Acoustical polaron in three dimensions: The ground-state energy and the self-trapping transition

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The interaction of an electron with acoustical phonons by the deformation potential is studied with the Feynman path-integral method for zero temperature. An upper bound to the polaron ground-state energy is obtained. The nature of the transition of the quasifree to the self-trapped electron state is discussed for different approximations to the polaron ground-state energy. We find that, within the Feynman approximation, which is the most reliable one for the ground-state energy, there exists a critical value (k_0^*) for the cutoff (k_0) in phonon wave-vector space such that for $k_0 < k_0^*$ ($k_0 > k_0^*$) the self-trapping transition is continuous (discontinuous) as a function of the electron-phonon coupling strength.

I. INTRODUCTION

The *self-trapping*[1] of an electron caused by its interaction with phonons has attracted renewed interest in recent years.[2–12] This problem is related to the localization problem.[13] In the latter the electron is localized by random potential fluctuations appearing in particular in disordered systems. In the present paper we discuss in detail the self-trapping of an electron due to its interaction with acoustical phonons of the host lattice. We limit ourselves to the study of an electron in a parabolic conduction band, moving in a three-dimensional (3D) lattice and interacting with the acoustical deformation potential. The problem under study is referred to as the *acoustical polaron problem.* As a first step the lattice temperature will be taken equal to zero. In the present paper we will study the ground-state energy of such an electron within different approximations. In a forthcoming paper the dynamical properties of this system will be derived. In particular the frequency-dependent mobility and the influence of the self-trapping transition will be studied.

The electron self-trapping problem already has a considerable history going back to Landau's paper in 1933. In recent years we noticed a revived interest because of the advent of new techniques (renormalization-group approaches,[11,14] Monte Carlo simulation techniques,[15] etc.) and the possibility of mapping certain physical systems onto an acoustical polaron-type problem (e.g., electrons on thin helium films,[7] etc.).

In this paper we consider the continuum model (i.e., "large polarons") but with a finite cutoff k_0 in the phonon k space which simulates the discreteness of the host lattice ($k_0 \sim 1/a$ with a the lattice constant). The opposite limit of a discrete lattice theory (the small polaron problem[15,16]) will not be discussed here.

The electron-phonon interaction will be described by a Fröhlich-type Hamiltonian

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

where

$$\omega_{\mathbf{k}}=sk \tag{2}$$

is the frequency of the acoustical phonons and

$$V_{\mathbf{k}}=\left[\frac{4\pi\alpha}{V}\right]^{1/2}\frac{\hbar^2}{m}k^{1/2} \tag{3}$$

with s the velocity of sound, V the volume of the crystal, and

$$\alpha=\frac{D^2m^2}{8\pi\rho\hbar^3 s} \tag{4}$$

is the dimensionless electron-phonon coupling constant where D is the deformation potential and ρ the mass density of the crystal. In our calculation the sum over the phonon wave vectors $\sum_{\mathbf{k}}$ will be replaced by the integral $[V/(2\pi)^3]\int d\mathbf{k}$ which is cutoff at k_0, the boundary of the first Brillouin zone.

Other authors used a slightly different notation for the electron-phonon coupling constant. Sumi and Toyozawa[2] introduced S_{ac} to characterize the strength of the electron-phonon interaction. The relation with our notation is $S_{ac}/N=(4\pi\alpha/Vk_0)(\hbar/\mathrm{ms})^2$ with N the number of unit cells in the crystal. Shoji and Tokuda[6] introduced a coupling constant α_3 which in our notation is given by $\alpha_3=\sqrt{2}\alpha$.

In the following we will express the energies in units of ms^2, the lengths in units of $\hbar/\mathrm{ms}$, and the phonon wave vector in units of $\mathrm{ms}/\hbar$. In doing so, all variables will be dimensionless.

In Ref. 2, Sumi and Toyozawa applied the Feynman path-integral method to study the ground-state energy and the polaron effective mass when the electron interacts simultaneously with the acoustical, as well as the optical, modes of the lattice vibrations. It was shown that the abrupt change of the polaron state from a nearly free electron state to the self-trapped state is caused by the short-range acoustical interaction and not by the long-range

LO-phonon interaction. In the present paper only the interaction with acoustical phonons is considered and we will concentrate on the phase diagram in (α,k_0) space and on the order of the self-trapping transition. One has to keep in mind that the self-trapping transition is not a phase transition in the strict sense because it is not a collective effect. But nevertheless there are, as we will demonstrate in the present paper, many similarities with the theory of phase transitions, and therefore we sometimes will adapt the language of phase transitions in the following.

