# Ground-state energy of a polaron in $n$ dimensions

F. M. Peeters, Wu Xiaoguang, and J. T. Devreese*
*University of Antwerp (Universitaire Instelling Antwerpen), Department of Physics, Universiteitsplein 1, B-2610, Antwerpen-Wilrijk, Belgium*
(Received 8 April 1985)

The Fröhlich Hamiltonian is generalized to the case of an electron moving in $n$ space dimensions. For $n=2$ and $n=3$ the familiar Fröhlich Hamiltonian is reobtained. The polaron ground-state energy is calculated up to fourth order in perturbation theory. We found that within the Feynman two-particle polaron model approximation the polaron ground-state energy satisfies the scaling relation $E_{n\text{D}}(\alpha)=(n/3)E_{3\text{D}}(\{\Gamma[(n-1)/2]3\sqrt{\pi}/2n\Gamma(n/2)\}\alpha)$, where $E_{n\text{D}}$ is the Feynman polaron ground-state energy for the polaron in $n$ dimensions and $E_{3\text{D}}$ the energy in three dimensions.

## I. INTRODUCTION

The study of the Fröhlich polaron problem has attracted interest over the last forty years (for a review we refer to Ref. 1). It was the first problem in solid-state physics which was treated within a field-theoretical framework. In recent years, there has been renewed interest in the polaron problem because (i) polaron effects have been observed in low-dimensional systems, e.g., $p$-type InSb metal-oxide-semiconductor structures[2] and (ii) certain physical problems can be mapped into a polaron-type problem, e.g., the interaction of an electron with the surface modes of a thin liquid-helium film can be mapped[3] into a two-dimensional (2D) acoustical polaron problem.

Over the years polaron effects have been studied in 3D and 2D (see, e.g., Ref. 4) systems. In the present paper we want to investigate the effect of the dimensionality of the system on the ground-state energy of the optical polaron. In order to do that we first extend the Fröhlich Hamiltonian to arbitrary dimensions. This generalization is not unique. We will follow a physical approach inspired by the formulation of the 2D optical polaron problem as obtained[5] from the 3D polaron Hamiltonian. More explicitly the Fröhlich Hamiltonian for lower-dimensional systems will be derived from the Fröhlich Hamiltonian of a higher-dimensional system by integrating out one or more dimensions. The basic interaction from which the polarization results will always be the same as in 3D, i.e., $1/r$ or Coulomb-like, but the electron motion will be embedded in an $n$-dimensional space. This approach has the property that in 3D and in 2D the present definition of the polaron Fröhlich Hamiltonian for $n$ dimensions reduces to the usual expression for the Fröhlich Hamiltonian.

In Sec. III we give a perturbation expansion of the polaron free energy which is based on a Feynman path-integral formulation of the polaron partition function. The polaron ground-state energy is obtained in Sec. IV up to second order in the electron-phonon coupling constant $\alpha$ (which corresponds to a fourth-order perturbation calculation in the electron-phonon interaction). For the 3D polaron we reobtain the result of Höhler and Mullensiefen[6] and in 2D we find our[7] recent result for the coefficient of the $\alpha^2$ term of the polaron ground-state energy. The exact ground-state energy to order $\alpha^2$ calculated for arbitrary dimensions is interesting for its own sake. We want (i) to study the effect of the dimensionality of the system on the polaron ground state energy and (ii) to investigate whether or not the Feynman approximation[8] to the polaron ground-state energy, generalized to arbitrary dimensions, gives a better description at higher dimensions. The latter question is studied in Sec. V where we also derive a scaling relation for the Feynman polaron ground-state energy. The explicit calculation of expectation values and of integrals are presented in the Appendixes.

## II. FRÖHLICH HAMILTONIAN FORMULATED IN $n$ DIMENSIONS

The form of the Fröhlich Hamiltonian[9] in $n$ dimensions is the same as in 3D,

$$H=\frac{\mathbf{p}^2}{2m}+\sum_{\mathbf{k}}\hbar\omega_{\mathbf{k}}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+\sum_{\mathbf{k}}(V_{\mathbf{k}}a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}+V_{\mathbf{k}}a_{\mathbf{k}}^{\dagger}e^{-i\mathbf{k}\cdot\mathbf{r}})\ , \quad (1)$$

except that now all vectors and operators are $n$ dimensional. $\mathbf{r}$ and $\mathbf{p}$ are the electron position and momentum operator, respectively. $a_{\mathbf{k}}^{\dagger}$ ($a_{\mathbf{k}}$) is the creation (annihilation) operator for a phonon with wave vector $\mathbf{k}$ and frequency $\omega_{\mathbf{k}}$. In the present paper we limit ourselves to dispersionless longitudinal optical phonons, i.e., $\omega_{\mathbf{k}}=\omega_0$. The electron-phonon interaction coefficient for coupling with wave vector $\mathbf{k}$ is denoted by $V_{\mathbf{k}}$. In the following units are chosen such that $\hbar=m=\omega_0=1$.

Now we have to address the question of the explicit form of the interaction coefficients $V_{\mathbf{k}}$ in $n$ dimensions. Therefore we remark that the electron-phonon interaction is a representation in second quantization of the electron interaction with the lattice polarization, which in 3D is essentially a Coulomb potential $1/r$. $|V_{\mathbf{k}}|^2$ is proportional to the Fourier transform of this potential, and as a consequence we have in $n$ dimensions

$$|V_{\mathbf{k}}|^2=\frac{A_n}{V_n k^{n-1}}\ , \quad (2)$$

with $V_n$ the volume of the $n$-dimensional crystal. In doing so we assume that the electron-polarization interaction is also $(1/r)$-like in $n$ dimensions but that the electron motion is embedded in $n$ space dimensions. To obtain the coefficient $A_n$ we note that $|V_l|^2$ in $n-1$ dimensions can be obtained from $|V_k|^2$ in $n$ dimensions by integrating out one of the dimensions explicitly,

