Polaron ground-state energy in d dimensions

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(Received 15 April 1994)

The polaron path integral introduced by Feynman is generalized to the case of an electron moving in d space dimensions. A scheme of systematic calculations of the obtained path integral is developed to estimate the ground-state energy of the polaron in the same way for different values of the electron-phonon coupling constant α. The leading-order term in this approach yields an upper bound to the polaron self-energy and improves Feynman's variational estimates for $d = 2$ and $d = 3$. A scaling relation between polaron self-energies for different space dimensions is obtained for this term. The next correction to this estimation is calculated by numerical integration for $d = 2$ and $d = 3$.

I. INTRODUCTION

The polaron problem embraces a wide range of questions concerning the behavior of the electron for conductance in polar crystals.[1–5] A field-theoretical formulation of polaron theory was proposed by Fröhlich[6] to describe the interaction of a single band electron with phonons, quanta associated with the longitudinal-optical branch of lattice vibrations. Since that time, the Fröhlich polaron model has attracted interest as a testing ground of various nonperturbative methods in quantum physics.

The main quasiparticle characteristics of the polaron are its ground-state energy (GSE) $E(\alpha)$, effective mass m_{eff},[7,8] and lifetime. The problem of finding the GSE of the Fröhlich Hamiltonian is of considerable significance because one can suppose that in comparing two approximate methods the one giving the better $E(\alpha)$ will likely give the better m_{eff}, which can be measured directly.[9] Second, experiments on the ionization energy of bound polarons[10] require theoretical estimation of the free-polaron GSE. Therefore, it is important to have good values for the free-polaron GSE.

Historically, the GSE of the polaron is investigated in the weak-,[6,11,12] intermediate-,[13] and strong-coupling regimes[14,15] by using different methods. An attempt to build a polaron theory, valid for arbitrary values of α, was made by Feynman[1] within the path-integral (PI) formalism.

The Feynman approach for the polaron has an advantage because the phonon coordinates are adequately eliminated and, as a consequence, the polaron problem is reduced to an effective one-particle problem with retarded interaction. Besides, the PI formalism allows one to build a class of exactly solvable models corresponding to quadratic functionals. Then one can use these functionals as bases for variational estimations. As a result, Feynman's PI approach gives good upper bounds on $E_0(\alpha)$ in the entire range of α in a unified way.

There arises the question whether Feynman's estimations of the polaron GSE can be improved by introducing some trial actions, more general than the quadratic action with two variational parameters used in Ref. 1. This question, in particular, has been studied within different variational approaches,[16,17] but given variational answers it could not estimate the next corrections to the values obtained.

Traditionally, the polaron problem has been investigated in three-dimensional ($d = 3$) space.[18,19] In recent years, however, polaron effects have been observed in low-dimensional systems,[20] and certain physical problems have been mapped into a two-dimensional ($d = 2$) polaron theory.[21] The possibility that an electron may be trapped on the surface of a dielectric material has attracted much interest.[22] The GSE of the polaron for $d = 2$ is discussed in Refs. 23–25.

In the present paper, we investigate the GSE of the polaron in the case of arbitrary space dimensions ($d > 1$) and try not only to improve Feynman's result, but also to estimate the next corrections, which allow one to test the accuracy and reliability of the obtained values. The paper is organized as follows. In Sec. II we formulate a generalization of the Feynman PI of the polaron to arbitrary spatial dimension ($d > 1$) and obtain a Gaussian-equivalent representation (GER) for this path integral. We transform the initial PI to the representation built so that all the quadratic part of the polaron action is concentrated entirely in the Gaussian measure of the PI which is defined from certain equations. Therefore the polaron interaction functional is purely non-Gaussian in this representation. The necessary equations defining the explicit polaron correlation function and the measure of PI in this representation are obtained here. In Sec. III the leading-order term of the polaron GSE, which represents an improvement of Feynman's upper bound, is obtained in d dimensions for arbitrary $\alpha > 0$. In Sec. IV, we obtain the next correction to the leading term

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of the polaron self-energy. In Sec. V, we derive scaling relations between our key equations for two and three dimensions. The numerical results obtained within our method in the entire range of $\alpha = 0$–∞ for $d = 2$ and $d = 3$ are given in Sec. VI and compared with the known data in each case.

II. POLARON PATH INTEGRAL IN *d* DIMENSIONS

The Fröhlich longitudinal-optical (LO) polaron model for $d = 3$ is determined by the Hamiltonian

$$H = \frac{1}{2m}\mathbf{p}^2 + \hbar\omega \sum_{\mathbf{k}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{k}} g_{\mathbf{k}} (a^\dagger_{\mathbf{k}} e^{-i\mathbf{kx}} - a_{\mathbf{k}} e^{i\mathbf{kx}}) ,$$

$$[a_{\mathbf{k}}, a^\dagger_{\mathbf{k}'}] = \delta_{\mathbf{kk}'} , \tag{1}$$

which describes the interaction of an electron (position and momentum vectors $\mathbf{x}$ and $\mathbf{p}$, band mass m) with the phonon field (creation and annihilation operators $a^\dagger_{\mathbf{k}}$,$a_{\mathbf{k}}$, quantization volume Ω, Plank constant $\hbar$) associated with a LO branch of lattice vibrations (wave vector $\mathbf{k}$ and frequency ω) in a polar crystal. The electron-phonon interaction coefficient for coupling with the wave vector $\mathbf{k}$ in (1) is defined as follows:

$$g_{\mathbf{k}} = \frac{i\hbar\omega(\hbar/2m\omega)^{1/4}(4\pi\alpha)^{1/2}}{|\mathbf{k}|} . \tag{2}$$

The dimensionless Fröhlich coupling constant reads

$$\alpha = \frac{e^2}{2}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)\frac{1}{\hbar\omega}\left(\frac{2m\omega}{\hbar}\right)^{1/2} , \tag{3}$$

where e is the electron charge, and ϵ_∞ and ϵ_0 are the high frequency and static dielectric constants of the crystal. In most real ionic crystals it takes the value $\alpha \sim 1$–20 (e.g., $\alpha \simeq 5$ for sodium chloride). In the following, units will be chosen such that $\hbar = m = \omega = 1$.

Until now, no nontrivial solution of $H\Psi_n = E_n\Psi_n$ was known. Various methods[1,14,26,13,27] have been used to calculate approximately the spectrum of H, and especially to obtain its GSE E_0 for selected (weak, intermediate, or strong) regions of α.

To extend the Fröhlich Hamiltonian (1) written for $d = 3$ to arbitrary spatial dimensions $d > 1$, we follow a physical approach[28,29] inspired by the formulation of a lower-dimensional polaron problem as obtained from the Fröhlich Hamiltonian of a higher-dimensional system by integrating out one or more dimensions. In this approach, the basic interaction characterizing the electron motion in d dimensions remains Coulomb-like ($\sim 1/r$), i.e., the same as for $d = 3$. In the particular cases of $d = 2$ and $d = 3$, this definition of a d-dimensional polaron Hamiltonian reduces to the standard expressions for the Fröhlich Hamiltonian.

Following Ref. 29 we suppose that the form of the Fröhlich Hamiltonian in d dimensions is the same as in (1) except that now all vectors and operators are d dimensional and the electron-phonon interaction coefficient $g_{\mathbf{k}}$ is redefined as follows:

$$|g_{\mathbf{k}}|^2 = \frac{\lambda_d^2}{|\mathbf{k}|^{d-1}} , \qquad \lambda_d^2 = \Gamma\left(\frac{d-1}{2}\right) 2^{d-3/2}\pi^{(d-1)/2}\alpha . \tag{4}$$

In particular,

$$|g_{\mathbf{k}}|^2 = \begin{cases} \dfrac{\sqrt{2}\,\pi\alpha}{|\mathbf{k}|} & \text{for } d = 2, \\ \dfrac{\sqrt{8}\,\pi\alpha}{|\mathbf{k}|^2} & \text{for } d = 3. \end{cases} \tag{5}$$

Accordingly, we write the PI representation of the free energy $F(\beta)$ of a polaron with a given temperature $\Theta = 1/\beta$ as follows:

$$\exp(-\beta F) = \mathrm{Tr}_{\mathrm{el}}\mathrm{Tr}_{\mathrm{ph}}\left[\exp(-\beta H)\right] , \tag{6}$$

where the Hamiltonian H in (1) should be written in terms of the coordinates and momenta. The "Trace" is here supposed to be taken over the whole space of states of the "electron + phonon" system.