The organization of the paper is as follows. In Sec. II different upper bounds to the polaron ground-state energy (E) are derived. We present results for the Feynman[17] approximation,[2] the Gaussian approximation, and the unitary transformation approximation discussed in Ref. 6. Numerical results for E and its derivatives $E'(\alpha)=\partial E/\partial\alpha$ and $E''(\alpha)=\partial^2 E/\partial\alpha^2$ are presented in Sec. III for the different approximations discussed in Sec. II. The phase diagram for the self-trapping transition is also given. Our conclusions are presented in Sec. IV.

II. DIFFERENT UPPER BOUNDS FOR THE GROUND-STATE ENERGY OF THE ACOUSTICAL POLARON

Various techniques have been used to calculate the ground-state energy of the polaron. In this section we summarize different approximations to the polaron ground-state energy: (1) approximations which are intended to be valid over the whole electron-phonon coupling range and (2) approximations which provide an upper bound to the exact polaron ground-state energy.

A. The Feynman approximation

Using the path-integral representation of the partition function and introducing an appropriate trial action, Feynman[17] derived an approximate expression for the optical polaron ground-state energy which today still constitutes one of the best approximations valid for the whole electron-phonon coupling range. Sumi and Toyozawa[2] adapted the Feynman approximation to the case of the three-dimensional acoustical polaron and found

$$E_F=\frac{3(v-w)^2}{4v}-\frac{2\alpha}{\pi}\int_0^\infty d\tau\int_0^{k_0} dk\,k^3 e^{-k\tau}e^{-k^2D(\tau)}, \tag{5}$$

where

$$D(\tau)=\frac{w^2}{2v^2}\tau+\frac{v^2-w^2}{2v^3}(1-e^{-v\tau}) \tag{6}$$

with v,w the two variational parameters of the Feynman polaron model.

The second-order perturbation-theory result for the polaron self-energy can be obtained from Eq. (5) by taking $v=w$ which leads to

$$E=-\frac{2\alpha}{\pi}\left[k_0^2-4k_0+8\ln\left[1+\frac{k_0}{2}\right]\right]. \tag{7}$$

The Feynman approximation also provides[10] higher-order terms in α.

In the strong-coupling limit $v\gg w$ and after a variational calculation one finds $v=2(\alpha/15\pi)^{1/2}k_0^{5/2}$ which results in the ground-state energy

$$E=-\frac{2\alpha}{3\pi}k_0^3+\left[\frac{3\alpha}{5\pi}\right]^{1/2}k_0^{5/2}. \tag{8}$$

The strong-coupling region is defined by the condition $\alpha\gg 15\pi/16k_0=2.95/k_0$. Note that for the acoustical polaron the ground-state energy in the strong-coupling limit is linear in the electron-phonon coupling constant α! This is different from the optical polaron where $E\sim-\alpha^2$ for $\alpha\to\infty$.

B. The Gaussian approximation

This approximation to the ground-state energy can be obtained from the Feynman result, Eq. (5), by taking the limit $w\to 0$:

$$E_G=\frac{3v}{4}-\frac{2\alpha}{\pi}\int_0^\infty d\tau\int_0^{k_0} dk\,k^3 e^{-k\tau}\times\exp\left[-k^2\frac{1-e^{-v\tau}}{2v}\right]. \tag{9}$$

Only one variational parameter, v, is left. In the Gaussian approximation the electron motion is approximated by the motion of a particle in a harmonic potential well. In the weak- and strong-coupling limits the same results are obtained as for the Feynman approximation to leading order in α. But in the weak-coupling limit there is an essential difference between E_F and E_G, namely, E_G gives Eq. (7) exactly—there are no higher orders in α—while E_F has higher-order terms in α. In the case of the 3D optical polaron a similar artifact of the Gaussian approximation was found in Ref. 10.

C. The approximation of Shoji and Tokuda

Using a generalization of the Lee-Low-Pines canonical transformation approach,[18] Shoji and Tokuda[6] found the following upper bound to the acoustical polaron ground-state energy:

$$E_{ST}=\frac{3}{4}\lambda-\frac{2\alpha}{\pi}\int_0^{k_0} dk\,k^2\frac{\exp\left[-(1-a)^2\frac{k^2}{2}\right]}{1+\frac{a^2}{2}k}, \tag{10}$$

where λ and a are two parameters which have to be determined by minimizing E_{ST}. For the limiting behavior of E_{ST} for $\alpha\ll 1$ and $\alpha\gg 1$ the same remarks can be made as for the Gaussian approximation.

