Exact and approximate results for the ground-state energy of a Fröhlich polaron in two dimensions

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The ground-state energy of a two-dimensional (2D) Fröhlich polaron is calculated to second order in the coupling constant (α) and gives $E/\hbar\omega_s=-(\pi/2)\alpha-0.063\,97\alpha^2$ with $\hbar\omega_s$ the surface optical-phonon energy. In the strong-coupling limit the adiabatic approximation is used and $E/\hbar\omega_s=-0.4047\alpha^2$ is found to leading order in α. The Feynman path-integral approximation, the Gaussian approximation, and the modified Lee-Low-Pines unitary transformation approximation to the polaron ground-state energy all satisfy the scaling relation $E_{2D}(\alpha)=\frac{2}{3}E_{3D}((3\pi/4)\alpha)$, where E_{2D} (E_{3D}) is the ground-state energy of the 2D (3D) polaron.

I. INTRODUCTION

An electron near the surface of an ionic or polar crystal interacts with the longitudinal surface optical- (SO) phonon mode. The electron with its virtual-phonon cloud in this situation is referred to as a "surface polaron" and has been studied by several authors.[1–4] They calculated the ground-state energy using several approximations. In Refs. 3 and 4 a "phase transition" of the surface polaron from a quasifree to a self-trapped state was found. In the present paper we will question this conclusion.

In this paper we discuss the ground-state energy of an electron moving in a two-dimensional (2D) space and which is coupled to SO phonons. The Hamiltonian for the interacting system of electron and SO phonons is given by[1]

$$H=\frac{\mathbf{p}^2}{2m}+\sum_{\mathbf{k}}\hbar\omega_s a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+\sum_{\mathbf{k}}(V_k e^{i\mathbf{k}\cdot\mathbf{r}}a_{\mathbf{k}}+V_k^{*}e^{-i\mathbf{k}\cdot\mathbf{r}}a_{\mathbf{k}}^{\dagger}) \tag{1}$$

with

$$V_k=-i\hbar\omega_s(\sqrt{2}\pi\alpha/Ak)^{1/2}(\hbar/m\omega_s)^{1/4}\,.$$

$\mathbf{p}$ and $\mathbf{r}$ are the electron momentum and position operators. $a_{\mathbf{k}}^{\dagger}$ ($a_{\mathbf{k}}$) is the creation (annihilation) operator of a SO phonon with wave vector $\mathbf{k}$ and energy $\hbar\omega_s$. The strength of the interaction between the electron and the SO phonon is represented by the coupling constant α.

The organization of the present paper is as follows. In Sec. II we calculate the exact ground-state energy: (i) to order α^2 in the weak-coupling limit and (ii) to leading order in α in the strong-coupling limit. In Sec. III we discuss different approximate theories valid for all α and we find a scaling relation between the ground-state energy of 2D and three-dimensional (3D) polarons. Our results are summarized and discussed in Sec. IV.

II. EXACT RESULTS

In this section we present exact results for the 2D polaron ground-state energy in the limit of weak and strong electron-phonon coupling.

A. Weak-coupling limit

The path-integral representation for the polaron partition function allows one to eliminate the phonon coordinates exactly.[5] The free energy (F) can be obtained from

$$e^{-\beta F}=e^{-\beta F_0}\langle e^{S_I[\mathbf{r}(t)]}\rangle_{S_0}\,, \tag{2}$$

where F_0 is the free energy of a free electron which is described by the action

$$S_0=-\frac{1}{2m}\int_0^{\beta}[\mathbf{r}(t)]^2dt\,.$$

The interaction part of the action is given by

$$S_I=\sum_{\mathbf{k}}|V_k|^2\int_0^{\beta}du\int_0^{\beta}du'G_{\omega_s}(u-u')e^{i\mathbf{k}\cdot[\mathbf{r}(u)-\mathbf{r}(u')]} \tag{3}$$

with

$$G_{\omega}(u)=\tfrac{1}{2}n(\omega)(e^{\omega|u|}+e^{\omega(\beta-|u|)})$$

the Green's function for the phonons. $\langle\ \rangle_{S_0}$ is a path-

integral average with weight e^{S_0}. We choose units such that $m=\omega_s=\hbar=1$ which results in $|V_k|^2=(\sqrt{2}\pi\alpha/A)(1/k)$.