$$\sum_{k_n} \frac{A_n}{V_n(k_n^2+l^2)^{(n-1)/2}} = \frac{A_{n-1}}{V_{n-1} l^{n-2}} , \tag{3}$$

with $\mathbf{k}=(\mathbf{l},k_n)$ an $n$-dimensional vector, $\mathbf{l}$, an $(n-1)$-dimensional vector, and $l^2=k_1^2+k_2^2+\cdots+k_{n-1}^2$. Replacing the sum by an integral, i.e.,

$$\frac{V_{n-1}}{V_n}\sum_{k_n} \to \frac{1}{2\pi}\int dk_n ,$$

we obtain

$$\frac{A_n}{2}\int_{-\infty}^{\infty} dk_n \frac{1}{(l^2+k_n^2)^{(n-1)/2}} = \frac{A_{n-1}}{l^{n-2}} , \tag{4}$$

which after performing the integral leads to

$$A_n = \frac{2\sqrt{\pi}\,\Gamma\left[\frac{n}{2}-\frac{1}{2}\right]}{\Gamma\left[\frac{n}{2}-1\right]} A_{n-1} , \tag{5}$$

where $\Gamma(x)$ is the $\Gamma$ function. Noting that in 3D the interaction coefficient is well known, i.e., $|V_{\mathbf{k}}|^2=(2\sqrt{2})\pi\alpha/Vk^2$, we can use the expressions (2) and (5) to obtain the interaction coefficient in $n$ dimensions:

$$|V_{\mathbf{k}}|^2 = \frac{\Gamma\left[\frac{n-1}{2}\right] 2^{n-3/2}\pi^{(n-1)/2}\alpha}{Vk^{n-1}} , \tag{6}$$

where $\alpha$ is the electron-phonon coupling constant and $V$ is the volume of the $n$-dimensional crystal.

In 2D, Eq. (6) reduces to

$$|V_{\mathbf{k}}|^2 = \frac{\sqrt{2}\pi\alpha}{Vk} , \tag{7}$$

which has been obtained earlier by others (see, e.g., Refs. 5 and 10).

## III. PERTURBATION EXPANSION OF THE POLARON FREE ENERGY

Since the pioneering work of Feynman[8] on the 3D polaron problem it has been well recognized that the Feynman path-integral formalism is a very convenient formalism for treating the polaron problem. The reason is that in this formalism as shown by Feynman the phonon coordinates can be eliminated exactly and as a consequence the polaron problem is reduced to a effective one-particle problem with retarded interaction. In the present paper we will use Feynman path integrals in order to calculate the polaron ground-state energy.

The partition function of the polaron system divided by the partition function of the noninteracting electron-phonon system is given by

$$Z = e^{-\beta F} = \langle e^{S_I[\mathbf{r}(t)]}\rangle_{S_0} , \tag{8}$$

with $F$ the electron-phonon interaction contribution to the polaron free energy and $\beta=1/k_BT$, with $k_B$ the Boltzmann constant and $T$ the lattice temperature. In the limit of zero temperature, the free energy $F$ reduces to the polaron ground-state energy $E$. The average in Eq. (8) is a path-integral average with weight function $\exp\{S_0[r(t)]\}$:

$$\langle A\rangle_{S_0} = \frac{\int d\mathbf{r}_0 \int\int \mathscr{D}\mathbf{r}(u) A[\mathbf{r}(u)] e^{S_0[\mathbf{r}(u)]}\delta(\mathbf{r}_0-\mathbf{r}(0))\delta(\mathbf{r}_0-\mathbf{r}(\beta))}{\int d\mathbf{r}_0 \int\int \mathscr{D}\mathbf{r}(u) e^{S_0[\mathbf{r}(u)]}\delta(\mathbf{r}_0-\mathbf{r}(0))\delta(\mathbf{r}_0-\mathbf{r}(\beta))} , \tag{9}$$

with $\int d\mathbf{r}_0$ an integral over the crystal volume $V$ and $\int\int \mathscr{D}\mathbf{r}(u)$ a Feynman path integral over all possible electron paths $\mathbf{r}(u)$ going through $\mathbf{r}_0$ at $u=0$ and at $u=\beta$. In Eq. (9) the phonon coordinates are already eliminated. The functionals appearing in Eq. (8) are

$$S_0 = -\frac{1}{2m}\int_0^\beta du\, \dot{\mathbf{r}}(u)^2 , \tag{10a}$$

the action of a free particle (for imaginary time) and

$$S_I = \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 \int_0^\beta du \int_0^\beta ds\, G_{\omega_{\mathbf{k}}}(u-s) e^{i\mathbf{k}\cdot[\mathbf{r}(u)-\mathbf{r}(s)]} , \tag{10b}$$

the action for the electron self-interaction. In Eq. (8) we introduced

$$G_\omega(u) = \tfrac{1}{2}n(\omega)(e^{\omega(u)}-e^{\omega(\beta-|u|)}) = \frac{\cosh(|u|-\beta/2)}{2\sinh(\beta/2)} , \tag{11}$$

the phonon Green's function where $n(\omega)=1/(e^{\beta\omega}-1)$ is the number of phonons with frequency $\omega$. $G_\omega(u)$ is independent of the dimensions of our system.