III. NUMERICAL RESULTS AND DISCUSSION

The three different approximations to the ground-state energy given in Sec. II are studied numerically in this section. In Fig. 1 we have plotted the ground-state energy and the first and second derivatives of the ground-state

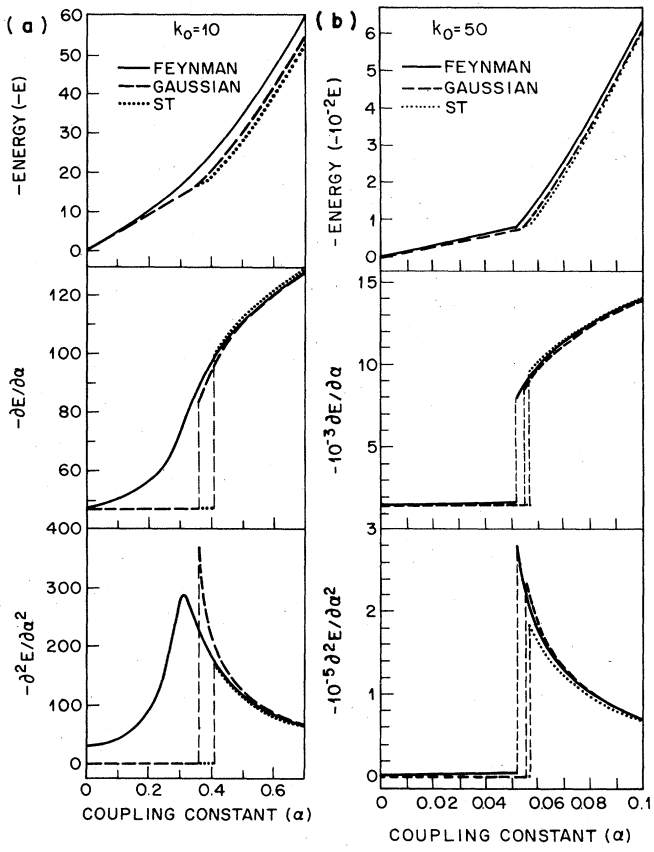

FIG. 1. Ground-state energy of the acoustical polaron in three dimensions and the first and second derivatives as a function of the electron-phonon coupling strength for two values of the cutoff [(a) $k_0=10$ and (b) $k_0=50$] for three different approximations.

energy with respect to the electron-phonon coupling, as a function of α for two values of the cutoff parameter, $k_0=10$ [Fig. 1(a)] and $k_0=50$ [Fig. 1(b)]. We note the following.

(1) For both values of k_0 the Feynman approximation gives the lowest value for the ground-state energy for all α. Consequently, in view of the variational character of the approximations the result of the Feynman approach is closest to the exact result.

(2) Note that in the limit $\alpha\rightarrow 0$ and for any value of k_0 all approaches give the same result for the ground-state energy (E) and its first derivative $E'(\alpha)=\partial E/\partial\alpha$. The reason for this is that in this limit the three approximations give the exact result up to first order in α. The second derivative $E''(\alpha)=\partial^2 E/\partial\alpha^2$ is different in the $\alpha\rightarrow 0$ limit because the Feynman approximation still gives a correction to order α^2, while in the other approximations there is no correction to order α^2 and consequently $\partial^2 E/\partial\alpha^2=0$. In fact, the Gaussian and the unitary transformation approaches give $\partial^2 E/\partial\alpha^2=0$ for $\alpha<\alpha_c$ where α_c depends on the approximation and the value of the cutoff k_0.

(3) In the strong-coupling limit, i.e., $\alpha\rightarrow\infty$, $E'(\alpha)=\partial E/\partial\alpha$ and $E''(\alpha)=\partial^2 E/\partial\alpha^2$ approach the same asymptotic result in the three approximations. The ground-state energy is the same up to leading order in α but the next correction terms are different for the three approximations.

(4) For $k_0=10$ the ground-state energy E_F and its derivatives to α are continuous for all values of α. This is in contrast with E_G and E_{ST} whose first and second derivatives to α are discontinuous at $\alpha_c=0.36$ and 0.41, respectively.