Since S_I is of order α, we may expand

$$e^{S_I}=1+S_I+S_I^2/2+\cdots .$$

To second order in α, Eq. (2) can then be written as

$$e^{-\beta(F-F_0)}=1+b_1\alpha+\frac{b_2}{2}\alpha^2 \tag{4a}$$

or

$$F=F_0-\frac{b_1}{\beta}\alpha-\frac{b_2-b_1^2}{2\beta}\alpha^2 \tag{4b}$$

with

$$b_1\alpha=\langle S_I[\mathbf{r}(t)]\rangle_{S_0}$$

and

$$b_2\alpha^2=\langle S_I[\mathbf{r}(t)]S_I[\mathbf{r}(t)]\rangle_{S_0} .$$

In the limit $\beta\to\infty$ (i.e., $T\to 0$, since $\beta=1/k_BT$) the free energy (F) equals the ground-state energy (E). The algebraic work involved in the calculation of the averages is presented in Appendix A. The result can be summarized by

$$E=-A\alpha-B\alpha^2+O(\alpha^3) \tag{5}$$

where A and B are given by

$$A=\frac{\sqrt{\pi}}{2}\int_0^\infty \frac{e^{-t}}{\sqrt{t}}dt=\frac{\pi}{2} , \tag{6}$$

$$B=-\frac{\pi^2}{8}-G+2\int_0^1 \frac{K(x)}{(1+x^2)^2}dx=0.063\,97 , \tag{7}$$

where

$$G=\sum_{m=0}^{\infty}\frac{(-1)^m}{(2m+1)^2}=0.915\,96$$

is Catalan's constant and $K(x)$ is the complete elliptic function. The coefficient $A=\pi/2$ was already obtained earlier.[1-3] The coefficient $B=0.063\,97$ is different from a result[6] obtained by Das Sarma and Mason using diagrammatic techniques. They found $B=0.057$. We have examined carefully (see Appendix B) their approximation and calculated B using their method, and found again $B=0.063\,97$, which is exactly our result which was obtained from expansion in α of E using path integrals.

B. Strong-coupling limit

In the $\alpha\gg 1$ limit the adiabatic approximation becomes exact. Following Pekar[7] we use the product ansatz $|\Phi\rangle=|\psi\rangle|\phi\rangle$ and optimize with respect to the phonon part $|\phi\rangle$. Following Miyake[8] the ground-state energy is given by the equation

$$\left[\frac{\mathbf{p}^2}{2}+\sum_{\mathbf{k}}\frac{\sqrt{2}\pi\alpha}{Ak}|\langle\psi|e^{i\mathbf{k}\cdot\mathbf{r}}|\psi\rangle|^2-2\sum_{\mathbf{k}}\frac{\sqrt{2}\pi\alpha}{Ak}\langle\psi|e^{i\mathbf{k}\cdot\mathbf{r}}|\psi\rangle e^{-i\mathbf{k}\cdot\mathbf{r}}\right]|\psi\rangle=E|\psi\rangle , \tag{8}$$

where $|\psi\rangle$ is the electron wave function. We may make a transformation[8] $\mathbf{r}\to\mathbf{r}/\sqrt{2}\alpha$, $\mathbf{k}\to\mathbf{k}\sqrt{2}\alpha$, which results in the following integro-differential equation:

$$\left[-\Delta-2\int d^2k\frac{\langle\psi|e^{i\mathbf{k}\cdot\mathbf{r}}|\psi\rangle}{2\pi k}e^{-i\mathbf{k}\cdot\mathbf{r}}\right]\psi=\left[\frac{E}{\alpha^2}+\bar{V}\right]\psi \tag{9}$$

with

$$\bar{V}=-\int d^2k\frac{|\langle\psi|e^{i\mathbf{k}\cdot\mathbf{r}}|\psi\rangle|^2}{2\pi k}$$

and Δ the Laplacian operator. In 2D the equation is hard to solve numerically. Therefore, we note that Eq. (9) is equivalent to a variational evaluation of

$$\frac{E}{\alpha^2}=-\langle\psi|\Delta|\psi\rangle-\int d^2k\frac{|\langle\psi|e^{i\mathbf{k}\cdot\mathbf{r}}|\psi\rangle|^2}{2\pi k} \tag{10}$$

with respect to the function $\psi(\mathbf{r})$.