It is well known from the original paper by Feynman[1] that the phonon trace $\mathrm{Tr}_{\mathrm{ph}}$ in (6) can be evaluated if one makes use of the PI technique. The result reads

$$\exp(-\beta F) = \int_{\mathbf{x}(0)=\mathbf{x}(\beta)} \delta\mathbf{x} \exp\left\{S[\mathbf{x}]\right\} , \tag{7}$$

where the action $S[\mathbf{x}]$ is

$$S[\mathbf{x}] = -\frac{1}{2}\int_0^\beta dt\, \dot{\mathbf{x}}^2(t) + \frac{\lambda_d^2}{8\pi}\int_0^\beta dt \int_0^\beta ds\, \frac{G(t-s)}{|\mathbf{x}(t) - \mathbf{x}(s)|} . \tag{8}$$

In (8), $G(t)$ is the temperature-dependent Green function of a harmonic oscillator,

$$G(t) = \frac{\exp(-|t|) + \exp(|t| - \beta)}{1 - \exp(\beta)} . \tag{9}$$

The free energy $F(\beta)$ tends to the GSE as $\beta \to \infty$ (zero temperature case)

$$E_0 = \lim_{\beta\to\infty} F(\beta) . \tag{10}$$

The path integral in (7) is not explicitly solvable due to the non-Gaussian character of S in (8). For its estimation (for $d = 3$) Feynman has proposed[1] a quadratic two-body trial action S_F instead of S:

$$S[\mathbf{x}] \longrightarrow S_F[\mathbf{x}] = -\frac{1}{2}\int_0^\beta dt\, \dot{\mathbf{x}}^2(t) + \frac{C}{2}\int_0^\beta dt \times \int_0^\beta ds\, \left[\mathbf{x}(t) - \mathbf{x}(s)\right]^2 \exp\{-w|t-s|\} . \tag{11}$$

Here C and w are variational parameters. With the quadratic trial action S_F in (7) one gets an exact solution for $F_F(\alpha, \beta)$. A variation over parameters C and w for finding the absolute minimum of $E_0^F(\alpha) = F_F(\alpha, \beta \to \infty)$ leads to a rigorous upper bound on the polaron GSE at arbitrary α, the known Feynman result.[30]

We consider the polaron GSE given by Eqs. (7)–(10). For further convenience, we choose the symmetrical region $-\beta/2 < t < \beta/2$ and change the variable of the PI in (7),

$$\mathbf{x}(t) \longrightarrow \mathbf{r}(t-T), \qquad T = \beta/2. \tag{12}$$

Accordingly, the GSE [further it will be denoted by $E(\alpha)$] of the Fröhlich polaron can be defined as follows:

$$E(\alpha) = -\lim_{T\to\infty} \frac{1}{2T} \ln Z_T(\alpha), \tag{13}$$

where

$$\begin{aligned} Z_T(\alpha) &= C_0 \int_{\mathbf{r}(-T)=\mathbf{r}(T)} \delta\mathbf{r} \exp\left\{ -\tfrac{1}{2}(\mathbf{r}, D_0^{-1}\mathbf{r}) + \frac{\alpha}{2} \int\int_{-T}^{T} dt\, ds\, V[\mathbf{r}(t)-\mathbf{r}(s); t, s] \right\} \\ &= \int d\sigma_0 \exp\left\{ \frac{\alpha}{2} \int\int_{-T}^{T} dt\, ds V[\mathbf{r}(t)-\mathbf{r}(s); t, s] \right\}. \end{aligned} \tag{14}$$

The standard normalization $E(0) = 0$ in (13) is satisfied under the condition

$$Z_T(0) = 1, \qquad \text{or} \qquad \int d\sigma_0 \times 1 = 1. \tag{15}$$

The free-electron system is described by the kinetic term

$$(\mathbf{r}, D_0^{-1}\mathbf{r}) = \int\int_{-T}^{T} dt\, ds\, \mathbf{r}(t) D_0^{-1}(t,s)\, \mathbf{r}(s), \tag{16}$$

$$D_0^{-1}(t,s) = -\frac{\partial^2}{\partial t^2}\delta(t-s).$$

The Green function D_0 corresponding to the differential operator D_0^{-1} and satisfying the periodic boundary conditions is

$$D_0(t,s) = -\tfrac{1}{2}|t-s| - \frac{ts}{2T}. \tag{17}$$

As we consider the GSE given in (13), the parameter T is supposed to be asymptotically large. In this limit one gets the Green function

$$D_0(t,s) \underset{T\to\infty}{\longrightarrow} D_0(t-s) = -\tfrac{1}{2}|t-s| \tag{18}$$

and its Fourier transform is

$$\begin{aligned} \tilde{D}_0(p) &= \int_{-\infty}^{\infty} dt\, e^{ipt} D_0(t) \\ &= \frac{1}{2}\left[\frac{1}{(p+i0)^2} + \frac{1}{(p-i0)^2}\right]. \end{aligned} \tag{19}$$

The normalization condition (15) leads to

$$C_0 = \frac{1}{\sqrt{\det D_0}} = \prod_p \sqrt{p^2}. \tag{20}$$

The Coulomb-like interaction part, the electron self-interaction, is given by the retarded potential

$$V[\mathbf{R}; t-s] = \frac{\Gamma(d/2 - 1/2)}{4\sqrt{2}\pi^{(d+1)/2}} e^{-|t-s|} \int \frac{d\mathbf{k}}{|\mathbf{k}|^{d-1}} \exp(i\mathbf{k}\mathbf{R}),$$

$$\mathbf{R} = \mathbf{r}(t) - \mathbf{r}(s). \tag{21}$$

with the electron position vector $\mathbf{r}(t)$ embedded into d dimensions.

III. THE LEADING-ORDER TERM OF THE POLARON GROUND-STATE ENERGY IN d DIMENSIONS

For α not too large, the PI in the initial presentation (14) may be estimated by using a perturbation expansion in α. The problem is to estimate $Z_T(\alpha)$ beyond the weak-coupling regime.

Our idea is the following. As α grows, $d\sigma_0$ with the initial kinetic part transforms to the new measure $d\sigma$ that also has a Gaussian character. The potential part is also changed into another interaction functional. The system goes to a new representation under strong enough interaction. Certain restrictions may be imposed on the representation. First, it is known that in quantum theory the main divergences given by "tadpole"-type vacuum diagrams may be efficiently eliminated out of consideration if the normal-ordered product of operators is introduced into the interaction Hamiltonian. We suppose that in the case of finite polaron theory without divergences, the main contribution to the finite background energy can also be taken into account if we require the normal-ordered form for the polaron interaction functional in the strong-coupling regime. Second, the system under consideration should be near its equilibrium state. Then any linear terms $\sim \mathbf{r}$ are absent here and quadratic configurations $\sim \mathbf{r}^2$ concentrated only in the Gaussian measure $d\sigma$ determine the Gaussian oscillator character of this equilibrium point. Therefore they should not appear in the interaction functional. Then the polaron action in the new representation of the PI consists of a new kinetic part $(\mathbf{r}, D^{-1}\mathbf{r})$ and a new non-Gaussian interaction functional which should be proportional to $\mathbf{r}^3$ as $|\mathbf{r}| \to 0$.

Following this idea, we introduce the Gaussian measure[31]

$$d\sigma \equiv C\delta\mathbf{r} \exp\{-\tfrac{1}{2}(\mathbf{r}, D^{-1}\mathbf{r})\}, \tag{22}$$

with the normalization condition $\int d\sigma \times 1 = 1$ satisfied by choosing the constant

$$C \equiv \sqrt{\det D^{-1}}. \tag{23}$$

The new correlation function $D(x-y)$ determined by

$$\int_{-\infty}^{\infty} dy\, D^{-1}(x,y)\, D(y,z) \;=\; \delta(x-z) \tag{24}$$

is supposed to be translationally invariant:

$$D(t,s) \;=\; D(t-s)\,. \tag{25}$$

First, we introduce the concept of the normal product $:\cdots:$ with respect to the Gaussian measure $d\sigma$ in the following way:[32]

$$\exp(i\mathbf{kR}) =: \exp(i\mathbf{kR}) : \exp\left\{-\mathbf{k}^2F(t-s)\right\}\,, \tag{26}$$

with the notation

$$F(t-s) \;\equiv\; D(0)-D(t-s)\,. \tag{27}$$

In particular, the relations

$$\int d\sigma : e^{i\mathbf{kR}} := 1\,, \tag{28}$$

$$r_i(t)r_j(s) \;=: r_i(t)r_j(s) : + \delta_{ij}D(t-s)\,, \qquad i,j=1,\ldots,d, \tag{29}$$

are satisfied. Then, we perform an identity transformation in (14)

$$(\mathbf{r},D_0^{-1}\mathbf{r}) = (\mathbf{r},D^{-1}\mathbf{r}) + : (\mathbf{r},[D_0^{-1}-D^{-1}]\mathbf{r}) : + ([D_0^{-1}-D^{-1}],D)\,. \tag{30}$$