(5) The discontinuity in $E'(\alpha)$ and $E''(\alpha)$ reflects a transition from a quasifree electron state ($\alpha<\alpha_c$) to a self-trapped electron state ($\alpha>\alpha_c$). In the Feynman approximation this transition is continuous when $k_0=10$. In that case it is characterized by a peak in $E''(\alpha)$ at $\alpha\approx 0.31$. For relatively large values of k_0 [see, e.g., Fig. 1(b) for $k_0=50$] the Feynman approximation also leads to a discontinuous transition, namely, at $\alpha_c=0.052$ ($E'_G(\alpha)$ [$E'_{ST}(\alpha)$] is discontinuous at $\alpha_c=0.055$ (0.057)).

(6) From the numerical results [Figs. 1(a) and 1(b)] it is apparent that for a given value of k_0 the critical coupling α_c at which the self-trapping transition occurs is smaller for approximations which give lower (i.e., better) values for the ground-state energy [if the transition is continuous we associate α_c with the position of the peak in $E''(\alpha)$].

From the above discussion we may conclude that our numerical results seem to *indicate* that the numerically calculated critical coupling α_c at which the self-trapping occurs is an upper bound to the exact α_c. This, of course, is a direct consequence of the fact that the calculated ground-state energy is an upper bound to the exact value of the ground-state energy. Indeed, the lower the calculated E the more binding there is and consequently the closer one is to the self-trapped state.

The phase diagram for the self-trapping transition is shown in Fig. 2. For each value of k_0 we plotted the α value at which the self-trapping occurs for the Feynman, the Gaussian, and the unitary transformation (ST) approaches. The unitary transformation approach gives a first-order transition [$E'(\alpha)$ is discontinuous] in the whole k_0 region which we investigated numerically (i.e., $k_0>0.4$). A more complicated phase diagram emerges for the Gaussian approximation which has a line of first-order transitions when $k_0>1.8$ and which continues into a line of second-order transitions [$E'(\alpha)$ is continuous but $E''(\alpha)$ is discontinuous] for $k_0\geq 1.8$. In the Feynman approximation the phase diagram consists of a line of first-order transitions which ends in the point $\alpha=0.151\pm 0.0005$, $k_0=18\pm 0.5$, at which point a second-order transition occurs. In the theory of phase transitions this point is analogous to a critical point. For $k_0<18$ there is *no* well-defined (i.e., discontinuous) self-trapping transition. In the limit $k_0\rightarrow\infty$ the line of first-order transitions could be fitted to $\alpha_c=2.56/k_0$.

The behavior of the first [$E'(\alpha)$] and second [$E''(\alpha)$] derivatives of the energy with respect to α close to the critical point is shown in Fig. 3 for E calculated within the Feynman approximation. Note that at the critical point $E'(\alpha)$ is continuous while $E''(\alpha)$ diverges. This divergent behavior for $k_0=18$ and $\alpha>0.151$ could be fitted to the power law $E''(\alpha)=-A(1-0.1508/\alpha)^{-\nu}$ with $A=930\pm 10$ and the exponent $\nu=0.61\pm 0.01$. For

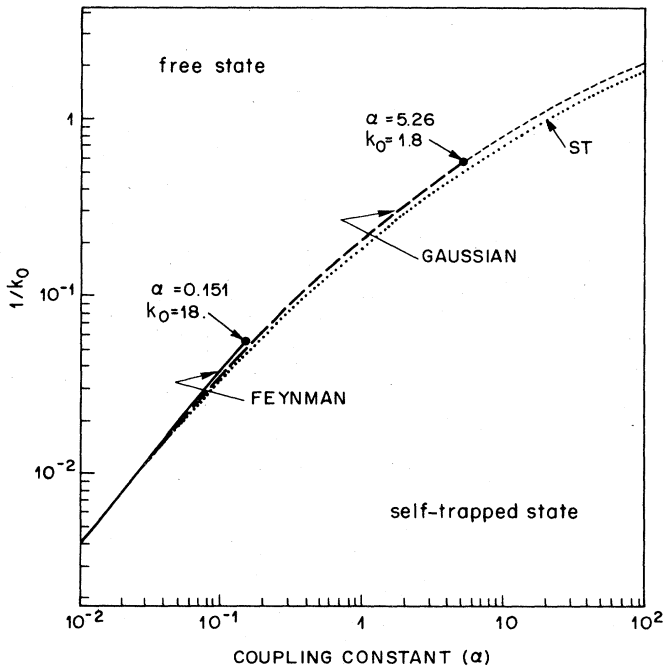

FIG. 2. Phase diagram for the self-trapping transition of the acoustical polaron in three dimensions within the three different approximations.