Now, we may choose different functional forms for $\psi(\mathbf{r})$ and make a variational calculation of Eq. (10) with respect to the parameters contained in $\psi(\mathbf{r})$. We take the following.

(1) A Gaussian trial wave function: $\psi=Ne^{-(\Lambda/2)r^2}$ which gives $\Lambda=\pi/8$ and $E=-\pi/8$ $\alpha^2=-0.3927\alpha^2$.

(2) An exponential trial function: $\psi=Ne^{-(\Lambda/2)r}$, where Λ becomes $\Lambda=3\pi/8$ and $E=-(3\pi/16)^2\alpha^2=-0.3470\alpha^2$.

(3) A Pekar-type ansatz: $\psi=N[1+br+a(br)^2]e^{-br}$, which after a numerical minimalization results in $a=0.367$, $b=1.45$ with the energy $E=-0.04046\alpha^2$.

In the 3D case Miyake[8] solved Eq. (9) numerically and showed that the Pekar wave function is accurate enough to give E/α^2 to an accuracy of 0.01%. In the 2D case it is much more difficult to solve Eq. (9) numerically. Therefore we proceeded as follows in order to get an idea of the accuracy of the Pekar wave function. In a successive way we incorporate more parameters and higher-order terms in r and investigate how E/α^2 changes. We found that the variational choice

$$\psi=N[1+br+a(br)^2+c(br)^3]e^{-br}$$

did not give a lower value for E because minimalization leads to $c=0$. Therefore we consider the following four-parameter wave function (which we will call the modified Pekar wave function):

$$\psi=N[1+br+a(br)^2+c(br)^3+d(br)^4]e^{-br} . \tag{11}$$

A numerical minimalization of the ground-state energy leads to $a=0.3606$, $b=1.2567$, $c=-0.083\,89$, $d=0.007\,464$, and $E=-0.4047\alpha^2$. The resulting ground-state energy E/α^2 is less than 0.02% different from the result obtained with Pekar's wave function and we may expect that $E=-0.4047\alpha^2$ corresponds to the exact result for the given digits. The normalized wave function for the above electron wave functions $\psi(\mathbf{r})$ is shown in Fig. 1. The difference between Pekar's wave function and the modified Pekar wave function is very small, as it is apparent from the inset of Fig. 1.

III. APPROXIMATE RESULTS

We will discuss three approximations which have been worked out for the 2D polaron ground-state energy and which are intended to be valid for the whole electron-phonon coupling range.

(1) Feynman's path-integral treatment of the 3D polaron problem[9] can be easily translated to the 2D case. Using the *Feynman polaron model* the following upper bound is obtained to the 2D polaron ground-state energy:[2]

$$E=\frac{(v-w)^2}{2v}-\frac{\alpha}{2}\left[\frac{\pi}{2}\right]^{1/2}\int_0^\infty dt\frac{e^{-t}}{\sqrt{D(t)}}\,, \tag{12}$$