For further convenience we introduce the notation

$$\int d\Omega \cdots \equiv \frac{\Gamma(d/2-1/2)}{4\sqrt{2}\pi^{(d+1)/2}} \int\int_{-T}^{T} dt\, ds \exp(-|t-s|) \times \int \frac{d\mathbf{k}}{|\mathbf{k}|^{d-1}} \exp\left\{-\mathbf{k}^2F(t-s)\right\}\cdots. \tag{31}$$

Then, we rewrite the functional integral in (14) in the following form:

$$Z_T(\alpha) = \frac{C_0}{C}\exp\left\{-\tfrac{1}{2}\left([D_0^{-1}-D^{-1}],D\right)+\alpha\int d\Omega\times 1\right\} \times \int d\sigma \exp\left\{-\tfrac{1}{2} : \left(\mathbf{r},[D_0^{-1}-D^{-1}]\mathbf{r}\right) : +\alpha\int d\Omega : e_2^{i(\mathbf{kR})} : -\frac{\alpha}{2}\int d\Omega : (\mathbf{kR})^2 : \right\}, \tag{32}$$

where

$$e_2^z = e^z - 1 - z - \frac{z^2}{2}\,. \tag{33}$$

In (32) we have used the identity

$$: \exp(i\mathbf{kR}) :=: e_2^{i(\mathbf{kR})} : + : 1 + i(\mathbf{kR}) - \tfrac{1}{2}(\mathbf{kR})^2 : \tag{34}$$

and relations

$$\int d\Omega\,(\mathbf{kR}) = 0\,, \qquad \int d\Omega\,(\mathbf{kR})^2 = \frac{1}{d}\int d\Omega\,\mathbf{k}^2\mathbf{R}^2\,. \tag{35}$$

Second, we include all quadratic terms ($\sim \mathbf{r}^2$) only into the Gaussian measure $d\sigma$ so that they should not arise in the remaining part of S in curly brackets in the right-hand side of (32). This goal is achieved by introducing the equation

$$: -\tfrac{1}{2}\left(\mathbf{r},[D_0^{-1}-D^{-1}]\mathbf{r}\right) - \frac{\alpha}{2d}\int d\Omega\,\mathbf{k}^2\mathbf{R}^2 := 0\,. \tag{36}$$

For $T\to\infty$ it becomes

$$\int\int_{-\infty}^{\infty} dt\, ds\left\{ : \mathbf{r}(t)[D_0^{-1}(t,s)-D^{-1}(t,s)]\mathbf{r}(s) : + \frac{\alpha\Gamma(d/2-1/2)}{4\sqrt{2}\pi^{(d+1)/2}d}\exp(-|t-s|) \times \int \frac{d\mathbf{k}}{|\mathbf{k}|^{d-1}}\mathbf{k}^2 \exp\left\{-\mathbf{k}^2F(t-s)\right\} : \mathbf{r}^2(t)+\mathbf{r}^2(s)-2\mathbf{r}(t)\mathbf{r}(s) : \right\} = 0\,, \tag{37}$$

Due to the symmetry $t \longleftrightarrow s$ we make the following substitutions in (37):

$$\mathbf{r}^2(t)+\mathbf{r}^2(s) \longrightarrow 2\mathbf{r}^2(t) = 2\mathbf{r}(t)\int_{-\infty}^{\infty} d\xi\, \delta(\xi-t)\mathbf{r}(\xi)\,. \tag{38}$$

Then, using the relation

$$\int \frac{d\mathbf{k}}{|\mathbf{k}|^{d-1}}\mathbf{k}^2 \exp\left\{-\mathbf{k}^2F(t-s)\right\} = \frac{\pi^{(d+1)/2}}{2\Gamma(d/2)F^{3/2}(t-s)}\,, \tag{39}$$

we rewrite (37) as follows:

$$\int\int_{-\infty}^{\infty} dt\, ds : \mathbf{r}(t)\left\{D_0^{-1}(t-s) - D^{-1}(t-s) + \alpha\frac{\Gamma(d/2-1/2)}{4\sqrt{2}\,d\,\Gamma(d/2)} \times \left[\delta(t-s)\int_{-\infty}^{\infty} d\xi\, \frac{\exp(-|t-\xi|)}{F^{3/2}(t-\xi)} - \frac{\exp(-|t-s|)}{F^{3/2}(t-s)}\right]\right\}\mathbf{r}(s) := 0\,. \tag{40}$$

This condition is satisfied if one sets

$$D_0^{-1}(t-s) - D^{-1}(t-s) + \alpha_d \Sigma(t-s) = 0\,. \tag{41}$$

Here we have introduced the "effective coupling constant"

$$\alpha_d = \alpha R_d\,, \qquad R_d = \frac{3\sqrt{\pi}\,\Gamma(d/2-1/2)}{2\,d\,\Gamma(d/2)} \tag{42}$$

and the function

$$\Sigma(t-s) \equiv \frac{1}{6\sqrt{2\pi}}\left\{\delta(t-s)\int_{-\infty}^{\infty} d\xi\,\frac{\exp(-|\xi|)}{F^{3/2}(\xi)} - \frac{\exp(-|t-s|)}{F^{3/2}(t-s)}\right\}. \tag{43}$$

Multiplying both sides of (41) by $D(s-x)$ and introducing integration over $\int_{-\infty}^{\infty} ds$, we arrive at the equation

$$-\Box_t D(t-x) - \delta(t-x) + \alpha_d \int_{-\infty}^{\infty} ds\,\Sigma(t-s)\,D(s-x) = 0\,. \tag{44}$$

It is convenient to use Fourier transforms defined as follows:

$$\tilde{D}(k) = \int_{-\infty}^{\infty} dx\, e^{ikx} D(x)\,, \tag{45}$$

$$\tilde{D}_0(k) = 1/k^2\,, \tag{46}$$

$$\tilde{\Sigma}(k) = \int_{-\infty}^{\infty} dt\, e^{-ikt}\Sigma(t) = \frac{1}{3\sqrt{2\pi}}\int_0^{\infty} dt \exp(-t)\,\frac{1-\cos(kt)}{F^{3/2}(t)}\,. \tag{47}$$

Accordingly, (44) becomes

$$k^2\tilde{D}(k) - 1 + \alpha_d\tilde{\Sigma}(k)\tilde{D}(k) = 0\,, \tag{48}$$

which leads to

$$\tilde{D}(k) = \frac{1}{k^2 + \alpha_d\,\tilde{\Sigma}(k)}\,. \tag{49}$$

Subsequently,

$$F(t) = D(0) - D(t) = \int_{-\infty}^{\infty}\frac{dk}{2\pi}\tilde{D}(k)\left(1-e^{ikt}\right) = \frac{1}{\pi}\int_0^{\infty} dk\,\frac{1-\cos(kt)}{k^2+\alpha_d\tilde{\Sigma}(k)}\,. \tag{50}$$

Due to Eqs. (47) and (50), in the new representation all the quadratic terms in the polaron action functional are concentrated only in the new Gaussian measure $d\sigma$.

The problem is to solve the nonlinear integral equations (47) and (50) for the two-point correlation function $D(x)$. Unfortunately, we are not able to solve them exactly in analytic form except the asymptotic cases $\alpha \to 0$ and $\alpha \to \infty$. In the intermediate range of $\alpha = 1$–40 we solve them by developing an iteration numerical scheme. We can easily find the asymptotical behavior of $F(t)$:

$$F(t) \sim t \quad \text{as} \quad t \to 0\,, \qquad F(t) \sim F_0 \quad \text{as} \quad t \to \infty \tag{51}$$

and $\tilde{\Sigma}(k)$:

$$\tilde{\Sigma}(k) \sim k^2 \quad \text{as} \quad k \to 0\,, \qquad \tilde{\Sigma}(k) \sim \tilde{\Sigma}_0 \quad \text{as} \quad k \to \infty\,, \tag{52}$$

where F_0 and $\tilde{\Sigma}_0$ are constants. These dependencies will be useful for correct numerical iterations to solve (47)–(50).

Note that, in the particular case of $d = 3$, equations similar to (47) were obtained in other approaches[33,25] from variational conditions. Our equations (47)–(50) may be used for a self-consistent estimation of $E(\alpha)$ for the d-dimensional optical polaron in the entire range of the electron-phonon coupling constant α.