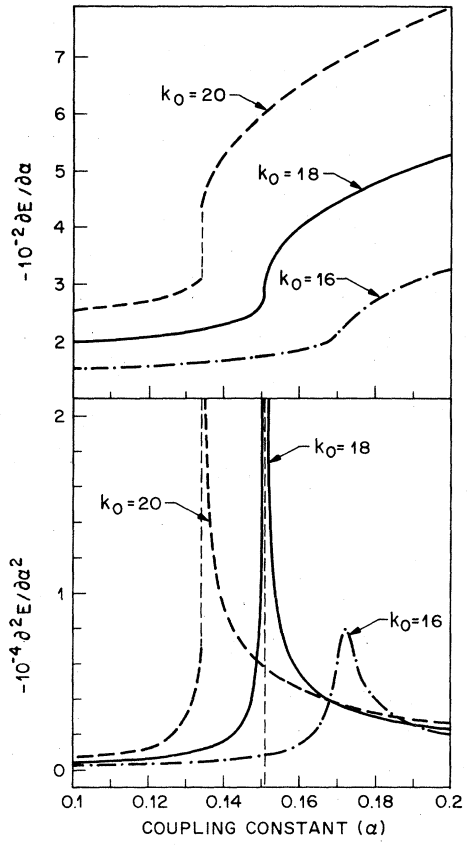

FIG. 3. First and second derivatives of the ground-state energy with respect to the electron-phonon coupling constant in the neighborhood of the critical point for the Feynman approximation.

$k_0 > 18$, $E'(\alpha)$ becomes discontinuous at a certain α_c where $E''(\alpha)$ exhibits a finite jump.

Experimentally, $E(\alpha)$, $E'(\alpha)$, and $E''(\alpha)$ are not directly measurable because α is a fixed quantity for each material. It is possible to observe the self-trapping transition by measuring the mobility $\mu \approx \tau/m^*$ which is inversely proportional to the polaron mass m^*. The scattering time τ does not change much at α_c as will be shown in a forthcoming paper. In Fig. 4 we plotted the mass of the Feynman polaron model $M=(v/w)^2$ as a function of α for different values of k_0. $M=(v/w)^2$ is a reasonably good approximation (within 10%) to the actual polaron mass m^* as will be shown in a forthcoming paper (see also Ref. 19). The differences between the quasifree-electron state and the self-trapped state are very clear. In the quasifree state, $M \approx 1$ and the electron mass is, within a few percent, equal to the bare electron mass. At sufficiently large α the polaron mass $M \gg 1$ and the polaron is dressed with a heavy phonon cloud which will severely limit the polaron mobility. For example, for $k_0=100$ the critical coupling is $\alpha_c=0.0256$ at which the mass M increases with three orders of magnitude and thus we expect that the mobility will decrease with several orders of magnitude.

For the strong-coupling limit $v \gg w$ and $D(\tau)$ can be approximated by $D(\tau) \simeq 1/2v$. In doing so we neglect the translational motion of the polaron [the term $\omega^2\tau/2v^2$ in $D(\tau)$ of Eq. (6)] and the virtual transitions to the different internal states [the term $(v^2-w^2)e^{-v\tau}/2v^3$ in $D(\tau)$ of Eq. (6)]. The ground-state energy

$$E_S=\frac{3v}{4}-\frac{2\alpha}{\pi}\int_0^\infty d\tau \int_0^{k_0} dk\, k^3 e^{-k\tau} e^{-k^2/2v} \qquad (11)$$

can then be presented as an analytic form

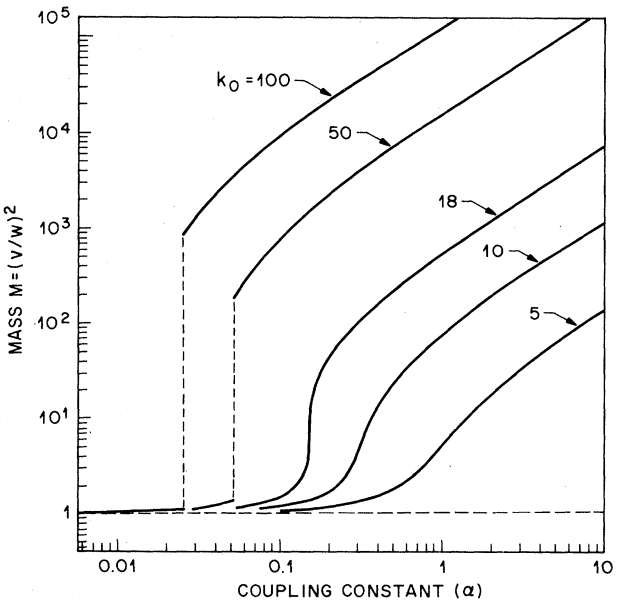

FIG. 4. Mass of the Feynman polaron model as function of the electron-phonon coupling and for different values of the cutoff k_0.