where

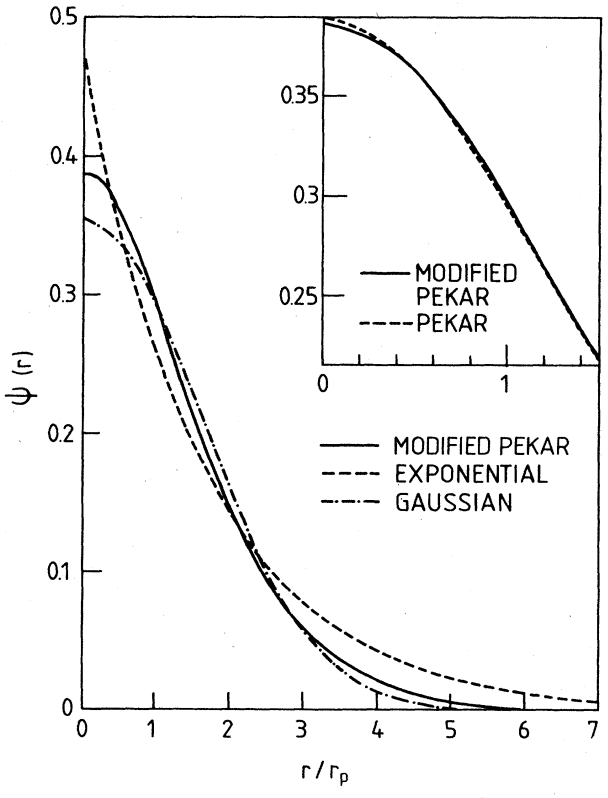

FIG. 1. Normalized polaron wave function for the 2D polaron in the strong-coupling limit $r_p=(\hbar/2m\omega_s)^{1/2}(1/\alpha)$.

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

and v and w are variational parameters which are chosen such that the smallest upper bound is obtained. For $\alpha\ll 1$, Eq. (12) gives to order α^2

$$E=-\frac{\pi}{2}\alpha-\frac{\pi^2}{216}\alpha^2\,. \tag{13a}$$

In the strong-coupling limit ($\alpha\gg 1$)

$$E=-\frac{\pi}{8}\alpha^2+O(\alpha^0) \tag{13b}$$

the leading term in α is identical to the result for a Gaussian wave function.

(2) Using the *Gaussian approximation,* which is a special case of the Feynman approximation (i.e., $w=0$), Farias *et al.*[3] found the following upper bound:

$$E=\frac{v}{2}-\frac{\alpha}{2}\sqrt{\pi}\sqrt{v}\int_0^\infty dt\frac{e^{-t}}{(1-e^{-vt})^{1/2}}\,, \tag{14}$$

where v is a variational parameter. When $\alpha\lesssim 2.48$ Eq. (14) gives $E=-(\pi/2)\alpha$ as a variational result. For $\alpha\gg 1$, $E=-(\pi/8)\alpha^2$ is obtained.

(3) Bodas *et al.*[4] recently applied an *extension* of the *Lee-Low-Pines unitary transformation* method and found the following upper bound to the polaron ground-state energy:

$$E=\frac{\lambda}{2}-\alpha\int_0^\infty dx\frac{\exp[-(1-\eta)^2x^2/\lambda]}{1+\eta^2x^2}\,, \tag{15}$$

where λ and η are two variational parameters. For $\alpha\lesssim 3.62$ the variational result leads to $E=-(\pi/2)\alpha$. In the strong coupling limit $E=-(\pi/8)\alpha^2$ is obtained.

The last two upper bounds to the 2D polaron ground-state energy, i.e., Eqs. (14) and (15), lead to a first-order phase-transition behavior, i.e., the first derivative of the ground-state energy to $\alpha(\partial E/\partial\alpha)$ exhibits a jump at a critical value α_c. The critical points are $\alpha_c=2.48$ for the Gaussian approximation and $\alpha_c=3.62$ for the unitary transformation approximation.

If we compare Eqs. (12), (14), and (15) for the 2D polaron ground-state energy with the equivalent results for the 3D polaron ground-state energy [see Eqs. (1), (4), and (6) of Ref. 10], we find the following scaling relation:

$$E_{2D}(\alpha)=\tfrac{2}{3}E_{3D}((3\pi/4)\alpha)\,. \tag{16}$$

Here E_{2D} and E_{3D} denote the 2D and 3D polaron ground-state energy, respectively. The scaling relation (16) is valid for the *approximate* upper bounds.