Finally we get the new representation (GER) of the GSE of the optical polaron in the form

$$E(\alpha) = E_0(\alpha) - \lim_{T\to\infty}\frac{1}{2T}\ln J_T(\alpha)\,, \tag{53}$$

where the function $E_0(\alpha)$, being the "leading-order energy," or the GSE in the zeroth approximation, is

$$E_0(\alpha) = -\lim_{T\to\infty}\frac{1}{2T}\left[\frac{1}{2}\ln\det\left(\frac{D}{D_0}\right) - \frac{1}{2}\left([D_0^{-1}-D^{-1}],D\right) + \alpha\int d\Omega\times 1\right]. \tag{54}$$

It is easy to show that

$$\frac{1}{2}\ln\frac{\det D}{\det D_0} = \frac{1}{2}\mathrm{Tr}\left[\ln\frac{D}{D_0}\right] = 2Td\int_0^{\infty}\frac{dk}{2\pi}\ln[k^2\tilde{D}(k)]\,, \tag{55}$$

$$-\frac{1}{2}\left([D_0^{-1}-D^{-1}],D\right) = -2Td\int_0^{\infty}\frac{dk}{2\pi}[k^2\tilde{D}(k)-1]\,, \tag{56}$$

$$\alpha\int d\Omega\times 1 = 2Td\,\frac{\alpha_d}{3\sqrt{2\pi}}\int_0^{\infty} dt\,\frac{\exp(-t)}{F^{1/2}(t)}\,. \tag{57}$$

Inserting these relations into (54) we obtain for $d > 1$ the leading term of the d-dimensional polaron GSE as follows:

$$E_0(\alpha) = -d\left\{\frac{1}{2\pi}\int_0^{\infty} dk\{\ln[k^2\tilde{D}(k)] - k^2\tilde{D}(k) + 1\} + \frac{\alpha_d}{3\sqrt{2\pi}}\int_0^{\infty} dt\,\frac{\exp(-t)}{F^{1/2}(t)}\right\}. \tag{58}$$

Our leading term (the zero-order approximation) $E_0(\alpha)$ gives an upper bound to the exact GSE of a polaron $E(\alpha)$. Really, applying Jensen's inequality to (53) one gets

$$\exp\{-2TE(\alpha)\} \geq \exp\{-2TE_0(\alpha)\} \tag{59}$$

because of

$$\int d\sigma : \exp(i\mathbf{kR}) - 1 + \tfrac{1}{2}(\mathbf{kR})^2 := 0\,. \quad (60)$$

Consequently,

$$E_0(\alpha) \geq E(\alpha)\,. \quad (61)$$

The high-order corrections $\Delta E(\alpha)$ in (53) can be obtained by evaluating the PI

$$e^{-2T\Delta E(\alpha)} = J_T(\alpha) = \int d\sigma \exp\left\{\alpha \int d\Omega : \exp(i\mathbf{kR}) - 1 + \frac{1}{2}(\mathbf{kR})^2 :\right\}. \quad (62)$$

It should be stressed that the representation (53) is completely equivalent to the initial representation (13) for asymptotically large $T \to \infty$. The Gaussian equivalent representation (53) gives the origin of various approximations differing from each other in the accuracy of deriving equations (47)–(50).

As a simple approximation of $\tilde{\Sigma}(k)$ obeying the asymptotics in (52), one can take the function

$$\tilde{\Sigma}^F(k) = \frac{\mu^2}{\alpha_d}\frac{k^2}{\xi^2 + k^2}\,, \quad (63)$$

where μ and ξ are parameters. Then, (50) becomes

$$F^F(t) = \frac{1}{\pi}\int_0^\infty dk\, \frac{1-\cos(kt)}{k^2}\left[1 - \frac{\mu^2}{\lambda^2 + k^2}\right] = \frac{\mu^2}{2\lambda^3}\left(1 - e^{-\lambda t} + \lambda t\,\frac{\xi^2}{\mu^2}\right), \quad (64)$$

$$\lambda = \sqrt{\mu^2 + \xi^2}\,.$$

These approximate solutions of (47)–(50) determine the leading term of the polaron self-energy in the following form:

$$E_0^F(\alpha) = -\frac{d}{2}\left[\xi - \lambda + \frac{\mu^2}{2\lambda}\right] - \frac{\alpha_d \lambda^{3/2} d}{3\mu\sqrt{\pi}} \times \int_0^\infty \frac{dt\, \exp(-t)}{\sqrt{1 - \exp(-\lambda t) + \lambda t \xi^2/\mu^2}}\,. \quad (65)$$

Minimizing the obtained energy over the parameters μ and ξ, one easily finds the Feynman variational upper bound in d dimensions. For $d = 3$ ($\alpha_3 = \alpha$) it explicitly reproduces the well-known Feynman variational upper bound to the polaron GSE:[30]

$$E^F(\alpha) = \min_\mu \min_\xi E_0^F(\alpha, d = 3)\,. \quad (66)$$

We stress that the extremal conditions on parameters μ, ξ in (66) are equivalent to a particular choice of the functions $\tilde{\Sigma}^F(k)$ and $F^F(t)$ in (63)–(64). However, the functions in (63)–(64) are not exact solutions of (47) and (50). It means that the Feynman trial quadratic action does not at all represent the Gaussian part of the polaron action for $d = 3$. Exact numerical solution of Eqs. (47) and (50) by the iteration procedure (shown below in Sec. VI) allows us to obtain $E_0(\alpha)$, more exactly, which improves the Feynman result $E^F(\alpha)$ in the entire range of α. The obtained numerical results $E_0(\alpha)$ for $d = 2$ and $d = 3$ as compared with Feynman's variational estimation are displayed in Tables I–VI below.

IV. THE CALCULATION OF THE SECOND-ORDER CORRECTION

According to (62) higher-order corrections $\Delta E(\alpha)$ to the polaron GSE are defined by the expression

$$\exp\{-2T\Delta E(\alpha)\} = \int d\sigma \exp\{W[\mathbf{r}]\}\,. \quad (67)$$

Here, the interaction functional written in the new representation is

$$W[\mathbf{r}] = \alpha_d \frac{\Gamma(d/2)\, d}{6\sqrt{2}\pi^{d/2+1}} \int\int_{-T}^{T} dt\, ds e^{-|t-s|} \times \int \frac{d\mathbf{k}}{|\mathbf{k}|^{d-1}} \exp\{-\mathbf{k}^2 F(t-s)\} : e_2^{i\mathbf{k}[\mathbf{r}(t)-\mathbf{r}(s)]} :\,. \quad (68)$$

It was shown in Ref. 32 that the main contribution to $E(\alpha)$ comes from $E_0(\alpha)$ as $\alpha \to \infty$. In the weak-coupling limit $\alpha \to 0$ the contribution of $E_0(\alpha)$ proportional to α is also dominant because the corrections generated by the functional integral in (68) vanish, being proportional to α^2. Then we can suppose that in the intermediate range of α, $E_0(\alpha)$ also gives the main contribution to the polaron self-energy. Corrections $\Delta E(\alpha)$ should be evaluated from the functional integral in (68) by expanding e^W in (67) in a series

$$\Delta E(\alpha) = \sum_{n=1}^{\infty} \Delta E_n(\alpha) = -\lim_{T\to\infty} \frac{1}{2T} \sum_{n=1}^{\infty} \frac{1}{n!} \int d\sigma\, \{W[\mathbf{r}]\}^n_{\text{connected}}\,. \quad (69)$$

We stress that (69) is not a standard perturbation series in the coupling constant α_d as α_d enters into W not only explicitly as a factor, but also implicitly through the function $F(t)$. The first term in (69) with $n = 1$ equals zero due to relations (28)–(29). Nontrivial corrections are given by terms with $n \geq 2$. For the second-order correction to $E_0(\alpha)$ we get

$$\Delta E_2(\alpha) = -\lim_{T\to\infty} \frac{1}{2T}\left\{\frac{\alpha_d^2}{2!}\left[\frac{\Gamma(d/2)\, d}{6\sqrt{2}\pi^{d/2+1}}\right]^2 \int\int_{-T}^{T} dt\, ds \int\int_{-T}^{T} dx\, dy e^{-|t-s|-|x-y|} \times \int \frac{d\mathbf{k}}{|\mathbf{k}|^{d-1}} \int \frac{d\mathbf{p}}{|\mathbf{p}|^{d-1}} \exp\{-\mathbf{k}^2 F(t-s) - \mathbf{p}^2 F(x-y)\} \int d\sigma : e_2^{i\mathbf{k}[\mathbf{r}(t)-\mathbf{r}(s)]} :: e_2^{i\mathbf{p}[\mathbf{r}(x)-\mathbf{r}(y)]} : \right\}. \quad (70)$$