$$E_S=\frac{3v}{4}-\frac{\alpha}{\pi}(2v)^{3/2}\left[\frac{\sqrt{\pi}}{2}\,\mathrm{erf}\left[\frac{k_0}{\sqrt{2v}}\right]-\frac{k_0}{\sqrt{2v}}e^{-k_0^2/2v}\right], \tag{12}$$

where $\mathrm{erf}(x)$ is the error function. In the self-trapped state, with increasing α and k_0 fixed, one has $v\to\infty$ and we may expand Eq. (12) in powers of $k_0/\sqrt{2v}\ll 1$:

$$E_S=\frac{3v}{4}-\frac{2\alpha}{\pi}\left[\frac{k_0^3}{3}-\frac{k_0^5}{10v}+\frac{k_0^7}{56v^2}+\cdots\right]. \tag{13}$$

The minimalization of Eq. (13) can thus easily be performed and gives

$$v=2\left[\frac{\alpha}{15\pi}\right]^{1/2}k_0^{5/2}\left[1-\frac{15}{56}\left[\frac{5\pi}{3\alpha}\right]^{1/2}\frac{1}{k_0^{1/2}}+\cdots\right] \tag{14}$$

which leads to the ground-state energy

$$E_S=-\frac{2\alpha}{3\pi}k_0^3+\frac{3\alpha}{5\pi}k_0^{5/2}-\frac{15}{112}k_0^2+\cdots. \tag{15}$$

The self-trapping transition occurs when the polaron ground-state energy in the self-trapped state becomes equal to the ground-state energy in the quasifree state. For k_0 large this implies $E_{\mathrm{QFS}}\simeq-(2\alpha/\pi)k_0^2$ from which we find

$$\alpha_c=\frac{9\pi}{160}(1+\sqrt{6})^2\frac{1}{k_0}=2.10/k_0 \tag{16}$$

which may be compared with our numerical result $\alpha_c=2.56/k_0$ of Sec. II. In deriving Eq. (16) it was assumed that $E_{\mathrm{QFS}}\simeq-(2\alpha/\pi)k_0^2$ which is only approximately valid. From our numerical analysis we found that in the quasifree-electron state (QFS) and for α near α_c (α_c is the electron-phonon coupling at which the self-trapping occurs), $v>w$ and this results in $E_{\mathrm{QFS}}<-(2\alpha/\pi)k_0^2$. Consequently, the self-trapping transition occurs for $\alpha_c>2.10/k_0$ which is in agreement with our numerical findings.

At the self-trapping transition the polaron mass jumps from $M_{\mathrm{QFS}}(v/w)^2\simeq 1$ to $M_S=(v/w)^2\simeq(4\alpha/15\pi)k_0^5\simeq 0.18k_0^4=3.49\alpha_c^4$ when $k_0\gg 1$. In the context of phase transitions one often introduces an order parameter. Within the Feynman approximation we define the quantity $\Delta(1/M)=1/M_{\mathrm{QFS}}-1/M_S$ which is plotted in Fig. 5. Note that $\Delta(1/M)$ has an analogous behavior with that of an order parameter in the theory of phase transitions.

For the Gaussian approximation we show in Fig. 6 the jump in the variational parameter v at the self-trapping transition. v measures the eigenfrequency of the quadratic electron potential. The above analysis of the ground-state energy in the Feynman approach is also valid for the Gaussian approximation because the dominant terms in E_S are independent of the value of w. For large k_0 we find approximately $\Delta v=2(\alpha/15\pi)^{1/2}k_0^{5/2}\simeq 0.42k_0^2=1.87/\alpha_c^2$. From our discussion on the coefficient in Eq. (16) we know that the coefficient in the relation $\Delta v\simeq 0.42k_0^2$ is correct within a factor of 2. Note also that in the Gaussian approximation for the QFS we have exactly $v=0$ while in the self-trapped state $v\neq 0$. For

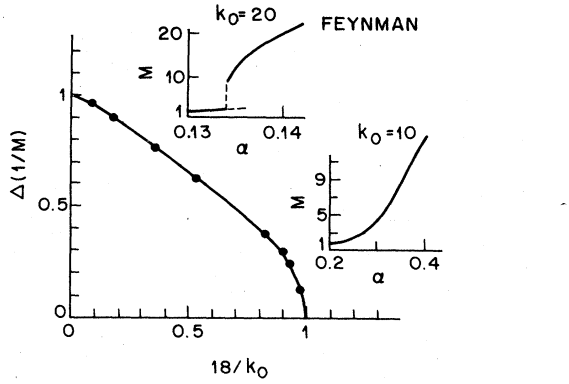

FIG. 5. Order parameter in the Feynman approximation. In the inset the Feynman polaron mass is given as a function of α for $k_0=10$ and 20.

