}.
\]

Since the polaron action is translationally invariant, the energy \( E(\alpha, p) \) is a continuous function of \( p \). By expanding it around small momentum we define the effective mass (EM)
of the polaron \( m^*(\alpha) \) as follows:

\[
E(\alpha, p) = E(\alpha) + \frac{p^2}{2m^*(\alpha)} + O(p^4).
\]  

(5)

With the new integration variable \( r(t) = \rho(t) - q(t) \), where \( q(t) = xt/\beta = yt \), one goes to conventional closed-end paths \( r(t) \) and rewrites (12) as follows:

\[
e^{-\beta E(\alpha, r)} = \sqrt{\frac{\beta}{2\pi}} \int dy e^{-i\beta py - \beta y^2/2} e^{-\beta F(\alpha, y^2)}, \quad e^{-\beta F(\alpha, y^2)} = \langle e^{\alpha W[r+q]} \rangle_0.
\]  

(6)

For \( \beta \to \infty \) the integral over \( y \) in (6) may be taken by the saddle point method. The saddle point \( y_0 = \sqrt{\xi} \) satisfies the equation

\[
-ip + \sqrt{\xi} [1 + 2F(\alpha, \xi)] = 0, \quad F(\alpha, \xi) = \frac{d}{d\xi}F(\alpha, \xi).
\]  

(7)

Then,

\[
E(\alpha, p) = ip\sqrt{\xi} + \frac{\xi}{2} + F(\alpha, \xi) = F(\alpha) + \frac{p^2}{2(1 + 2F(\alpha))} + O(p^4),
\]  

(8)

where \( F(\alpha) = F(\alpha, 0) \) and \( F(\alpha) = F(\alpha, 0) \). Comparing (6) with (8) we find

\[
E(\alpha) = F(\alpha), \quad m^*(\alpha) = 1 + 2F(\alpha).
\]  

(9)

To evaluate \( F(\alpha) \) we use the expansion

\[
W[r + q] = W[r] + iy V_1[r] - \frac{y^2}{2} V_2[r] + O(y^3),
\]  

\[
V_1[r] = \int d\Omega_{tsk} e^{ikR(t,s)} k(t - s), \quad V_2[r] = \int d\Omega_{tsk} e^{ikR(t,s)} k^2(t - s)^2.
\]

Neglecting terms \( \sim O(y^3) \) we obtain

\[
e^{-\beta F(\alpha, y^2)} = Z_\beta(\alpha) \exp \left\{ -y^2 \frac{Y_\beta(\alpha)}{Z_\beta(\alpha)} \right\}, \quad Y_\beta(\alpha) = \frac{1}{2} \langle e^{\alpha W[r]} \left(V_1^2[r] + V_2[r]\right) \rangle_0.
\]  

(10)

Hence,

\[
F(\alpha) = -\lim_{\beta \to \infty} \frac{1}{\beta} \ln Z_\beta(\alpha), \quad F(\alpha) = \lim_{\beta \to \infty} \frac{Y_\beta(\alpha)}{Z_\beta(\alpha)}.
\]  

(11)

3. The average number of virtual phonons (ANVP) excited by the electron-lattice interaction is given by

\[
N(\alpha) = \langle 0 | \sum_k a_k^\dagger a_k | 0 \rangle = \left. \frac{\partial H}{\partial \omega_0} \right|_{\omega_0=1} = -\frac{1}{\beta} \frac{\partial}{\partial \omega_0} \ln \text{Tr} e^{-\beta H} \bigg|_{\omega_0=1}.
\]  

(12)

The differentiation in (12) should not affect the interaction term in \( H \). We obtain

\[
N(\alpha) = \frac{\alpha}{\sqrt{2}} \int_0^\infty d\tau \int_{-\infty}^\infty \frac{X(\alpha, k, \tau)}{Z_\beta(\alpha)}, \quad X(\alpha, k, \tau) = \langle e^{i k R(t,s) + \alpha W[r]} \rangle_0.
\]  

(13)

where \( \tau = t - s \). Note, the following relation between the ANVP and GSE takes place

\[
N(\alpha) = \left( 1 - \frac{3}{2} \alpha \frac{\partial}{\partial \alpha} \right) E(\alpha).
\]  