We calculate

$$\int d\sigma : \exp\{i\mathbf{k}[\mathbf{r}(t)-\mathbf{r}(s)]\} :: \exp\{i\mathbf{p}[\mathbf{r}(x)-\mathbf{r}(y)]\} := \exp\{-\mathbf{kp}\Xi\}\,, \tag{71}$$

where the four-point correlation function Ξ is introduced as follows:

$$\Xi(t,s,x,y) = D(t-x)+D(s-y)-D(s-x)-D(t-y)\,. \tag{72}$$

Expanding $\exp(-\mathbf{kp}\Xi)$ into a series and taking into account the relation

$$\int\int d\mathbf{k}\,d\mathbf{p}\,f(\mathbf{k}^2,\mathbf{p}^2)\,(\mathbf{kp})^{2n} = \frac{4\pi^{d-1/2}\Gamma(n+1/2)}{\Gamma(d/2)\Gamma(n+d/2)}\int_0^\infty dk\int_0^\infty dp\,(kp)^{d-1+2n}f(k^2,p^2) \tag{73}$$

for arbitrary function $f(\mathbf{k}^2,\mathbf{p}^2)$, one finally gets

$$\Delta E_2(\alpha) = -\lim_{T\to\infty}\frac{1}{2T}\frac{\alpha_d^2\Gamma(d/2)\,d^2}{144\pi^{3/2}}\int\int_{-T}^{T}dt\,ds\int\int_{-T}^{T}dx\,dy e^{-|t-s|-|x-y|} \times\sum_{n=2}^{\infty}\frac{\Xi^{2n}\,\Gamma(n+1/2)\,[(2n-1)!!]^2}{(2n)!\,4^n\,\Gamma(n+d/2)\,[F(t-s)F(x-y)]^{n+1/2}}\,. \tag{74}$$

Remember that the function $F(t)$ is a solution of Eqs. (47)–(50). Using the symmetry behaviors of the functions $F(t-s)F(x-y)$ and $\Xi(t,s,x,y)$ we can reduce the four-dimensional integration volume in (74) into a three-dimensional volume. We obtain

$$\Delta E_2(\alpha) = -\alpha_d^2\frac{\Gamma(d/2)\,d^2}{18\pi^{3/2}}\sum_{n=2}^{\infty}Q_nR_n(\alpha)\,, \tag{75}$$

$$Q_n = \frac{(2n)!\,\Gamma(n+1/2)}{16^n(n!)^2\Gamma(n+d/2)}\,,$$

$$R_n = \int\int\int_0^\infty dadbdc\left\{e^{-a-c}\frac{[F(a+b)+F(b+c)-F(a+b+c)-F(b)]^{2n}}{[F(a)F(c)]^{n+1/2}} + e^{-a-2b-c}\frac{[F(a)+F(c)-F(a+b+c)-F(b)]^{2n}}{[F(a+b)F(b+c)]^{n+1/2}} + e^{-a-2b-c}\frac{[F(a+b)+F(b+c)-F(a)-F(c)]^{2n}}{[F(a+b+c)F(b)]^{n+1/2}}\right\}.$$

We stress that expression (75) can further be simplified, but we keep this form for clarity.

Finally, we get the following expression for the GSE of the polaron:

$$E^{(2)}(\alpha) = E_0(\alpha) + \Delta E_2(\alpha)\,, \tag{76}$$

which can be evaluated numerically for arbitrary α and different space dimensions d.

Notice that $E_0(\alpha)$ in (58) is of the order of α^i ($i = 0,1,2,\ldots$) while $\Delta E_2(\alpha)$ in (75) is only of the order of α^j ($j=2,3,\ldots$).

V. SCALING RELATIONS

The theory under consideration has two parameters α and d. In general, all our expressions should depend on both of them. Notice that key expressions in (47), (49), and (50), completely defining the functions $F(t)$ and $\tilde{\Sigma}(k)$, depend only on the effective coupling constant α_d. This means that the relations

$$F^{[n]}(\alpha_m,t) = F^{[m]}(\alpha_n,t)\,,$$
$$\tilde{\Sigma}^{[n]}(\alpha_m,k) = \tilde{\Sigma}^{[m]}(\alpha_n,k), \qquad n,m>1, \tag{77}$$

hold, where the numbers of space dimensions n and m are in square brackets $[\cdots]$. In the particular case of $d=2$ and $d=3$, we found

$$F^{[2]}(\alpha,t) = F^{[3]}\left(\frac{3\pi\alpha}{4},t\right),$$
$$\tilde{\Sigma}^{[2]}(\alpha,k) = \tilde{\Sigma}^{[3]}\left(\frac{3\pi\alpha}{4},k\right). \tag{78}$$

Then, considering (58), one easily finds that this scaling relation is also valid for $\frac{1}{d}E_0(\alpha_d)$. We have

$$E_0^{[2]}(\alpha) = \frac{2}{3}\,E_0^{[3]}\left(\frac{3\pi\alpha}{4}\right). \tag{79}$$

Note that the relation (79) was obtained earlier in Refs. 29 and 25. But this scaling is not valid beyond E_0 because the interaction functional $W[\mathbf{r}]$ depends not only on α_d, but also on d in a complicated way. In particular, for $d=2$ and $d=3$ we can rewrite (75) as

$$\Delta E_2^{[2]}(\alpha) = -\frac{\pi\alpha^2}{8}\sum_{n=2}^{\infty}\frac{(2n)!\,\Gamma(n+1/2)}{16^n\,(n!)^3}\,R_n(\alpha_2)\,, \tag{80}$$

$$\Delta E_2^{[3]}(\alpha) = -\frac{9\pi\alpha^2}{32}\sum_{n=2}^{\infty}\frac{(2n)!}{16^n(n!)^2\,(2n+1)}\,R_n(\alpha_3)\,, \tag{81}$$

which show that the scaling relation (58) is no longer satisfied above $E_0(\alpha)$.

Let us consider the asymptotic limits of spatial dimensions d at fixed finite α. The lowest value of the parameter under consideration is $d = 1 + 2\epsilon$ with $\epsilon \to +0$. For this case we easily find that

$$\lim_{d\to 1} \alpha_d = \frac{3\alpha}{d-1} \to \infty . \tag{82}$$

On the other hand, considering large space dimensions, we find that

$$\lim_{d\to\infty} \alpha_d = \frac{3\alpha\sqrt{\pi e}}{\sqrt{2}\, d^{3/2}} \to 0 . \tag{83}$$

Taking into account (82) and (83) we can conclude that as d becomes larger, α_d decreases fast and in fact we deal with the effective weak-coupling regime $\alpha_d \ll 1$ even for α not too small. For example, the second-order correction $\Delta E_2(\alpha)$ behaves as follows (see Eq. (93) in Sec. VI):

$$\Delta E_2(\alpha) \underset{d\to\infty}{\longrightarrow} -\frac{1}{8\pi}\alpha_d^2 . \tag{84}$$

In other words, our leading-order energy term $E_0(\alpha)$ tends to the exact GSE $E(\alpha)$ as d grows because the role of $\Delta E(\alpha)$ becomes insignificant.

VI. NUMERICAL RESULTS

In this section, we present numerical values of $E_0(\alpha)$ and $E^{(2)}(\alpha)$ estimated within the GER method and compare them with known results obtained in various (weak, strong, and intermediate) ranges of α. The results obtained are given in Tables I–VI and shown in Figs. 1 and 2 below.

A. Weak-coupling limit

Among the known numerical results concerning the GSE of the polaron, those obtained for $\alpha \to 0$ are more accurate. In this limit the problem has been investigated by Fröhlich in a pioneering work.[33] Lee, Low, and Pines[25] applied to this problem the variational principle and Tomonaga method. As $\alpha \to 0$, one can apply either the standard perturbation approach,[34] or canonical transformations of the Hamiltonian with subsequent variational estimations.[36,26,37,35,13,38] Below, we calculate the exact GSE of the d-dimensional polaron to order α^2 in the weak-coupling limit and compare the accuracy of the results obtained with exact perturbation estimations presented in Refs. 26, 39, 40, 24, 41, and 29 for $d = 2$ and $d = 3$.