$k_0>1.8$ there is a jump in v at the transition point while for $k_0<1.8$ v is continuous but $\partial v/\partial\alpha$ is discontinuous at the self-trapping transition point.

IV. CONCLUSION

In earlier work[10] we pointed out that the Gaussian approximation can be obtained from the Feynman approximation by taking one of the variational parameters, namely w, equal to zero. Physically this means that the translational degrees of freedom are not taken into account; the electron is localized in a potential well for $v\neq 0$. Next we will try to obtain the Shoji-Tokuda result from the Feynman approximation. For that purpose we disregard the exponential term in the function $D(\tau)$ [Eq. (6)] and insert $D(\tau)=[(v^2-w^2)/2v^3]+(w^2/2v^2)\tau$ into Eq. (5). This allows one to perform the τ integral explicitly and results in

$$E=\frac{3}{4}\frac{(v-w)^2}{v}-\frac{2\alpha}{\pi}\int_0^{k_0}dk\frac{k^2}{1+\frac{w^2}{2v^2}k}e^{-k^2(v^2-w^2)/2v^3}. \tag{17}$$

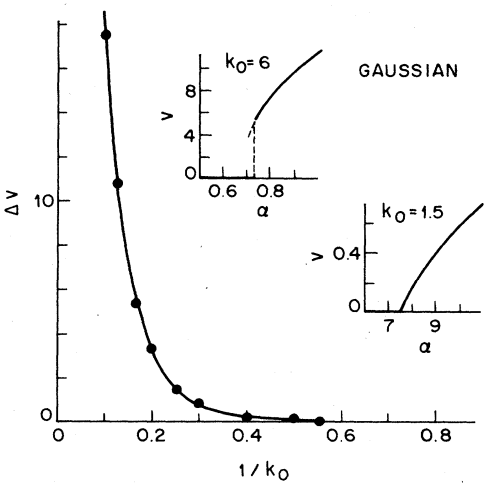

FIG. 6. Discontinuity of the variational parameter v in the Gaussian approximation. In the inset the variational parameter is shown as a function of α for $k_0=1.5$ and 6 in the neighborhood of the self-trapping transition.

Comparing this equation with the Shoji-Tokuda result [Eq. (10)], one sees that both expressions are very similar. We can make the identification $a=w/v$ and $\lambda=(v-w)^2/v$ but then the exponential in the integral of Eq. (10) is $e^{-k^2/v}$ which is different from the one in Eq. (17) which still contains $1-w^2/v^2$. Another possibility is to choose $a=w/v$ and $\lambda=v(v-w)^2/(v^2-w^2)$ which makes the terms with the integral in Eqs. (10) and (17) identical to each other, but then the first term in Eq. (10), $\frac{3}{4}\lambda=(3/4v)(v-w)^2/[1-(w/v)^2]$, is larger than the corresponding term in Eq. (17), $(3/4v)(v-w)^2$, and consequently Eq. (17) gives a result which is lower than $E_{\rm ST}$. In conclusion, the integral term in the ground-state energy of the Shoji-Tokuda result can be obtained from the Feynman approach by neglecting the transitions to the different internal states, retaining the translational degrees of freedom with an effective mass $a^{-2}=(v/w)^2$. Even after this approximation the resulting kinetic-energy term is still smaller than the corresponding term in the ST result.

In earlier work on the self-trapping transition by Toyozawa and Shinozuka,[4] the dependence of the discreteness of the self-trapping transition on the dimensionality of the system, on the type of the interaction, and on the phonon dispersion was studied within the adiabatic approximation for large values of the cutoff k_0. In the case of the 3D acoustical polaron problem their results are reobtained here and are given by Eq. (13). The extension to finite k_0 values of the results of Ref. 4 was given recently by Das Sarma[12] whose result for the 3D acoustical polaron is reobtained here and is given by Eq. (12). In the present work we confirm that for large values of the cutoff k_0 the adiabatic approximation gives the correct behavior for the self-trapping transition. But for smaller values of k_0 a more detailed approximation is needed. The Feynman path-integral approximation is most suited for it because it is able to describe, within the same approximation, a continuous and a discontinuous self-trapping transition.