The objective of the present paper is to obtain a perturbative expansion of the ground-state energy in $\alpha$, the electron-phonon coupling constant. Note that $|V_{\mathbf{k}}|^2\sim\alpha$ and thus $S_I\sim\alpha$. Consequently expanding $e^{S_I}$ in Eq. (8) implies a perturbative expansion of the partition function,

$$Z=\sum_{m=0}^{\infty}\frac{1}{m!}\langle\{S_I[\mathbf{r}(u)]\}^m\rangle_{S_0}\ , \tag{12}$$

which we may write as

$$Z=\sum_{m=0}^{\infty}a_m(n,\beta)\frac{\alpha^m}{m!}\ , \tag{13}$$

where $a_0(n,\beta)\equiv 1$ and $n$ is the dimension of the space we are working in. One can make a similar expansion for the free energy,

$$F=\sum_{m=1}^{\infty}b_m(n,\beta)\alpha^m\ . \tag{14}$$

Using the definition $Z=e^{-\beta F}$ the expansion coefficients of $F$ can be expressed in terms of the expansion coefficients of $Z$, e.g.,

$$b_1(n,\beta)=-\frac{a_1(n,\beta)}{\beta}\ , \tag{15a}$$

$$b_2(n,\beta)=\frac{1}{2\beta}[a_1^2(n,\beta)-a_2(n,\beta)]\ , \tag{15b}$$

$$b_3(n,\beta)=\frac{1}{6\beta}\{a_1(n,\beta)[3a_2(n,\beta)-2a_1^2(n,\beta)]-a_3(n,\beta)\}\ , \tag{15c}$$

which is the familiar cumulant expansion for the free energy.

Inserting Eq. (10b) into Eq. (12) we obtain for $m\geq 1$

$$a_m(n,\beta)=\frac{1}{\alpha^m}\sum_{\mathbf{k}_1}\cdots\sum_{\mathbf{k}_m}\prod_{j=1}^{m}|V_{\mathbf{k}_j}|^2\int_0^{\beta}du_j\int_0^{\beta}ds_j G_{\omega(\mathbf{k}_j)}(u_j-s_j)\left\langle\exp\left[i\sum_{j=1}^{m}\mathbf{k}_j\cdot[\mathbf{r}(u_j)-\mathbf{r}(s_j)]\right]\right\rangle_{S_0}\ . \tag{16}$$

The expectation value in Eq. (16) is calculated in Appendix A and is given by Eq. (A8). Thus formally we know the expansion coefficients of the partition function,

$$\begin{aligned}a_m(n,\beta)=\frac{1}{\alpha^m}\sum_{\mathbf{k}_1}\cdots\sum_{\mathbf{k}_m}\prod_{i=1}^{m}|V_{\mathbf{k}_i}|^2\int_0^{\beta}du_i\int_0^{\beta}ds_i G_{\omega(\mathbf{k}_i)}(u_i-s_i)e^{-k_i^2D(u_i-s_i)}\\ \times\exp\left[-\sum_{i=0}^{m}\sum_{j=1}^{i-1}\mathbf{k}_i\cdot\mathbf{k}_j[D(s_j-u_i)+D(u_j-s_i)\right.\\ \left.-D(u_j-u_i)-D(s_j-u_i)]\right]\ ,\end{aligned} \tag{17}$$

where $\omega(\mathbf{k})=\omega_{\mathbf{k}}$, $\sum_{j=1}^{i-1}=0$ if $i=1$, and $D(\tau)=(|\tau|/2)(1-|\tau|/\beta)$.

## IV. SECOND- AND FOURTH-ORDER PERTURBATION RESULT FOR THE POLARON GROUND-STATE ENERGY

The ground-state energy to second order in perturbation theory is given by the term linear in $\alpha$ in the free energy $F$ for $\beta\to\infty$. One therefore should calculate

$$a_1(n,\beta)=\frac{1}{\alpha}\sum_{\mathbf{k}}|V_{\mathbf{k}}|^2\int_0^{\beta}du\int_0^{\beta}ds\ G_{\omega_{\mathbf{k}}}(u-s)e^{-k^2D(u-s)}\ . \tag{18}$$

Noting the property $D(\tau)=D(\beta-\tau)$ and $G_\omega(\tau)=G_\omega(\beta-\tau)$, one of the integrals is trivially done:

$$a_1(n,\beta)=\frac{\beta}{\alpha}\sum_{\mathbf{k}}|V_{\mathbf{k}}|^2\int_0^{\beta}du\ G_{\omega_{\mathbf{k}}}(u)e^{-k^2D(u)}\ . \tag{19}$$

This expression can further be simplified to

$$\begin{aligned}a_1(n,\beta)&=\frac{\beta}{\alpha}\frac{V}{(2\pi)^n}\frac{2\pi^{n/2}}{\Gamma(n/2)}\int_0^{\infty}dk\,k^{n-1}|V_{\mathbf{k}}|^2\int_0^{\beta}du\ G_{\omega_{\mathbf{k}}}(u)e^{-k^2D(u)}\\ &=\beta\frac{\Gamma\left[\frac{n-1}{2}\right]}{\sqrt{2\pi}\Gamma(n/2)}\int_0^{\beta}du\ G_{\omega_0}(u)\int_0^{\infty}dk\ e^{-k^2D(u)}\\ &=\beta\frac{\Gamma\left[\frac{n-1}{2}\right]}{2\sqrt{2}\Gamma\left[\frac{n}{2}\right]}\int_0^{\beta}du\frac{G_{\omega_0}(u)}{\sqrt{D(u)}}=\beta^{3/2}\frac{\pi\Gamma\left[\frac{n-1}{2}\right]}{4\Gamma\left[\frac{n}{2}\right]}\frac{I_0(\beta/2)}{\sinh(\beta/2)}\ ,\end{aligned}$$

with $I_0(x)$ the modified Bessel function of order zero.