For α not too large, the polaron self-energy $E(\alpha)$ has the form

$$E(\alpha) = \alpha C_{w1} + \alpha^2 C_{w2} + O(\alpha^3) . \tag{85}$$

The coefficients C_{w1} and C_{w2} are known with good accuracy for $d = 2$ (Ref. 29) and $d = 3$.[39,29] In our approach, the coefficient C_{w1} arises only from $E_0(\alpha)$ in (58); whereas C_{w2} arises from both $E_0(\alpha)$ and $\Delta E_2(\alpha)$ in (75).

Since we are interested only in calculating the coefficients C_{w1} and C_{w2} in (85), it is enough to solve the functions $F(t)$ and $\tilde{D}(k)$ up to α. From (50) and (47) we get

$$\tilde{\Sigma}(k) = \frac{2}{3\sqrt{\pi}}\int_0^\infty dt e^{-t}\, \frac{1-\cos(kt)}{t^{3/2}} + O(\alpha) , \tag{86}$$

$$F(t) = \frac{1}{\pi}\int_0^\infty dk\, \{1-\cos(kt)\}\, \tilde{D}(k) = \frac{t}{2} - \alpha_d f(t) + O(\alpha^2) , \tag{87}$$

where

$$\tilde{D}(k) = \frac{1}{k^2}\left(1 - \alpha_d \frac{\tilde{\Sigma}(k)}{k^2}\right) + O(\alpha^2) , \tag{88}$$

$$f(t) = \frac{1}{\pi}\int_0^\infty dk\, \frac{1-\cos(kt)}{k^2}\, \frac{\tilde{\Sigma}(k)}{k^2} + O(\alpha^2) . \tag{89}$$

Substituting these expressions into (58), we get

$$E_0(\alpha) = -\alpha\frac{R_d d}{3} - \alpha^2 \frac{R_d^2\, d}{36}\left(1 - \frac{8}{3\pi}\right) + O(\alpha^3) . \tag{90}$$

In (90) we made use of the following relation:

$$\frac{2\sqrt{\pi}}{3}\int_0^\infty dt \exp(-t)\, \frac{f(t)}{t^{3/2}} = \int_0^\infty dk \left[\frac{\tilde{\Sigma}(k)}{k^2}\right]^2 = \frac{\pi}{9}\left(1 - \frac{8}{3\pi}\right) . \tag{91}$$

Equation (90) defines the coefficient C_{w1} exactly as

$$C_{w1} = -\frac{R_d}{3} d \tag{92}$$

and also contributes to C_{w2}. Concerning the coefficient C_{w2}, we should also take into account corrections coming from $\Delta E_2(\alpha)$. Inserting (87) into (75) and going to variables $x = 1 + a/b$ and $y = 1 + c/b$, we get

$$\Delta E_2(\alpha) = -\alpha^2 \frac{R_d^2\, \Gamma(d/2) d^2}{9\pi^{3/2}} \times \sum_{n=2}^{\infty} \frac{(2n)!\,\Gamma(n+1/2)}{4^n (n!)^2\, \Gamma(n+d/2)} B_n + O(\alpha^3) , \tag{93}$$

$$B_n = \int\int_1^\infty dx\, dy\, \frac{1}{(x+y)^2}\left[\frac{1}{(xy)^{n+1/2}} + \frac{1}{(x+y-1)^{n+1/2}}\right] .$$

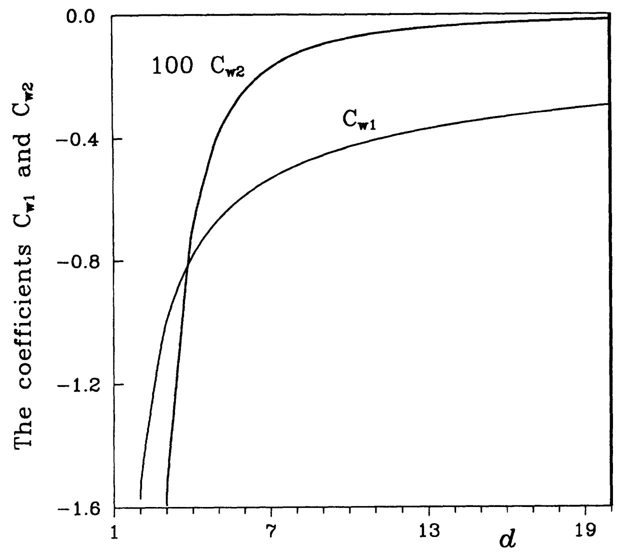

FIG. 1. The behavior of the coefficients C_{w1} and C_{w2} of the polaron ground-state energy in expansion $E(\alpha) = \alpha C_{w1} + \alpha^2 C_{w2} + O(\alpha^3)$ at weak-coupling limit $\alpha \to 0$ in dependence on number of space dimensions d. Curves correspond to 1 – C_{w1} and 2 – $100C_{w2}$.

The remaining higher-order corrections $\Delta E_{n>2}(\alpha)$ are proportional to $\sim \alpha^3$, and therefore they do not contribute to C_{w1} and C_{w2}. We have

$$C_{w2} = -\frac{R_d^2 d}{36}\left(1 - \frac{8}{3\pi}\right) - \frac{R_d^2 \Gamma(d/2)\, d^2}{9\pi^{3/2}} \times \sum_{n=2}^{\infty} \frac{(2n)!\,\Gamma(n+1/2)}{4^n (n!)^2\, \Gamma(n+d/2)} B_n\,. \tag{94}$$

The dependence of the coefficients C_{w1} and C_{w2} on the space dimension number d is shown in Fig. 1. Note that $C_{w1} = -\sqrt{\pi/2d}$ as $d \to \infty$, implying that polaron effects decrease in large space dimensions. On the contrary, this effect is considerable for $d = 2$. We stress that our results in (92) and (94) coincide with those obtained in Ref. 29.

In two dimensions $\alpha_2 = 3\pi\alpha/4$ and one rewrites (90) and (93) as

$$E_0(\alpha) = -\alpha\frac{\pi}{2} - \alpha^2 \frac{9\pi^2}{288}\left(1 - \frac{8}{3\pi}\right) + O(\alpha^3) = -\frac{\alpha}{2}\pi - \alpha^2 0.046\,626 + O(\alpha^3)\,, \tag{95}$$

$$\Delta E_2(\alpha) = -\alpha^2 \frac{\pi}{4} \sum_{n=2}^{\infty} \frac{[(2n)!]^2}{16^n (n!)^4} \cdot B_n + O(\alpha^3) = -\alpha^2 0.017\,348 + O(\alpha^3)\,. \tag{96}$$

As a result, we obtain

$$E^{(2)}(\alpha) = -\alpha\frac{\pi}{2} - \alpha^2 0.063\,974 + O(\alpha^3) \tag{97}$$

for the exact GSE of the two-dimensional polaron up to the order α^2. For comparison, in Table I we give the known results for $d = 2$ as $\alpha \to 0$. One can see from Table I that our C_{w2} obtained only from $E_0(\alpha)$ improves the Feynman's estimate about 2%. Adding the next correction calculated from ΔE_2 results in $C_{w2} = -0.063\,974$, which is in good agreement with the exact value in Ref. 29. Note, ΔE_2 contributes about 27% to the total value of C_{w2}.

In three dimensions, highly accurate results have been obtained in Ref. 29. Notice that $\alpha_3 = \alpha$. Then, we get from (90) and (93)

$$E_0(\alpha) = -\alpha - \alpha^2 \frac{1}{12}\left(1 - \frac{8}{3\pi}\right) + O(\alpha^3) = -\alpha - \alpha^2 0.012\,598 + O(\alpha^3)\,. \tag{98}$$

and

$$\Delta E_2(\alpha) = -\frac{\alpha^2}{\pi} \sum_{n=2}^{\infty} \frac{(2n)!}{4^n (n!)^2 (2n+1)} B_n + O(\alpha^3) = -\alpha^2 0.003\,321 + O(\alpha^3)\,. \tag{99}$$

Summing them, we have

$$E^{(2)}(\alpha \to 0) = -\alpha - \alpha^2 0.015\,919 + O(\alpha^3)\,. \tag{100}$$

TABLE I. Comparison of known weak-coupling results for the polaron ground-state energy $E(\alpha) = \alpha C_{w1} + \alpha^2 C_{w2} + O(\alpha^3)$ in two dimensions.