(14)
3 Generalized Gaussian Approximation

For finite $\alpha$, the nonlocality and $\delta$-singularity arising in (3) prevent any explicit evaluation of $Z_\beta(\alpha)$, $Y_\beta(\alpha)$ and $X_\beta(\alpha, k, \tau)$. Below we represent a nonvariational approximation method, which isolates completely the Gaussian contributions from these Pls. The remaining non-Gaussian corrections turn to be relatively small (at least for the energy) and may be systematically estimated to improve the leading-order approximations.

i. First, we demonstrate the basic idea of our method by evaluating $Z_\beta(\alpha)$. Note, the initial representation (2) is optimal only for $\alpha \to 0$. To describe the system more efficiently at finite $\alpha$ we introduce a functional integration weighted with the most general Gaussian measure $d\sigma[r]$ as follows

$$\langle (\ldots) \rangle = \int d\sigma[r] (\ldots), \quad d\sigma[r] = \delta r e^{-\frac{1}{2}(r, D^{-1}r)}, \quad (1) = 1. \quad (15)$$

We assume that all Gaussian configurations of the system is totally concentrated in $d\sigma[r]$. This imposes specific requirements on $D^{-1}(t, s)$ (and on its Green function $D(t, s)$) that will be discussed later. Obviously, the following relations take place

$$\langle r(t) r(s) \rangle = D(t, s), \quad \langle e^{ikR(t,s)} \rangle = e^{-k^2F(|t-s|)}, \quad F(t, s) = \frac{D(t, t) + D(s, s)}{2} - D(t, s).$$

Then, we rewrite (2) in the new representation as follows

$$Z_\beta(\alpha) = \exp \left\{ \frac{1}{2} \text{Tr} \ln \frac{D}{D_0} \right\} \left\{ \exp \left\{ \frac{1}{2} \int_0^\beta dt ds r(t) D^{-1}(t, s) r(s) - S_0[r] + \alpha W[r] \right\} \right\}. \quad (16)$$

Let us introduce the conception of the normal-ordered form of functionals with respect to $d\sigma[r]$. In particular, we use the following normal forms:

$$:r(t) r(s): = r(t) r(s) - D(t, s), \quad :e^{ikR(t,s)}: = e^{ikR(t,s)} e^{k^2F(t,s)} \quad (17)$$

so that

$$\langle :r(t) r(s) : \rangle = 0, \quad \langle :e^{ikR(t,s)} : \rangle = 0, \quad e^z = e^z - 1 - z - \frac{z^2}{2}. \quad (18)$$

Functional $W[r]$ may be decomposed as follows:

$$W[r] = \int d\Lambda_{tsk} :e^{ikR(t,s)} : = W[0] + iW_1[r] - \frac{1}{2} W_2[r] + W_{int}[r],$$

$$W_1[r] = \int d\Lambda_{tsk} k :R(t, s), \quad W_2[r] = \int d\Lambda_{tsk} k^2 :R^2(t, s), \quad (19)$$

$$W_{int}[r] = \int d\Lambda_{tsk} :e^{ikR(t,s)} : \quad d\Lambda_{tsk} = d\Omega_{tsk} e^{-k^2F(t,s)}.$$

Since all quadratic configurations of the polaron action in the new representation is totally included in $d\sigma[r]$, any extra quadratic parts should be eliminated as follows

$$\frac{1}{2} \int_0^\beta dt ds : r(t) [D^{-1}(t, s) - D_0^{-1}(t, s)] r(s) : + \alpha W_2[r] = 0, \quad \forall r. \quad (20)$$
This requirement leads to the following constraint equations for function $F(t)$:

$$F(t) = \frac{1}{\pi} \int_0^\infty dk \left[ 1 - \cos(kt) \right] \tilde{D}(k),$$

$$\tilde{D}(k) = \left( k^2 + \frac{\alpha}{\sqrt{2\pi}} \int_0^\infty dt \, e^{-\frac{1 - \cos(kt)}{F^{3/2}(t)}} \right)^{-1},$$

where $\tilde{D}(k)$ is the Fourier transform of $D(t)$. Note, $\tilde{D}_0(k) = 1/k^2$. Taking into account (20) we rewrite (16)

$$Z_{\beta}(\alpha) = e^{-\beta E_0(\alpha)} \cdot J_{\beta}(\alpha), \quad J_{\beta}(\alpha) = \langle e^\alpha W_{\text{int}}[r] \rangle,$$

$$E_0(\alpha) = -\frac{1}{2\pi} \int_0^\infty dk \left[ \ln \left( k^2 \tilde{D}(k) \right) - k^2 \tilde{D}(k) + 1 \right] + \frac{\alpha}{\sqrt{2\pi}} \int_0^\infty dt \frac{\exp(-t)}{F^{1/2}(t)},$$

where $E_0(\alpha)$ is the Gaussian leading-order contribution to the GSE of the polaron confined in one dimension. The non-Gaussian corrections associated with $J_{\beta}(\alpha)$ can be estimated systematically. Equations (16)-(22) serve as the basis of the Generalized Gaussian Approximation (GGA) method applied to $Z_{\beta}(\alpha)$.