The coefficient of the term linear in $\alpha$ appearing in the free energy is [see Eqs. (14) and (15a)]

$$b_1(n,\beta)=-\frac{\pi}{4}\frac{\Gamma\left[\frac{n-1}{2}\right]}{\Gamma\left[\frac{n}{2}\right]}\sqrt{\beta}\frac{I_0(\beta/2)}{\sinh(\beta/2)}, \quad (20)$$

which in the limit of zero temperature reduces to

$$b_1(n,\beta)=-\frac{\sqrt{\pi}}{2}\frac{\Gamma\left[\frac{n-1}{2}\right]}{\Gamma\left[\frac{n}{2}\right]}. \quad (21)$$

Note that for $n=1$ the result is not defined. For $n=2,3,\ldots$, one obtains $b_1(2,\infty)=-\pi/2$, $b_1(3,\infty)=-1$, $b_1(4,\infty)=-\pi/4$, $b_1(5,\infty)=-2\pi/3$, $b_1(6,\infty)=-3\pi/16$, $\ldots$, and in the asymptotic limit $n\to\infty$ we may apply Stirling's formula to find $b_1(n,\infty)=-\sqrt{\pi/2n}$, which tends to zero (as $n$ tends to infinity). We are then led to the conclusion that polaron effects decrease with increasing dimensionality. Furthermore, note that to order $\alpha$ [see Eq. (20)] temperature effects and the dimensionality factor out separately. The polaron ground-state energy to order $\alpha$ has been obtained earlier for the case $n=3$ (see Ref. 1) and for $n=2$ (see Ref. 4). Equation (21) is a generalization of these standard results to arbitrary dimensions.

Now we will consider the next term in the expansion of the free energy with respect to $\alpha$. This term can be obtained by fourth-order perturbation theory. From Eqs. (14) and (15b) we see that we have to calculate $a_2(n,\beta)$ which is given by Eq. (17):

$$a_2(n,\beta)=\frac{1}{\alpha^2}\sum_{\mathbf{k}_1}\sum_{\mathbf{k}_2}|V_{\mathbf{k}_1}|^2|V_{\mathbf{k}_2}|^2 \times\int_0^\beta du_1\int_0^\beta ds_1\int_0^\beta du_2\int_0^\beta ds_2 G_{\omega(\mathbf{k}_1)}(u_1-s_1)G_{\omega(\mathbf{k}_2)}(u_2-s_2)e^{-k_1^2D(u_1-s_1)} \times e^{-k_2^2D(u_2-s_2)}e^{-\mathbf{k}_1\cdot\mathbf{k}_2C(u_1,s_1,u_2,s_2)}, \quad (22)$$

with

$$C(u_1,s_1,u_2,s_2)=D(u_1-s_1)+D(s_2-u_2)-D(u_1-u_2)-D(s_1-s_2). \quad (23)$$

In Appendix B we evaluate the sum over the wave vectors $k_1$ and $k_2$. This reduces Eq. (22) to

$$a_2(n,\beta)=\frac{1}{8}\left[\frac{\Gamma\left[\frac{n-1}{2}\right]}{\Gamma\left[\frac{n}{2}\right]}\right]^2\int_0^\beta du_1\int_0^\beta ds_1\int_0^\beta du_2\int_0^\beta ds_2\frac{G_{\omega_0}(u_1-s_1)}{[D(u_1-s_1)]^{1/2}}\frac{G_{\omega_0}(u_0-s_2)}{[D(u_2-s_2)]^{1/2}} \times F\left[\frac{1}{2},\frac{1}{2};\frac{n}{2};\frac{C^2(u_1,s_1,u_2,s_2)}{D(u_1-s_1)D(u_2-s_2)}\right], \quad (24)$$

with $F(a,b;c;z)$ the hypergeometric function. In Appendix C it is shown how this fourfold integral can be reduced further. Inserting the explicit expressions for $a_1(n,\beta)$ and $a_2(n,\beta)$ into Eq. (15b) and taking the limit $\beta\to\infty$, we find (cf. Appendix C) the expression

$$b_2(n,\beta)=-\frac{\Gamma\left[\frac{n-1}{2}\right]}{\sqrt{\pi}\Gamma\left[\frac{n}{2}\right]}\left[\frac{\pi^{3/2}}{8}\frac{\Gamma\left[\frac{n-1}{2}\right]}{\Gamma\left[\frac{n}{2}\right]}+\frac{1}{2}\int_0^1 dx\left[1-\frac{4}{(1+x^2)^2}\right]F(n,x)\right], \quad (25)$$

where

$$F(n,x)=\int_0^{\pi/2}d\theta\frac{\sin^{n-2}\theta}{(1-x^2\cos^2\theta)^{1/2}}. \quad (26)$$

In Table I numerical results are given for the coefficients $b_1(n,\infty)$ and $b_2(n,\infty)$ for different values of the dimensions $n$. The results for $n=3$ and $n=2$ coincide with the results of Refs. 6 and 7, respectively. In 3D the integral in Eq. (25) can be done analytically

$$b_2(3,\infty)=-\ln[1+3/(2\sqrt{2})]+1/\sqrt{2},$$

which is the result of Ref. 6. From Eqs. (21) and (25) it is apparent that $b_1(n,\infty)$ and $b_2(n,\infty)$ are infinite for $n=1$. But the ratio $b_2(n,\infty)/b_1^2(n,\infty)$ is defined for

TABLE I. Expansion parameters for the exact perturbation result (up to the given digits) of the polaron ground-state energy $E=b_1\alpha+b_2\alpha^2$ for different dimensions $n$.

| $n$ | $-b_1$ | $-b_2$ |
|---|---|---|
| 2 | 1.570 796 3 | 0.063 974 0 |
| 3 | 1.000 000 0 | 0.015 919 6 |
| 4 | 0.785 398 2 | 0.007 009 6 |
| 5 | 0.666 666 7 | 0.003 910 6 |
| 6 | 0.589 048 6 | 0.002 486 3 |
| 7 | 0.533 333 3 | 0.001 717 5 |
| 8 | 0.490 873 9 | 0.001 256 5 |
| 9 | 0.457 142 9 | 0.000 958 6 |
| 10 | 0.429 514 6 | 0.000 755 2 |
| 20 | 0.291 336 5 | 0.000 167 1 |
| 30 | 0.234 749 2 | 0.000 071 3 |

$n=1$; we found

$$-\frac{b_2(1,\infty)}{b_1^2(1,\infty)}=\frac{3}{\sqrt{8}}-1=0.060\,660\,17\ldots . \tag{27}$$