Authors	C_{w1}	C_{w2}
Das Sarma and Mason (Ref. 39)	$-\pi/2$	−0.062
Feynman's theory (Ref. 40)	$-\pi/2$	−0.04569
4th-, 6th-order pert. theory (Ref. 40)	$-\pi/2$	−0.06397
Peeters *et al.* (Ref. 29)	$-\pi/2$	−0.0639740[a]
Hipolito (Ref. 41)	$-\pi/2$	−0.0245
Present $E_0(\alpha)$	$-\pi/2$	−0.046626
Present $E_0(\alpha) + \Delta E_2$	$-\pi/2$	−0.063974

[a]The exact value.

TABLE II. Comparison of known weak-coupling results for the polaron ground-state energy $E(\alpha) = \alpha C_{w1} + \alpha^2 C_{w2} + O(\alpha^3)$ in three dimensions.

Authors	C_{w1}	C_{w2}
Das Sarma and Mason (Ref. 39)	−1	−0.016
Feynman's theory (Ref. 40)	−1	−0.012347
Röseler (Ref. 35)	−1	−0.0159196[a]
Lee *et al.* (Ref. 26)	−1	−0.014
Larsen (Ref. 13)	−1	−0.016
Present $E_0(\alpha)$	−1	−0.012598
Present $E_0(\alpha) + \Delta E_2$	−1	−0.015919

[a]The exact value.

TABLE III. Comparison of obtained estimations of the coefficient C_s of the polaron ground-state energy $E(\alpha) = \alpha^2 C_s + O(1)$ for $d = 2$ as $\alpha \to \infty$.

Authors	C_s
Das Sarma and Mason (Ref. 39)	−0.392699
Feynman's theory (Ref. 40)	−0.392699[a]
Xiaoguang *et al.* (Ref. 40)	−0.4047[b]
Hipolito (Ref. 41)	−0.392699
Smondyrev (Ref. 25)	−0.4099
Present $E_0(\alpha)$	−0.392699
Present $E_0(\alpha) + \Delta E_2$	−0.400538

[a]Estimated in Ref. 39.
[b]Adiabatic approximation.

Our results are displayed in Table II together with the known results of the polaron GSE for $d = 3$ in the weak-coupling limit. Our leading term of energy $E_0(\alpha)$ improves the Feynman variational estimation of C_{w2} by 2%. The next correction (99) results in $C_{w2} = -0.015\,919$, which is in good agreement with the exact value in Ref. 29. Note, for $d = 3$ our ΔE_2 contributes about 21% (smaller than for $d = 2$) to the total value of C_{w2}. Comparing (84), (97), and (100) with the results for $d = 2$ and $d = 3$, we conclude that higher-order corrections (the second-order one in our case) coming from $J_T(\alpha)$ are substantially more important for $d = 2$ than for $d = 3$. In other words, the polaron effect is stronger in low space dimensions [see Eq. (84)]. This effect was noted earlier in Refs. 29 and 25.

B. Strong-coupling regime

The GSE of the polaron in the strong electron-phonon coupling regime has been considered by Landau and Pekar[41] in the Born-Oppenheimer approach and by Bogoliubov and Tjablikov[43] in the adiabatic approximation. Special perturbative analyses can also be performed as $\alpha \to \infty$.[14,44,38,45,15]

It is well known that in this limit

$$E(\alpha) = \alpha^2 C_s + O(1)\,. \tag{101}$$

At large α, the functions $F(t)$ and $\tilde{\Sigma}(k)$ behave as constants except in the vicinities of the points $t = 0$ and $k = 0$. Starting with the assumed functions

$$F(t) = A\,, \qquad \tilde{\Sigma}(k) = B \tag{102}$$

and substituting these into (47)–(50), one gets the following expressions for the constants A and B:

$$A = \frac{1}{\pi}\int_0^\infty dk\,\frac{1}{k^2 + \alpha_d B} = \frac{1}{2\mu}\,, \tag{103}$$

$$B = \frac{1}{3\sqrt{2\pi}}\int_0^\infty dt e^{-t}\frac{1}{A^{3/2}} = \frac{2\mu^{3/2}}{3\sqrt{\pi}}\,, \tag{104}$$

where

$$\mu = \frac{4\alpha_d^2}{9\pi}\,. \tag{105}$$

Substituting these functions into (47) and (50) we have

$$F(t) = \frac{1}{\pi}\int_0^\infty dk\,\frac{1-\cos(kt)}{k^2+\alpha_d B} = \frac{1-\exp(-\mu|t|)}{2\mu}\,, \tag{106}$$

so

$$\tilde{D}(k) = \frac{1}{k^2+\mu^2}\,, \qquad \tilde{\Sigma}(k) = B\,\frac{k^2}{1+k^2}\,. \tag{107}$$

We substitute (106) and (107) into (58) and obtain the leading term of the polaron GSE in the strong-coupling regime as

$$\begin{aligned} E_0(\alpha) &= -\frac{d}{2\pi}\int_0^\infty dk\left[\ln\left(\frac{1+k^2}{1+k^2+\mu^2}\right) + \frac{\mu^2}{1+k^2+\mu^2}\right] \\ &\quad - \frac{\alpha_d\sqrt{\mu}}{3\sqrt{\pi}}\int_0^\infty dt\,\frac{\exp(-t)}{\sqrt{1-\exp(-\mu\, t)}} \\ &= -\alpha_d^2\,\frac{d}{9\pi} + O(1)\,. \end{aligned} \tag{108}$$

Concerning $\Delta E_2(\alpha)$ we have found that only the first term in curly brackets $\{\cdots\}$ in (75) could give a nonvanishing contribution as $\mu \to \infty$ and there we can make the substitution

$$\exp(-a-c)\,\frac{[F(a+b)+F(b+c)-F(a+b+c)-F(b)]^{2n}}{[F(a)F(c)]^{n+1/2}} \longrightarrow 8\mu\exp(-a-c-2n\mu b) + O(1) \tag{109}$$

TABLE IV. Comparison of obtained estimations of the coefficient C_s of the polaron ground-state energy $E(\alpha) = \alpha^2 C_s + O(1)$ for $d = 3$ as $\alpha \to \infty$.

Authors	C_s
Schultz (Ref. 49)	−0.1061
Pekar [by Miyake (Ref. 15)]	−0.108504[a]
Miyake (Ref. 15)	−0.108513[b]
Luttinger and Lu (Ref. 46)	−0.1066
Marshall and Mills (Ref. 51)	−0.1078
Sheng and Dow (Ref. 52)	−0.1065
Adamowski *et al.* (Ref. 33)	−0.1085128
Feranchuk and Komarov (Ref. 53)	−0.1078
Efimov and Ganbold (Ref. 32)	−0.10843

[a]Estimated in Ref. 15.
[b]The exact value.

in (75). Performing integrations over da, db, and dc one gets

$$\Delta E_2(\alpha) = -\alpha_d^2 \frac{2\,\Gamma(d/2)\,d^2}{9\pi^{3/2}} \times \sum_{n=2}^{\infty} \frac{(2n)!\,\Gamma(n+1/2)}{16^n (n!)^2\, n\,\Gamma(n+d/2)} + O(1). \quad (110)$$

Adding it to (108) we finally obtain

$$E^{(2)}(\alpha) = -\alpha_d^2 \left\{ \frac{d}{9\pi} + \frac{2\,\Gamma(d/2)\,d^2}{9\pi^{3/2}} \times \sum_{n=2}^{\infty} \frac{(2n)!\,\Gamma(n+1/2)}{16^n (n!)^2\, n\,\Gamma(n+d/2)} \right\} + O(1). \quad (111)$$

In two dimensions $\alpha_2 = 3\alpha\pi/4$ and (110) becomes

$$E^{(2)}(\alpha) = -\alpha^2 \left\{ \frac{\pi}{8} + \frac{\pi}{2} \sum_{n=2}^{\infty} \frac{[(2n)!]^2}{64^n (n!)^4 n} \right\} + O(1) = -\alpha^2 0.400\,538 + O(1). \quad (112)$$

For comparison, in Table III we give our result with the known results of the polaron GSE for $d = 2$ in the strong-coupling regime $\alpha \to \infty$.

In three dimensions $\alpha_3 = \alpha$ and from (110) and (111) we get

$$E^{(2)}(\alpha) = -\alpha^2 \left\{ \frac{1}{3\pi} + \frac{2}{\pi} \sum_{n=2}^{\infty} \frac{(2n)!}{16^n (n!)^2 n(2n+1)} \right\} + O(1) = -\alpha^2 0.107\,766 + O(1). \quad (113)$$

This value is obtained by developing a specific perturbation expansion in (69) up to the order $\sim 1/2! \int d\sigma \{W[\mathbf{r}]\}^2$.