This scaling relation (16) implies that the numerical results for the ground-state energy and the first $(\partial E/\partial\alpha)$ and the second $(\partial^2E/\partial\alpha^2)$ derivatives of E to α for the above approximate results are, up to a simple rescaling of E and α, identical to those of the 3D case which were presented in Ref. 10. The analysis concerning a possible phase transition of the 2D polaron can thus be taken over from Ref. 10, which suggests that the phase transitions found in Refs. 1, 3, and 4 *are rather a consequence of their*

approximation than an intrinsic property of the Fröhlich Hamiltonian.

The Fröhlich polaron in 2D, as studied in the present paper, behaves essentially different from the 2D acoustical polaron as was discussed in Ref. 11. The latter one shows a discontinuous transition from the quasifree to the self-trapped polaron state, when studied within the Feynman polaron model, in contrast to the 2D Fröhlich polaron which behaves continuously as function of α. This is suggestive for the fact that the dispersionless nature of the polaron spectrum is crucial for the continuous nature of the quasifree to self-trapped state transition.

We will supplement the numerical results given in Ref. 10 by calculating the third derivative, i.e., $\partial^3 E/\partial\alpha^3$, which shows even more dramatically the difference between the Feynman, Gaussian, and unitary transformation approximation (see Fig. 2). In the Feynman approximation $\partial^3 E/\partial\alpha^3$ turns out to be continuous. For $\alpha \lesssim 4.1$, $\partial^3 E/\partial\alpha^3$ is negative. With increasing α, $\partial^3 E/\partial\alpha^3$ decreases first and reaches its minimal value at $\alpha \simeq 2.7$. Then it increases and at $\alpha \simeq 4.1$, $\partial^3 E/\partial\alpha^3$ becomes positive. At a slightly higher α value, $\partial^3 E/\partial\alpha^3$ reaches a maximum after which it continuously decreases to zero when $\alpha \to \infty$. The Gaussian ($\alpha_c \simeq 2.48$) and the unitary transformation approximation ($\alpha_c \simeq 3.62$) to E gives $\partial^3 E/\partial\alpha^3 = 0$ for $\alpha < \alpha_c$. For $\alpha > \alpha_c$, $\partial^3 E/\partial\alpha^3$ is positive and a continuous decreasing function with increasing α.

Including the temperature dependence within the above approximative results would not alter the scaling relation (16). The temperature dependence of the internal energy, the entropy, and the specific heat can therefore be easily obtained, within Feynman's approximation, from Sec. IV of Ref. 12 using the scaling relation (16).

IV. CONCLUSION

In the first part of this conclusion we will digress on the scaling relation

$$E_{2D}(\alpha) = \tfrac{2}{3} E_{3D}((3\pi/4)\alpha) \tag{17}$$

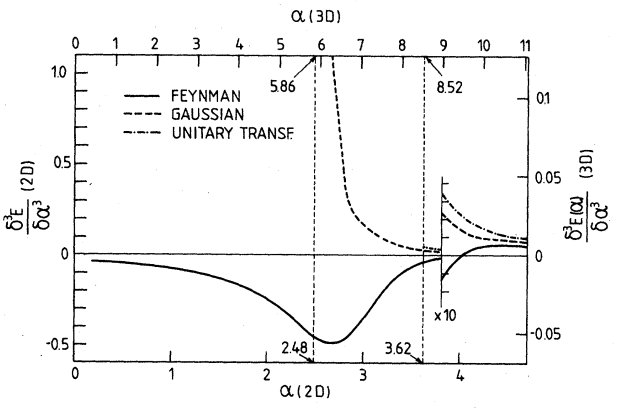

FIG. 2. Third derivative of the ground-state energy with respect to the coupling constant α for different polaron theories. Left and lower scale is for the 2D polaron, right and upper scale is for the 3D polaron.