In the limit of large dimensions, one can make a series expansion which yields

$$-\frac{b_2(n,\infty)}{b_1^2(n,\infty)}=\left[\frac{1}{2}-\frac{4}{3\pi}\right]\frac{1}{n}+\frac{9}{8}\left[\frac{24}{5\pi}-\frac{3}{2}\right]\frac{1}{n\left[\frac{n}{2}+1\right]}+\cdots . \tag{28}$$

## V. DISCUSSION AND CONCLUSION

The results for the polaron ground-state energy of previous sections which are exact to order $\alpha^2$ can be compared with the ground-state energy calculated within the Feynman two-particle polaron model approximation. The latter approximation gives

$$E=\frac{n}{4}\frac{(v-w)^2}{v}-\frac{\Gamma\left[\frac{n-1}{2}\right]}{\Gamma\left[\frac{n}{2}\right]}\frac{\alpha}{2\sqrt{2}}\int_0^\infty dt\frac{e^{-t}}{[D_0(t)]^{1/2}} , \tag{29}$$

with

$$D_0(t)=\frac{w^2}{2v^2}t+\frac{v^2-w^2}{2v^3}(1-e^{-vt}) , \tag{30}$$

where $v$ and $w$ are the parameters of the Feynman polaron model which are determined by minimizing the energy (29) with respect to $v$ and $w$. Comparing Eq. (29) with the Feynman result[8] for the 3D polaron we note the following scaling relation,

$$E_{n\mathrm{D}}(\alpha)=\frac{n}{3}E_{3\mathrm{D}}\left[\frac{\Gamma\left[\frac{n-1}{2}\right]}{\Gamma\left[\frac{n}{2}\right]}\frac{3\sqrt{\pi}}{2n}\alpha\right] , \tag{31}$$

between the energy of the $n$D polaron ($E_{n\mathrm{D}}$) and the 3D polaron ($E_{3\mathrm{D}}$). This scaling relation is *not* an exact relation. It is valid for the Feynman polaron energy and also for the ground state energy to order $\alpha$. The next-order term (i.e., $\alpha^2$) no longer satisfies Eq. (31). The reason is that in the exact calculation (to order $\alpha^2$) the electron motion in the different space directions is coupled by the electron-phonon interaction. No such coupling is taken into account in the Feynman theory; and this is the underlying reason for the validity of the scaling relation for the Feynman approximation. A more elaborate discussion of the approximate validity of Eq. (31) was given by the present authors in Ref. 7 for the case of the 2D polaron.

The Feynman approximation to the polaron ground-state energy (29) gives an upper bound to the exact ground-state energy. By expansion of Eq. (29) for small $\alpha$ we obtain

$$E=-\frac{\sqrt{\pi}}{2}\frac{\Gamma\left[\frac{n-1}{2}\right]}{\Gamma\left[\frac{n}{2}\right]}\alpha-\frac{1}{27n}\left[\frac{\Gamma\left[\frac{n-1}{2}\right]}{\Gamma\left[\frac{n}{2}\right]}\frac{\sqrt{\pi}}{2}\right]^2\alpha^2 . \tag{32}$$

The first term on the right-hand side (i.e., the term in $\alpha$) equals the exact result as obtained from second-order perturbation theory. The second term on the right-hand side (i.e., the term in $\alpha^2$) is smaller than the exact result (see Table I) which was obtained by fourth-order perturbation theory. Let us introduce

$$\alpha'=\frac{\sqrt{\pi}}{2}\frac{\Gamma\left[\frac{n-1}{2}\right]}{\Gamma\left[\frac{n}{2}\right]}\alpha .$$

Equation (32) then takes the simple form

$$E=-\alpha'-\lambda_n^F(\alpha')^2 , \tag{33}$$

where

$$\lambda_n^F=\frac{1}{27n} . \tag{34}$$

With this normalization of the electron-phonon coupling constant, finite results are obtained for $n=1$! The coefficient of the $(\alpha')^2$ term in the expansion of the ground-state energy is shown in Fig. 1 for the exact result and for the Feynman approximation. In order to plot Fig. 1 we calculated $\lambda_n$ for $n$ generalized to a real number. For $n\rightarrow\infty$ the exact result reads

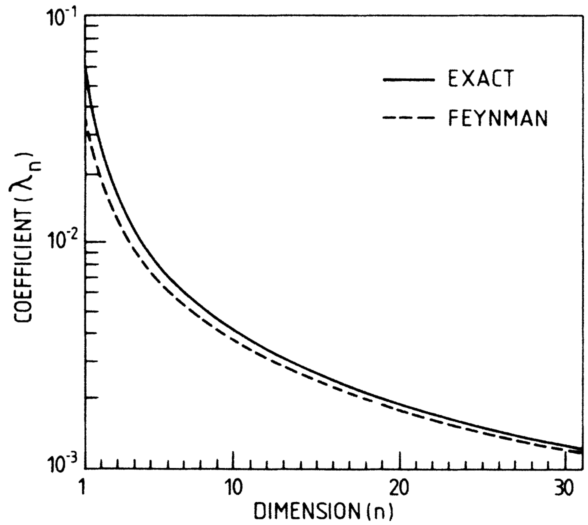


FIG. 1. Coefficient of the $(\alpha')^2$ term in the polaron ground-state energy $E=-\alpha'-\lambda_n(\alpha')^2$ as function of the dimension of the system for the exact perturbation result and for the Feynman approximate polaron theory.

$$\lambda_n=\left[\frac{1}{4}-\frac{2}{3\pi}\right]\frac{1}{n}=0.037\,793\,4\,\frac{1}{n}\ , \tag{35}$$

while the Feynman result is given by

$$\lambda_n^F=0.037\,037\,04\,\frac{1}{n}\ . \tag{36}$$

Note that the coefficient of the $1/n$ term of $\lambda_n$ is only a factor 1.02 larger than the corresponding Feynman result.