Jackson and Platzman[7] applied the Feynman approximation to the two-dimensional (2D) acoustical polaron problem. In their study they fixed k_0 and only varied the electron-phonon coupling constant α. It is interesting to note that their results are qualitatively similar to ours when we take $k_0>18$. These authors also investigated[20] the influence of temperature on the self-trapping transition and found that the transition becomes smoother with increasing temperature. A similar behavior is expected for the 3D acoustical polaron problem.

The following question still exists: Is the self-trapping transition continuous or discontinuous for the 3D acoustical polaron? The present study shows that the better the approximation the more continuous the self-trapping transition is. A similar situation was found for the 3D (Ref. 10) and the 2D (Ref. 21) optical polarons. At present we can only say that the best approximation yet studied (namely, the Feynman approximation) gives a continuous self-trapping transition for $k_0<18$ while for $k_0>18$ the self-trapping transition is a discrete one.

It would be interesting to see if an even better approximation than the Feynman two-parameter polaron model (e.g., a general harmonic approximation with an infinite number of variational parameters as discussed in Ref. 22 for the 3D optical polaron) does lead to an even larger critical value $k_0=18$. But within a variational approach one is never able to prove whether the self-trapping transition is continuous or discontinuous. A totally different approach to the problem would be a Monte Carlo calculation of the ground state (see, e.g., Refs. 15 and 23). This approach, in principle, is exact but is limited by, e.g., statistical errors induced by the finite simulation time. The latter one will limit the conclusion drawn from such a calculation on the discreteness of the self-trapping transition.

In the present work the ground-state properties of an electron interacting with acoustical phonons via the deformation potential were investigated. In real crystals the interaction with LO phonons can also be important and may change the present results qualitatively, but it is not expected (see, e.g., Ref. 2) to be the determining factor for the occurrence of self-trapping. Consequently, we can make a qualitative comparison between the present results and experimental results and indicate the main trends between groups of materials.

The semiconductors Si and Ge have a lattice constant of $a=5.43$ and 5.66 Å, respectively, which is much smaller than the unit of length introduced in our calculation: $\hbar/{\rm ms}=830$ Å for Si and 5100 Å for Ge. The energy scale is ${\rm ms}^2=0.7$ meV (Si) and 0.07 meV (Ge). The parameters determining the behavior of the acoustical polaron are $k_0=480$ (Si) and 2800 (Ge) and $\alpha=7.5\times10^{-5}$ (Si) and 1.1×10^{-6} (Ge), which gives $\alpha k_0=0.036$ (Si) and 0.031 (Ge) but which is too small to have self-trapping. Thus the electrons in Si and Ge cannot be self-trapped as is indeed observed in these materials.

For the III-V compounds similar results are found. As an example we take GaAs which has $a=5.65$ Å; the units in our problem are ${\rm ms}^2=0.11$ meV and $\hbar/{\rm ms}=3200$ Å. The coupling constant $\alpha=6.3\times10^{-6}$ is very small while the cutoff in wave-vector space $k_0=1800$ Å is such that we are in the large k_0 limit. The relevant quantity $\alpha k_0=0.011$ tells us that the electrons in GaAs are free as is well known experimentally.

For the alkali halides the product αk_0 is an order of magnitude larger, and we found $\alpha k_0\sim0.19$–0.26. As an example, let us take NaCl, which has a lattice constant of $a=5.6$ Å; the units in our problem are, for the energy, ${\rm ms}^2=0.57$ meV, and the length, $\hbar/{\rm ms}=5.6$ Å. Furthermore, $k_0=310$, $\alpha=7.7\times10^{-4}$ and thus the product $k_0=0.24$ is still an order of magnitude too small to have self-trapping for the electrons. The holes in alkali halides are found experimentally to be self-trapped. This can be explained from the present formalism and appears to be mainly a consequence of their larger effective mass. The effective mass of holes is a factor of 3–4 larger than the electron effective mass, and consequently [see Eq. (4)] the coupling constant α will be a factor of 10 larger and thus the product $\alpha k_0>2.4$ is sufficiently large to have self-trapping.

The present results are consistent with the experiments and with earlier theoretical calculations.[2,24,25]

In the present work we did not discuss the self-trapping of excitons. The Hamiltonian (1) should then be modified in order to account for the electron-hole interaction. The interested reader is referred to, e.g., Refs. 24–26.

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