derived in this paper, which is satisfied by the approximate theories[2–4] [see Eqs. (12), (14), and (15)]. It should be noted that *the exact result* for the weak-coupling expansion up to α^2 [see Eqs. (5)–(7)] and the exact strong-coupling limit *do not satisfy this scaling relation.* Thus the scaling relation (16) is only approximately valid. Note that the weak-coupling expansion of the polaron ground-state energy up to order α satisfies the scaling relation. But the scaling relation breaks down for higher orders in α. The reason is that in the approximate theories and for the coefficient of α in a weak-coupling expansion of E one has to calculate integrals of the form

$$I_{3D} = \int d^3k \frac{1}{k^2} e^{-Ak^2} = \frac{4\pi}{\sqrt{A}} \frac{\sqrt{\pi}}{2} \tag{18a}$$

and

$$I_{2D} = \int d^2k \frac{1}{k} e^{-Ak^2} = \frac{2\pi}{\sqrt{A}} \frac{\sqrt{\pi}}{2}, \tag{18b}$$

which differs only by a constant factor. However, in the exact perturbation expansion to order α^2 and in the exact strong-coupling limit the corresponding integrals are of the form

$$I_{3D} = \int d^3k_1 \int d^3k_2 e^{-B(k_1^2+k_2^2)-A\mathbf{k}_1\cdot\mathbf{k}_2} \tag{19a}$$

and

$$I_{2D} = \int d^2k_1 \int d^2k_2 e^{-B(k_1^2+k_2^2)-A\mathbf{k}_1\cdot\mathbf{k}_2}, \tag{19b}$$

which contain integrals over the angle ϕ ($\cos\phi = \mathbf{k}_1\cdot\mathbf{k}_2/k_1k_2$) which are different in three dimensions:

$$\int_0^\pi d\phi \sin\phi\, e^{-Ak_1k_2\cos\phi},$$

from those in the two-dimensional case:

$$\int_0^{2\pi} d\phi\, e^{-Ak_1k_2\cos\phi}.$$

The difference is no longer a simple constant factor. In the approximate theories no coupling between the different directions in space exists [cf. Eqs. (18a) and (18b) with Eqs. (19a) and (19b)]. This is the underlying reason for the validity of the scaling relation for the approximate theories.

For the same reason there exists a similar scaling relation for the approximate Feynman expression of the polaron mass m^*:

TABLE I. Ground-state energy in the weak-coupling limit to order α^2.

	$-E/\hbar\omega_s$
Exact	$\frac{\pi}{2}\alpha + 0.063\,97\alpha^2$
Feynman	$\frac{\pi}{2}\alpha + 0.045\,69\alpha^2$
Gaussian	$\frac{\pi}{2}\alpha$

TABLE II. Ground-state energy in the strong-coupling limit to leading order in α.

	$-E/\hbar\omega_s$
Exact	$0.4047\alpha^2$
Pekar	$0.4046\alpha^2$
Feynman (Gaussian)	$0.3927\alpha^2$
Exponential	$0.3470\alpha^2$

$$m^*_{2D}(\alpha)/m_{2D}=m^*_{3D}((3\pi/4)\alpha)/m_{3D}\ , \tag{20}$$

where m^*_{3D} (m_{3D}), m^*_{3D} (m_{2D}) is the polaron (electron band) mass of the 3D (2D) polaron.

To summarize, we have calculated the exact 2D polaron ground-state energy up to second order in the Fröhlich coupling constant α and to leading order in α in the case of the strong-coupling limit (i.e., $\alpha \gg 1$). These results are summarized in Tables I and II and are compared with the corresponding expansions of some approximate theories. We found that the ground-state energy (and also the polaron mass) of the approximate theories can easily be obtained from the corresponding 2D results by applying the scaling relation

$$E_{2D}(\alpha)=\tfrac{2}{3}E_{3D}((3\pi/4)\alpha)\ .$$

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APPENDIX A

In this Appendix we present a detailed calculation of the 2D polaron ground-state energy to second order in the Fröhlich coupling constant α. The calculation relies on a path-integral representation of the partition function. This calculation is similar to the 3D case as given in Ref. 13 but with the difference that in the 2D case not all integrals can be done in the zero-temperature limit.