In conclusion we have generalized the Fröhlich Hamiltonian for the polaron to $n$ dimensions. The generalization is such that the Fröhlich Hamiltonian in the next lower dimension can be obtained by integrating out one of the dimensions. In 3D and 2D the well-known expressions for the Fröhlich Hamiltonian are reobtained. A formal perturbation expansion was presented for the polaron free energy in $n$ dimensions. In the limit of zero temperature, the ground-state energy was calculated up to fourth order in perturbation theory or equivalently to second order in the electron-phonon coupling constant $\alpha$. We found that polaron effects in the ground-state energy decrease with increasing dimensionality. This conclusion generalizes an earlier result by Das Sarma[5] and Larsen[11] who found that polaron effects are enhanced in 2D systems in comparison with 3D systems. Within the Feynman approximation we find that the polaron ground-state energy of an $n$-dimensional polaron can be obtained from the 3D result by a simple scaling relation.

## ACKNOWLEDGMENTS

This work is partially sponsored by Fonds voor Kollektief Fundamenteel Onderzoek, Belgium, Project No. 2.0072.80. One of the authors (F.M.P.) acknowledges financial support from the Belgian National Fund for Scientific Research. Wu Xiaoguang wishes to thank the International Culture Cooperation of Belgium for support.

## APPENDIX A

In this appendix we calculate the path-integral average

$$f(u_1,s_1,\ldots,u_m,s_m;\mathbf{k}_1,\ldots,\mathbf{k}_m)=\langle\exp\{i\mathbf{k}_1\cdot[\mathbf{r}(u_1)-\mathbf{r}(s_1)]+\cdots+i\mathbf{k}_m\cdot[\mathbf{r}(u_m)-\mathbf{r}(s_m)]\}\rangle_{S_0}$$
$$=\left\langle\exp\left[i\sum_{j=1}^{m}\mathbf{k}_m\cdot[\mathbf{r}(u_j)-\mathbf{r}(s_j)]\right]\right\rangle_{S_0}\ , \tag{A1}$$

where $0\le s_j$, $s_j\le\beta$. This expression may be written as (we put $m=\hbar=\omega_0=1$)

$$f(\{u_i,s_i\};\{k_i\})=\frac{1}{Z_0}\int d\mathbf{r}_0\int\int_{\mathbf{r}_0=\mathbf{r}(0)}^{\mathbf{r}_0=\mathbf{r}(\beta)}\mathscr{D}\mathbf{r}(t)\exp\left[-\tfrac{1}{2}\int_0^\beta dt\,\dot{\mathbf{r}}(t)^2+i\sum_{j=1}^{m}k_m[\mathbf{r}(u_j)-\mathbf{r}(s_j)]\right]\ , \tag{A2}$$

where

$$Z_0=\int d\mathbf{r}_0\int\int_{\mathbf{r}_0=\mathbf{r}(0)}^{\mathbf{r}_0=\mathbf{r}(\beta)}\mathscr{D}\mathbf{r}(u)\exp\left[-\tfrac{1}{2}\int_0^\beta du\,\dot{\mathbf{r}}(u)^2\right]\ . \tag{A3}$$

Introducing the Lagrangian for imaginary time,

$$L=-\tfrac{1}{2}\dot{\mathbf{r}}(t)^2+i\sum_{j=1}^{m}\mathbf{k}_j\cdot\mathbf{r}(t)[\delta(t-u_j)-\delta(t-s_j)]\ , \tag{A4}$$

Eq. (A2) can be written as

$$f(\{u_i,s_i\};\{k_i\})=\frac{1}{Z_0}\int d\mathbf{r}_0\int\int_{\mathbf{r}_0=\mathbf{r}(0)}^{\mathbf{r}_0=\mathbf{r}(\beta)}\mathscr{D}\mathbf{r}(t)\exp\left[\int_0^\beta dt\,L(\dot{\mathbf{r}}(t),\mathbf{r}(t),t)\right]\ . \tag{A5}$$

The Lagrangian (A4) describes a free particle which interacts with the imaginary electric field $\mathbf{E}\sim i\sum_{j=1}^{m}\mathbf{k}_j[\delta(t-u_j)-\delta(t-s_j)]$. Note that the Lagrangian (A4) is quadratic in the electron position coordinates and consequently[12] only the classical path and quadratic fluctuations around it contribute to the path integral of Eq. (A5).

The classical equation of motion corresponding to the Lagrangian (A4),

$$\ddot{\mathbf{r}}(t)+i\sum_{j=1}^{m}\mathbf{k}_j[\delta(t-u_j)-\delta(t-s_j)]=0\ , \tag{A6}$$

has to be solved with the boundary conditions $\mathbf{r}(0)=\mathbf{r}(\beta)=\mathbf{r}_0$ and where $0\le u_j,\ s_j\le\beta$. The solution is

$$\mathbf{r}(t)=\mathbf{r}_0+\dot{\mathbf{r}}(0)t+i\sum_{j=1}^{m}\mathbf{k}_j[(u_j-t)\Theta(t-u_j)-(s_j-t)\Theta(t-s_j)]\ , \tag{A7}$$

where the electron velocity at $t=0$ is given by

$$\dot{\mathbf{r}}(0)=-\frac{i}{\beta}\sum_{j=1}^{m}\mathbf{k}_j(u_j-s_j)\ , \tag{A8}$$

with $\Theta(x)=0\ (x<0),\ 1\ (x>0)$.