Note, $E_0(\alpha)$ represents a upper bound to the true GSE of the one-dimensional polaron. Indeed, $\langle W_{\text{int}}[r] \rangle = 0$. Then, by using the Jensen-Peierls inequality one obtains

$$J_{\beta}(\alpha) \geq e^{\alpha(W_{\text{int}}[r])} = 1 \quad \text{so,} \quad E(\alpha) \leq E_0(\alpha).$$

ii. Now we evaluate $Y_{\beta}(\alpha)$ within the GGA method. Remember, transformations (19)-(22) affect only the exponent in (10), but not any prefactor of the exponential. Therefore, despite the factor $(V_1^2[r] + V_2[r])/2$, all steps of the GGA method may be directly applied to $Y_{\beta}(\alpha)$. Constraint equations (21) remain without any change. We obtain

$$Y_{\beta}(\alpha) = e^{-\beta E_0(\alpha)} \cdot \frac{1}{2} \langle e^{\alpha W_{\text{int}}[r]} \left( V_1^2[r] + V_2[r] \right) \rangle = e^{-\beta E_0(\alpha)} \left\{ \mathcal{F}_\xi^0(\alpha) + \frac{1}{2} J_{\beta}(\alpha) \right\},$$

where

$$\mathcal{F}_\xi^0(\alpha) = \frac{1}{2} \int d\Lambda_{tsk} k^2 (t - s)^2, \quad J_{\beta}(\alpha) = \langle e^{\alpha W_{\text{int}}[r]} \cdot Q[r] \rangle,$$

$$Q[r] = \int d\Lambda_{tsk} k^2 (t - s)^2 \left( e^{ikR(t,s)} - 1 \right) + \left[ \int d\Lambda_{tsk} k (t - s) \left( e^{ikR(t,s)} - 1 \right) \right]^2.$$

Substituting (24) into (11) and (8) we obtain the leading-order (Gaussian) approximation to the polaron EM as follows

$$m_0^*(\alpha) = 1 + 2\mathcal{F}_\xi^0(\alpha) = 1 + \frac{\alpha}{2\sqrt{2\pi}} \int_0^\infty dt \frac{t^2 \exp(-t)}{F^{3/2}(t)}.$$

Higher-order (non-Gaussian) corrections to the EM are given by

$$\Delta m^*(\alpha) = \lim_{\beta \rightarrow \infty} \frac{J_{\beta}(\alpha)}{J_{\beta}(\alpha)} - 2 \mathcal{F}_\xi^0(\alpha) \cdot [J_{\beta}(\alpha) - 1].$$
iii. Note, the additional linear term \( ikR(t, s) \) standing in the exponent in (13) affects neither the normal ordering, nor the elimination of the quadratic path configurations. Hence, the constraint equations (21) do not change for the ratio \( X_\beta(\alpha, k, t)/Z_\beta(\alpha) \). So, we write

\[
\frac{X_\beta(\alpha, k, \tau)}{Z_\beta(\alpha)} = e^{-k^2F(\tau)} + \text{non-Gaussian part}.
\]

Substituting (28) into (13) and neglecting the non-Gaussian part we obtain the leading-order approximation to the ANVP as follows

\[
N_0(\alpha) = \frac{\alpha}{\sqrt{2\pi}} \int_0^\infty dt e^{-t} \frac{t}{F^{1/2}(t)}.
\]

4 Non-Gaussian Corrections

To improve the obtained Gaussian approximations we use the following expansions

\[
J_\beta(\alpha) = \sum_{n=2}^{\infty} \frac{\alpha^n}{n!} \langle W_{\text{int}}^{n}[r] \rangle, \quad J_\beta(\alpha) = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} \langle W_{\text{int}}^{n}[r] Q[r] \rangle.
\]

These are not plain perturbation expansions over \( \alpha \) because each of terms in angle brackets contains \( \alpha \) in a complicated way so that these series converge fast even for large \( \alpha \). Taking into account higher-order non-Gaussian contributions, we obtain corrected values