The coefficient of order α is given by [see Eqs. (3) and (4b)]

$$A=\frac{b_1}{\beta}=\frac{1}{\alpha\beta}\langle S_I[\mathbf{r}(t)]\rangle_{S_0} \tag{A1}$$

$$=\frac{1}{\alpha\beta}\sum_{\mathbf{k}}|V_k|^2\int_0^\beta du\int_0^\beta du' G_{\omega_s}(u-u')\langle e^{i\mathbf{k}\cdot[\mathbf{r}(u)-\mathbf{r}(u')]}\rangle_{S_0} \tag{A2}$$

where $\langle\ \rangle_{S_0}$ is a path-integral average with weight e^{S_0}. One readily finds

$$\langle e^{i\mathbf{k}\cdot[\mathbf{r}(u)-\mathbf{r}(u')]}\rangle_{S_0}=e^{-k^2D(u-u')} \tag{A3}$$

with

$$D(t)=\frac{|t|}{2}\left[1-\frac{|t|}{\beta}\right]\ . \tag{A4}$$

Inserting Eq. (A3) into Eq. (A2) and performing as many integrals as possible gives

$$A=\left[\frac{\pi}{2}\right]^{1/2}\int_0^\beta du\frac{G_{\omega_s}(u)}{D(u)}\left[1-\frac{u}{\beta}\right]\ . \tag{A5}$$

In the zero-temperature limit we obtain the well-known result

$$\lim_{\beta\to\infty}A=\frac{\sqrt{\pi}}{2}\int_0^\infty dt\frac{e^{-t}}{\sqrt{t}}=\frac{\pi}{2}\ . \tag{A6}$$

The coefficient of the α^2 term is [see Eqs. (3) and (4b)]

$$B=\frac{1}{2\beta}(b_2-b_1^2)\ , \tag{A7}$$

where

$$b_2=\frac{1}{\alpha^2}\langle S_I[\mathbf{r}(t)]S_I[\mathbf{r}(t)]\rangle_{S_0} \tag{A8}$$

$$=\frac{1}{\alpha^2}\sum_{\mathbf{k}_1}\sum_{\mathbf{k}_2}|V_{k_1}|^2|V_{k_2}|^2\int_0^\beta du_1\int_0^\beta du_1'\int_0^\beta du_2\int_0^\beta du_2' G_{\omega_s}(u_1-u_1')G_{\omega_s}(u_2-u_2') \times\langle e^{i\mathbf{k}_1\cdot[\mathbf{r}(u_1)-\mathbf{r}(u_1')]}e^{i\mathbf{k}_2\cdot[\mathbf{r}(u_2)-\mathbf{r}(u_2')]}\rangle_{S_0} . \tag{A9}$$

The average in Eq. (A9) can be found in Ref. 13 and is given by

$$\langle e^{i\mathbf{k}_1\cdot[\mathbf{r}(u_1)-\mathbf{r}(u_1')]}e^{i\mathbf{k}_2\cdot[\mathbf{r}(u_2)-\mathbf{r}(u_2')]}\rangle=\exp[-k_1^2D(u_1-u_1')-k_2^2D(u_2-u_2')-\mathbf{k}_1\cdot\mathbf{k}_2M(u_1,u_1',u_2,u_2')] , \tag{A10}$$

where

$$M(u_1,u_1',u_2,u_2')=D(u_1-u_2')+D(u_2-u_1')-D(u_1-u_2)-D(u_1'-u_2') . \tag{A11}$$

By inserting Eq. (A10) into Eq. (A9) and performing the transformation

$$\begin{bmatrix}u_1\\u_1'\\u_2\\u_2'\end{bmatrix}=\begin{bmatrix}1&\frac{1}{2}&\frac{1}{2}&0\\1&\frac{1}{2}&-\frac{1}{2}&0\\1&-\frac{1}{2}&0&\frac{1}{2}\\1&-\frac{1}{2}&0&-\frac{1}{2}\end{bmatrix}\begin{bmatrix}R\\r\\\tau_1\\\tau_2\end{bmatrix} \tag{A12}$$

and performing as many integrals as possible, we ended up with the following expression:

$$b_2=4\beta\int_0^{\beta/2}d\tau_1\frac{G_{\omega_s}(\tau_1)}{[D(\tau_1)]^{1/2}}\int_0^{\tau_1}d\tau_2\frac{G_{\omega_s}(\tau_2)}{[D(\tau_2)]^{1/2}}\left[(\tau_1-\tau_2)K(x_2)+(\beta-\tau_1-\tau_2)K(x_1)+2[D(\tau_1)D(\tau_2)]^{1/2}\int_{-x_1}^{x_2}dx\,K(x)\right] , \tag{A13}$$

where $x_1=\tau_1\tau_2/\beta[D(\tau_1)D(\tau_2)]^{1/2}$, $x_2=\tau_2(1-\tau_1/\beta)/[D(\tau_1)D(\tau_2)]^{1/2}$, and $K(x)$ is the complete elliptic function. In the limit of zero temperature we obtain

$$B=-\tfrac{1}{2}\int_0^\infty d\tau_1\frac{e^{-\tau_1}}{(\tau_1)^{1/2}}\int_0^\infty d\tau_2\frac{e^{-\tau_2}}{(\tau_2)^{1/2}}\left[(\tau_1-\tau_2)\left[K(x_{12})-\frac{\pi}{2}\right]+2(\tau_1\tau_2)^{1/2}\int_0^{x_{12}}dx\left[K(x)-\frac{\pi}{2}\right]\right] \tag{A14}$$

with $x_{12}=(\tau_2/\tau_1)^{1/2}$. This expression can be further simplified to

$$B=-\frac{\pi^2}{8}-G+2\int_0^1 dx\frac{K(x)}{(1+x^2)^2} , \tag{A15}$$

where $G=\sum_{m=0}^\infty(-1)^m/(2m+1)^2$.

APPENDIX B

In this Appendix we apply conventional fourth-order perturbation theory to obtain the correction $-B\alpha^2$ to the 2D polaron ground-state energy to second order in the Fröhlich coupling-constant α. One obtains the following form:[6]

$$B=I_1+I_2+I_3 \tag{B1}$$

with

$$I_1=\frac{1}{(2\pi)^2}\int\frac{d^2p}{p}\int\frac{d^2q}{q}\frac{1}{(p^2+1)^2[(\mathbf{p}+\mathbf{q})^2+2]} , \tag{B2}$$

$$I_2=\frac{1}{(2\pi)^2}\int\frac{d^2p}{p}\int\frac{d^2q}{q}\frac{1}{(p^2+1)(q^2+1)[(\mathbf{p}+\mathbf{q})^2+2]} , \tag{B3}$$

$$I_3=\frac{1}{(2\pi)^2}\int\frac{d^2p}{p}\int\frac{d^2q}{q}\frac{1}{(p^2+1)^2(q^2+1)} , \tag{B4}$$

where I_1,I_2,I_3 is the contribution of the nested, crossing, and reducible diagrams, respectively.

I_3 can easily be calculated; we obtained $I_3=-\pi^2/8$. To calculate I_1 we may integrate first over q, which results in

$$I_1=\int_0^\infty dp\frac{1}{(p^2+1)^2(p^2+2)^{1/2}}K\left[\frac{p}{(p^2+2)^{1/2}}\right]. \quad \text{(B5)}$$

With the transformation $x^2=p^2/(p^2+2)$, Eq. (B5) becomes

$$I_1=\int_0^1 dx\frac{1-x^2}{(1+x^2)^2}K(x)\,. \quad \text{(B6)}$$

A numerical evaluation of the integral in Eq. (B6) gives the result $I_1=0.822\,93$.

Performing the q integration in Eq. (B3), I_2 can be written as a twofold integral which we were unable to reduce further:

$$I_2=\int_0^\infty dp\int_0^{\pi/2}d\phi\frac{1}{(p^2+1)^2+4p^2\cos^2\phi}\times\left[1-\frac{1-p^2\cos2\phi}{(p^2+2-p^2\cos^2\phi)^{1/2}}\right]. \quad \text{(B7)}$$

We have calculated numerically $I_2=0.474\,74$. Finally we obtain

$$B=0.063\,97\,. \quad \text{(B8)}$$

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