Inserting the classical path (A6) into the Lagrangian (A4) gives the expectation value (A5),

$$f(\{u_i,s_i\};\{\mathbf{k}_i\})=\exp[-D(\{u_i,s_i\};\{\mathbf{k}_i\})]\ , \tag{A9}$$

where

$$D(\{u_i,s_i\};\{k_i\})=-\frac{1}{2\beta}\left[\sum_{j=1}^{m}\mathbf{k}_j(u_j-s_j)\right]^2+\sum_{j,l=1}^{m}\mathbf{k}_j\cdot\mathbf{k}_l[u_l(\Theta(u_j-u_l)-\Theta(s_j-u_j))-s_l(\Theta(u_j-s_l)-\Theta(s_j-s_l))]\ . \tag{A10}$$

This expression can also be written in a slightly different form,

$$D(\{u_i,s_i\};\{\mathbf{k}_i\})=\sum_{j=1}^{m}\mathbf{k}_j^2D(u_j-s_j)+\sum_{j<l=2}^{m}\mathbf{k}_j\cdot\mathbf{k}_l[D(s_j-u_l)+D(u_j-s_l)-D(u_j-u_l)-D(s_j-s_j)]\ , \tag{A11}$$

with

$$D(\tau)=\frac{|\tau|}{2}\left[1-\frac{|\tau|}{\beta}\right]\ , \tag{A12}$$

which has the property $D(\beta-\tau)=D(\tau)$. In Eq. (A11) we defined $\sum^{m}{}_{j,l \atop j<l=2}=0$ when $m=1$. For $m=2$, Eqs. (2.12) and (2.14) of Ref. 13 are obtained with $\Lambda(\tau)=2D(\tau)$.

## APPENDIX B

The $2n$-fold sum,

$$A=\frac{1}{\alpha^2}\sum_{\mathbf{k}_1}\sum_{\mathbf{k}_2}|V_{\mathbf{k}_1}|^2|V_{\mathbf{k}_2}|^2e^{-\mathbf{k}_1^2a}e^{-\mathbf{k}_2^2b}e^{-\mathbf{k}_1\cdot\mathbf{k}_2c}\ , \tag{B1}$$

will be evaluated in this appendix. Replace the sum $(1/V)\sum_{\mathbf{k}}\to[1/(2\pi)^n]\int d\mathbf{k}$ by an $n$-fold integral, introduce spherical coordinates,[14] and insert Eq. (6). This results in

$$A=\left[\frac{\Gamma\left[\frac{n-1}{2}\right]2^{(n-3)/2}\pi^{(n-1)/2}}{(2\pi)^n}\right]^2\frac{2\pi^{n/2}}{\Gamma\left[\frac{n}{2}\right]}\frac{2\pi^{(n-1)/2}}{\Gamma\left[\frac{n-1}{2}\right]}\int_0^\infty dk_1\int_0^\infty dk_2\int_0^\pi d\theta\sin^{n-2}\theta e^{-k_1^2a}e^{-k_2^2b}e^{-ck_1k_2\cos\theta}\ ; \tag{B2}$$

performing the $k_2$ integral one finds

$$A=\frac{\Gamma\left[\frac{n-1}{2}\right]}{2\pi\sqrt{\pi}\Gamma\left[\frac{n}{2}\right]}\left[\frac{\pi}{b}\right]^{1/2}\int_0^{\pi/2}d\theta\sin^{n-2}\theta\int_0^\infty dk_1e^{-k_1^2a}e^{+c^2k_1^2\cos^2\theta/4b}\ . \tag{B3}$$

This can further be simplified to

$$A=\frac{\Gamma\left[\frac{n-1}{2}\right]}{2\sqrt{\pi}\Gamma\left[\frac{n}{2}\right]}\int_0^{\pi/2}d\theta\frac{\sin^{n-2}\theta}{(4ab-c^2\cos^2\theta)^{1/2}}\ . \tag{B4}$$

By a change of variable we readily find

$$A=\frac{\Gamma\left[\frac{n-1}{2}\right]}{2\sqrt{\pi}\Gamma\left[\frac{n}{2}\right]}\int_0^1 dx\frac{(1-x^2)^{(n-3)/2}}{(4ab-c^2x^2)^{1/2}}\,, \tag{B5}$$

which can be expressed in terms of a hypergeometric function

$$A=\left[\frac{\Gamma\left[\frac{n-1}{2}\right]}{\Gamma\left[\frac{n}{2}\right]}\right]^2\frac{1}{8\sqrt{ab}}F\left[\frac{1}{2},\frac{1}{2};\frac{n}{2};\frac{c^2}{4ab}\right]. \tag{B6}$$

## APPENDIX C

In this appendix we present details of the calculation of the coefficient of the $\alpha^2$ term in the $n$D polaron ground-state energy. This coefficient is given by [see Eq. (15b)]

$$b_2(n,\beta)=\frac{1}{2\beta}[a_1^2(n,\beta)-a_2(n,\beta)]\,, \tag{C1}$$

where the limit $\beta\to\infty$ must still be taken. The term $a_1(n,\beta)$ was calculated in Sec. IV. We will give an outline of the calculation of $a_2(n,\beta)$. Similar calculations have been performed in Refs. 13 and 7 for the 3D and 2D polarons, respectively.

$a_2(n,\beta)$ is given by

$$\begin{aligned}a_2(n,\beta)=\frac{1}{\alpha^2}\sum_{\mathbf{k}_1}\sum_{\mathbf{k}_2}|V_{\mathbf{k}_1}|^2|V_{\mathbf{k}_2}|^2 &\times\int_0^\beta du_1\int_0^\beta ds_1\int_0^\beta du_2\int_0^\beta ds_2 G(u_1-s_1)G(u_2-s_2)e^{-k_1^2D(u_1-s_1)}\\ &\times e^{-k_2^2D(u_2-s_2)}e^{-\mathbf{k}_1\cdot\mathbf{k}_2C(u_1,s_1,u_2,s_2)}\,,\end{aligned} \tag{C2}$$

where $D(\tau)$ and $C(u_1,s_1,u_2,s_2)$ have been defined in Secs. III and IV. First, make the transformation

$$\begin{bmatrix}u_1\\ s_1\\ u_2\\ s_2\end{bmatrix}=\begin{bmatrix}1 & \frac{1}{2} & \frac{1}{2} & 0\\ 1 & \frac{1}{2} & -\frac{1}{2} & 0\\ 1 & -\frac{1}{2} & 0 & \frac{1}{2}\\ 1 & -\frac{1}{2} & 0 & -\frac{1}{2}\end{bmatrix}\begin{bmatrix}R\\ r\\ \tau_1\\ \tau_2\end{bmatrix} \tag{C3}$$