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

\[
m^*_n(\alpha) = m^*_0(\alpha) + \Delta m^*_2(\alpha) + \ldots + \Delta m^*_n(\alpha),
\]

\[
N_n(\alpha) = N_0(\alpha) + \Delta N_2(\alpha) + \ldots + \Delta N_n(\alpha).
\]

In particular,

\[
\Delta E_2(\alpha) = -\frac{\alpha^2}{2\beta} \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty dt ds dx dy e^{-|t-s|-|x-y|} \rho^{1/2}(t, s, x, y) \frac{e^{-|t-s|-|x-y|}}{\rho^{1/2}(t, s, x, y)} \{ (t-s)^2 F(x-y) 
\]

\[
+ (x-y)^2 F(t-s) + |t-s| |x-y| \Xi(t,s,x,y) \},
\]

\[
\rho(t, s, x, y) = 4 F(t-s) F(x-y) - \Xi^2(t, s, x, y),
\]

\[
\Xi(t, s, x, y) = F(t-x) + F(s-y) - F(s-x) - F(t-y).
\]

Note, the integrations over \( s \) and \( y \) in (32) may be taken explicitly. The remaining double integrals can be derived analytically in the weak- and strong-coupling limit, and numerically for finite \( \alpha \).

5 Exact and Numerical Results

We admit that the accuracy reached with the second- and third-order non-Gaussian corrections in (31) is sufficient for our consideration. Below we have represented exact analytical solutions in the weak- and strong-coupling limit and reasonable numerical data for finite \( \alpha \).
Weak coupling
For \( \alpha \to 0 \) the solution of the constraint equations (21) reads

\[
\widetilde{D}(k) = \left\{ k^2 + 2 \alpha \left( \sqrt{2} \sqrt{1 + \sqrt{1 + k^2} - 2} + \alpha^2 \chi(k^2) \right) \right\}^{-1} + O(\alpha^3),
\]

where \( \chi(k^2) \) is a monotonically increasing positive function. Then, we obtain the exact GSE, EM and ANVP of the one-dimensional polaron up to the \( \alpha^3 \)-order. The results read

\[
E_3(\alpha) = -\alpha - \left( \frac{3}{\sqrt{8}} - 1 \right) \alpha^2 - \left( 5 - \frac{63\sqrt{2} - 19\sqrt{3}}{16} - \frac{29\sqrt{6}}{48} \right) \alpha^3 + O(\alpha^4),
\]

\[
m^*_3(\alpha) = 1 + \frac{1}{2} \alpha + \left( \frac{5}{8\sqrt{2}} - \frac{1}{4} \right) \alpha^2 + 0.0691096281 \alpha^3 + O(\alpha^4),
\]

\[
N_3(\alpha) = \frac{1}{2} \alpha + \left( \frac{3}{\sqrt{2}} - 2 \right) \alpha^2 - \frac{7}{2} \left( 5 - \frac{63\sqrt{2} - 19\sqrt{3}}{16} - \frac{29\sqrt{6}}{48} \right) \alpha^3 + O(\alpha^4).
\]

A refined weak-coupling method based on the three-phonon correction has resulted in

\[
E_{CW}(\alpha) = -\alpha - 0.06066 \alpha^2 - 0.00844 \alpha^3,
\]

\[
m^*_{CW}(\alpha) = 1 + 0.5 \alpha + 0.19194 \alpha^2 - 0.06912 \alpha^3,
\]

\[
N_{CW}(\alpha) = 0.5 \alpha + 0.12132 \alpha^2 + 0.02954 \alpha^3.
\]

Our weak-coupling results (34) improve the known data [8, 7] on the one-dimensional polaron. Note, a recent attempt by considering an additional confining dot potential has resulted in the binding energy and effective mass diverging in one dimension [10].

Strong coupling
In the strong-coupling limit the solution of (21) looks like

\[
\widetilde{D}(k) = (k^2 + \mu^2)^{-1}, \quad \mu = 4\alpha^2/\pi.
\]

The Gaussian leading-order and the corrected estimates for the GSE, EM and ANVP become

\[
E_0(\alpha) = -\left( 1/\pi \right) \alpha^2, \quad m^*_0(\alpha) = \left( 16/\pi^2 \right) \alpha^4, \quad N_0(\alpha) = \left( 2/\pi \right) \alpha^2,
\]

\[
E_2(\alpha) = -0.327014 \alpha^2, \quad m^*_2(\alpha) = 1.858065 \alpha^4, \quad N_2(\alpha) = 0.654028 \alpha^2,
\]

\[
E_3(\alpha) = -0.330205 \alpha^2, \quad m^*_3(\alpha) = 1.966430 \alpha^4, \quad N_3(\alpha) = 0.660410 \alpha^2.
\]