The estimation of the next higher-order corrections for the coefficient C_s was obtained by the authors earlier in Ref. 32:

$$C_s \leq -0.108\,431. \quad (114)$$

The exact coefficient obtained numerically by Miyake[15] is

$$C_s^M = -0.108\,513. \quad (115)$$

The comparison of the known results for the coefficient C_s for $d = 3$ is displayed in Table IV.

C. Intermediate-coupling range

In the intermediate-coupling regime the main tool for obtaining polaron properties is the variational approach.[26,1] For $d = 3$, the Feynman variational method based on a trial oscillator-type action gives an upper bound on the polaron free energy, valid for arbitrary α. Generalizations of the Feynman action for $d = 3$ to the arbitrary density function[16] and arbitrary quadratic action[17] have improved this upper bound. In our opinion, the resul[17] obtained for $d = 3$ is the best variational upper bound in the whole range of α. But this variational method does not give the next corrections to this bound. Other numerical methods dealing with this problem [46, 47] require specific complicated schemes of calculations which may introduce statistical errors. Estimations of both the upper and lower bounds for the polaron self-energy obtained in Refs. 13 and 48 should be improved.

Considering intermediate values of α, we have derived Eqs. (47) and (50) numerically, by the following iteration scheme:

$$F_{n+1}(t) = \boldsymbol{\Phi}_t[\tilde{\Sigma}_n], \quad \tilde{\Sigma}_n(k) = \boldsymbol{\Omega}_k[F_n], \quad n \geq 0, \quad (116)$$

starting from reasonable assumed functions $F_0(t)$ and $\tilde{\Sigma}_0(k)$ as defined in (106) and (107). Both the series $F_n(t)$ and $\tilde{\Sigma}_n(k)$ turned out to be rapidly convergent and the

TABLE V. The obtained estimations of the polaron ground-state energy $E_0(\alpha)$ and $E^{(2)}(\alpha)$ for $d = 2$ in the intermediate range of α compared with known results obtained in Refs. 41, 54, and 39.

α	Feynman[a]	Hipolito (Ref. 41)	Huybrecht (Ref. 54)	Das Sarma and Mason (Ref. 39)	Present E_0	Present $E_0 + E_2$
0.6364	−1.0198	−1.0266	−1.0201	−1.0405	−1.020	−1.028
1.909	−3.2247	−3.2263	−3.2263	−3.5690	−3.231	−3.250
3.183	−5.9191	−6.0902	−5.9193	−6.9688	−5.928	−6.039
4.450	−9.6935	−9.8723	−9.7154	−11.388	−9.710	−9.871

[a]Our estimation by Feynman's variational method.

TABLE VI. The obtained estimations of the polaron ground-state energy $E_0(\alpha)$ and $E^{(2)}(\alpha)$ for $d = 3$ in the intermediate range of α compared with known results obtained in Refs. 33, 49, 48, and 13. Our $E_0(\alpha)$ coincides exactly with the upper bound obtained in Ref. 33.

	Osc. (Ref. 33)	Feynman (Ref. 49)	Smondyrev (Ref. 48)		Larsen (Ref. 13)		Present	
α	upper	upper	upper	lower	upper	lower	E_0	$E_0 + E_2$
0.5	−0.5	−0.5032	−0.5041	−0.5041	−0.5040	−0.5052	−0.504	−0.5041
1.0	−1.0	−1.0130	−1.0167	−1.0175	−1.0160	−1.0270	−1.014	−1.017
1.5	−1.5	−1.5302			−1.5361	−1.576	−1.532	−1.539
2.0	−2.0	−2.0554			−2.0640	−2.172	−2.058	−2.071
2.5	−2.5	−2.5894			−2.5995	−2.872	−2.593	−2.614
3.0	−3.0	−3.1333	−3.1645	−3.2122	−3.1421		−3.138	−3.167
4.0	−4.0	−4.2565			−4.2771		−4.265	−4.305
5.0	−5.0	−5.4401	−5.4945	−5.7767			−5.452	−5.528
7.0	−7.356	−8.1127	−8.0406	−8.8832			−8.137	−8.255
9.0	−10.72	−11.486	−10.834	−12.654			−11.54	−11.69
11.0	−14.94	−15.710	−13.905	−17.165			−15.83	−16.04
20.0	−44.53	−45.283					−45.33	−45.99
30.0	−97.58	−98.328					−98.52	−99.86
40.0	−171.9	−172.60					−173.4	−175.1

value of the leading term $E_0(\alpha)$ is actually not changed since $n \geq 6$. The results for $E_0(\alpha)$ and $E^{(2)}(\alpha)$ in two dimensions are presented in Table V. The values of $E_0(\alpha)$ and $E^{(2)}(\alpha)$ for $d = 3$ are given in Table VI and shown in Fig. 2 in comparison with the known data.[13,49,17,48] For clarity, in Fig. 2 we show only the deviation of the quoted polaron energies from the standard "oscillator-potential" approximation result. Our $E_0(\alpha)$ for $d = 3$ coincides with the upper bound obtained in Ref. 17. We have made preliminary estimations which indicate that the decreasing series in (69) was alternating. Then one can expect that the third-order correction $\Delta E_3(\alpha)$ may slightly increase the value of $E^{(2)}(\alpha)$ and inclusion of higher-order corrections $\Delta E_{n>2}(\alpha)$ might result in insignificant oscillation of $E^{(n>2)}(\alpha)$ between $E_0(\alpha)$ and $E^{(2)}(\alpha)$. In other words, the obtained $E^{(2)}(\alpha)$ may be accepted as a lower bound of the ground-state energy of the polaron. Note that numerical results obtained in Ref. 50 at three points ($\alpha = 1, 3, 5$) by the method of "partial averaging" lie exactly between our curves for $E_0(\alpha)$ and $E^{(2)}(\alpha)$.

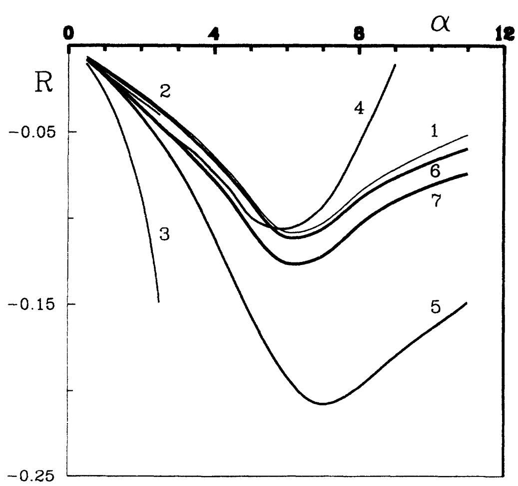

FIG. 2. Some known results of the polaron ground-state energy E (for three dimensions) plotted as function of the electron-phonon coupling constant α. For clarity, the ratio $R = (E_* - E_{\rm harm})/|E_{\rm harm}|$ is shown, where E_* are estimations obtained in Refs. 33, 49, 48, and 13 and $E_{\rm harm}$ is the "harmonic-oscillator" approximation (Ref. 33). In these units the curve for $E_{\rm harm}$ coincides with the abscissa axis. Curves correspond to estimations (1) Feynman's upper; (2) and (3), Larsen's upper and lower; (4) and (5), Smondyrev's upper and lower; (6) our $E_0(\alpha)$; and (7) our $E^{(2)}(\alpha)$.

VII. CONCLUSION

A scheme of systematic calculations has been proposed to estimate the ground-state energy of the polaron in the same way for different values of the electron-phonon coupling constant α. The polaron path integral by Feynman has been generalized to the case of an electron moving in d space dimensions. We transform this path integral to a representation built so that all the quadratic part of the polaron action is concentrated entirely in the Gaussian measure, which is defined from certain equations. The interaction part of the polaron action is purely non-Gaussian in this representation. The leading-order term in this approach yields an upper bound to the polaron self-energy and improves the Feynman variational estimates for $d = 2$ and $d = 3$. A scaling relation between polaron self-energies for different space dimensions is obtained for this term. The next correction to this estimation is calculated by numerical integration for $d = 2$ and $d = 3$. Our results obtained within the proposed method provide a reasonable description of both two- and three-dimensional polarons at arbitrary coupling α. The consideration could be extended to computing the other characteristics of the polaron, the effective mass, and the average number of phonons, as well as to estimating the energy of the polaron in the presence of the magnetic field due to the validity of the proposed method for the complex functionals.

ACKNOWLEDGMENTS

The authors are grateful to Professor H. Leschke for useful discussions. One of us (G.G.) would also like to thank Professor S. Ranjibar-Daemi, the IAEA, and UNESCO for hospitality at the ICTP, Trieste.

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