and perform the $R$ integration. This simplifies Eq. (C2) to

$$\begin{aligned}a_2(n,\beta)=\frac{8}{\alpha^2}\sum_{\mathbf{k}_1}\sum_{\mathbf{k}_2}|V_{\mathbf{k}_1}|^2|V_{\mathbf{k}_2}|^2 &\times\int_0^\beta d\tau_1\int_0^{\tau_1}d\tau_2 G(\tau_1)G(\tau_2)e^{-k_1^2D(\tau_1)}e^{-k_2^2D(\tau_2)}\\ &\times\left[2\int_0^{1/2(\tau_1-\tau_2)}d\tau(\beta-\tau_1)+2\int_{(1/2)(\tau_1-\tau_2)}^{\beta-(1/2)(\tau_1+\tau_2)}dr[\beta-\tfrac{1}{2}(\tau_1+\tau_2)-r]\right]\\ &\times e^{-\mathbf{k}_1\cdot\mathbf{k}_2C(\tau_1,\tau_2,r)}\,,\end{aligned} \tag{C4}$$

where we introduced the function

$$C(\tau_1,\tau_2,r)=\begin{cases}\tau_2(1-\tau_1/\beta), & 0<r<\frac{1}{2}(\tau_1-\tau_2)\\ \frac{1}{2}(\tau_1+\tau_2)-\frac{\tau_1\tau_2}{\beta}-r, & \frac{1}{2}(\tau_1-\tau_2)<r<\frac{1}{2}(\tau_1+\tau_2)\\ -\frac{\tau_1\tau_2}{\beta}, & \frac{1}{2}(\tau_1+\tau_2)<r\,.\end{cases}$$

Next, perform the $\mathbf{k}_1,\mathbf{k}_2$ integrations (see also Appendix B) and one ends up with

$$a_2(n,\beta)=\frac{8\beta}{\sqrt{\pi}}\frac{\Gamma\left[\frac{n-1}{2}\right]}{\Gamma\left[\frac{n}{2}\right]}\times\int_0^\beta d\tau_1\int_0^{\tau_1}d\tau_2\frac{G(\tau_1)G(\tau_2)}{[4D(\tau_1)D(\tau_2)]^{1/2}}\times\left[\tfrac{1}{2}(\tau_1-\tau_2)F(n,x_2)+\tfrac{1}{2}[\beta-(\tau_1+\tau_2)]F(n,x_1)+[4D(\tau_1)D(\tau_2)]^{1/2}\int_{-x_1}^{x_2}dx\,F(n,x)\right], \quad (C5)$$

where $x_2=\tau_2(1-\tau_1/\beta)/[4D(\tau_1)D(\tau_2)]^{1/2}$, $x_1=\tau_1\tau_2/\beta[4D(\tau_1)D(\tau_2)]^{1/2}$, and

$$F(n,x)=\int_0^{\pi/2}d\theta\frac{\sin^{n-2}\theta}{(1-x^2\cos^2\theta)^{1/2}} . \quad (C6)$$

Inserting the expressions for $a_1(n,\beta)$ and $a_2(n,\beta)$ into Eq. (B1) and taking the limit $\beta\to\infty$, one finds

$$b_2(n,\beta)=-\frac{\pi}{8}\left[\frac{\Gamma\left[\frac{n-1}{2}\right]}{\Gamma\left[\frac{n}{2}\right]}\right]^2-\frac{1}{2\sqrt{\pi}}\frac{\Gamma\left[\frac{n-1}{2}\right]}{\Gamma\left[\frac{n}{2}\right]}\int_0^1 dx\,F(n,x)+\frac{2}{\sqrt{\pi}}\frac{\Gamma\left[\frac{n-1}{2}\right]}{\Gamma\left[\frac{n}{2}\right]}\int_0^1 dx\frac{F(n,x)}{(1+x^2)^2} , \quad (C7)$$

which we have evaluated numerically for different values of $n$.

---

*Also at University of Antwerp (Rijksuniversitair Centrum Antwerpen), B-2020 Antwerpen and Eindhoven University of Technology, Department of Physics, NL-5600 MB Eindhoven, The Netherlands.

[1] *Polarons and Excitons,* edited by C. G. Kuper and G. D. Whitfield (Oliver and Boyd, Edinburgh, 1963); *Polarons in Ionic Crystals and Polar Semiconductors,* edited by J. T. Devreese (North-Holland, Amsterdam, 1972); *Polarons and Excitons in Polar Semiconductors and Ionic Crystals,* edited by J. T. Devreese and F. M. Peeters (Plenum, New York, 1984).

[2] M. Horst, U. Merkt, and J. P. Kotthaus, Phys. Rev. Lett. **50**, 754 (1983).

[3] S. A. Jackson and P. M. Platzman, Phys. Rev. B **24**, 499 (1981).

[4] S. Das Sarma and B. A. Mason, Ann. Phys. (N.Y.) (to be published).

[5] S. Das Sarma, Phys. Rev. B **27**, 2590 (1983).

[6] G. Höhler and A. M. Mullensiefen, Z. Phys. **157**, 159 (1959).

[7] Wu Xiaoguang, F. M. Peeters, and J. T. Devreese, Phys. Rev. B **31**, 3420 (1985).

[8] R. P. Feynman, Phys. Rev. **97**, 660 (1955).

[9] H. Fröhlich, Adv. Phys. **3**, 325 (1954).

[10] J. Sak, Phys. Rev. B **6**, 3981 (1972).

[11] D. M. Larsen, Phys. Rev. B **30**, 4807 (1984).

[12] See, e.g., R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).

[13] K. Arisawa and M. Saitoh, Phys. Status Solidi B **120**, 361 (1983).

[14] The representation of an $n$-dimensional integral in spherical coordinates can be found, e.g., in Appendix A of G. 't Hooft and M. Veltman, Nucl. Phys. **44*B***, 189 (1972).