Rigorous studies of the strong-coupling regime of the polaron in one dimension have been performed, particularly, in [4, 5]. Within the Pekar adiabatic approximation [7] efficient for \( \alpha \to \infty \), one arrives at the following variational task with a normalized wave function \( \Psi(x) \):

\[
E_A(\alpha) = -\alpha^2 \int dx \left\{ \Psi(x) \Delta \Psi(x) + 2 |\Psi(x)|^4 \right\}, \quad m^*_A(\alpha) = \alpha^4 \frac{4}{\pi} \int dk k^2 |\langle \Psi | e^{ikx} | \Psi \rangle|^2.
\]

A modified polynomial placed instead of \( \Psi(x) \) in [4] has resulted in \( E_{PS} = -0.3330877 \alpha^2, \) \( m^*_{PS} = 2.1254 \alpha^4 \) and \( N_{PS} = 0.6661754 \alpha^2 \). Fortunately, problem (38) admits explicit analytic solutions (obtained first in [4] with a re-scaled coupling) as follows:

\[
\Psi(x) = \sqrt{2}/(e^x + e^{-x}), \quad E_A(\alpha) = -\alpha^2/3, \quad m_A^*(\alpha) = 32 \alpha^4/15, \quad N_A(\alpha) = 2 \alpha^2/3.
\]
We see that our Gaussian (leading-order) approximations $E_0(\alpha)$, $m_0^*(\alpha)$ and $N_0(\alpha)$ differ from the adiabatic results (39). However, these gaps have been systematically narrowed by involving higher-order non-Gaussian contributions in (37).

**Intermediate coupling**

For finite $\alpha$ we have solved numerically the constraint equations in (21). The obtained numerical results for the Gaussian leading-order contributions $E_0(\alpha)$ and $m_0^*(\alpha)$ as well as for the next-to-leading corrected data are plotted in Fig. 1 in comparison with the Feynman estimates [6]. In Fig. 2 we have represented $N_0(\alpha)$ calculated by formula (29). According to our results, the number of virtual phonons increases fast as $\alpha$ grows and hence, the three-phonon correlation method [8] should be used carefully for $\alpha \geq 2.5$.

The ground-state energy and effective mass of the one-dimensional polaron normalized to the corresponding Feynman estimates (dotted horizontal lines) versus the coupling constant $\alpha$. Dashed lines represent the leading-order Gaussian approximations and solid curves correspond to the corrected results taking into account the second-order non-Gaussian contributions.

Note, that the Feynman-type estimation [6] represents a partial case of the Gaussian leading-order approximation, when a trial convex function $\tilde{D}_F(k) = w/k^2 + (1-w)/(k^2+\mu^2)$ is used instead of the exact solution $\tilde{D}(k)$. Therefore, the Feynman estimate is less exact than the general Gaussian result, in particular, $E_{0F}(\alpha) > E_0(\alpha)$.

In conclusion, the ground-state characteristics of the large optical polaron confined in one dimension have been calculated by using the generalized Gaussian approximation method. Exact analytic solutions for the GSE, EM and ANVP have been obtained up to the order $\alpha^3$ in the weak-coupling limit. In the strong coupling limit, our Gaussian leading-order results deviate (e.g., by 0.9 percent for the energy) from the adiabatic data obtained within the Pekar Ansatz, but the gaps have been systematically narrowed by involving the higher-order corrections. For finite coupling, the leading-order Gaussian GSE improves the Feynman variational estimate [8] and represents the lowest upper bound available for the one-dimensional polaron. Our result for the number of excited phonons limits the validity region of the few-phonon approximation methods. The next-to-leading non-Gaussian contributions have been calculated to correct the Gaussian approximations for finite $\alpha$. 

Fig. 1

![Graph showing ground-state energy and effective mass versus coupling constant \(\alpha\).](image-url)
The Gaussian approximation to the average number of virtual phonons $N_0(\alpha)$ versus the coupling constant $\alpha$.

Applied to the polaron confined in one dimension, the GGA method provides reliable results rather quickly in the entire range of coupling. Therefore, it will be reasonable to apply the GGA method to improve the Lieb-Yamazaki type lower-bound estimate (see, e.g. [9]) of the polaron self-energy.

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