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The polaron–bipolaron transition for acoustical three-dimensional polarons

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Abstract. The ground-state energy of an acoustical bipolaron in three dimensions (3D) is studied within the Feynman path integral method. The acoustical polaron exhibits a transition from the quasi-free state to the self-trapped state. Depending on the value of the Debye cut-off (k_0) in phonon wavevector space this transition can be continuous or discontinuous. If two electrons are present a second transition becomes possible: the transition to the bipolaron state in which the two electrons are self-trapped around the same position. The corresponding phase diagram is calculated as function of the cut-off (k_0), the electron–phonon coupling strength (α), and the repulsion (U) between the electrons. We found that: (i) the bipolaron transition is a first-order transition; (ii) it is also possible between two polarons which are in the quasi-free state, i.e. are not self-trapped; and (iii) the effective particle mass increases substantially at the transition point.

1. Introduction

We consider a model describing non-relativistic particles, which we shall call electrons for definiteness, which interact with phonons [1]. The quasi-particle consisting of the electron and the self-induced phonon cloud is called a *polaron*. Using path integral techniques it is possible to eliminate the field variables (i.e. the phonons) exactly, which reduces it to a non-local one-particle problem. In the present paper, we follow the original idea of the Feynman polaron model [2], in which in zeroth order the virtual phonon cloud surrounding the electron is replaced by a fictitious particle which is bound to the electron through a spring, and generalize it to the bipolaron case. The parameters characterizing the Feynman polaron and bipolaron model are determined through a minimization of the ground-state energy.

The discovery of high-temperature superconductors, which exhibit strong electron–phonon interaction, has revived interest in the generalization of the polaron concept [3–5]. One possible mechanism put forward is the condensation of *bipolarons* into a superconducting phase [3, 6]. The necessary precondition for this to happen is that bipolarons exist. Previous work on *large* optical bipolarons indicated that they can only exist for extremely large electron–phonon coupling, which is probably not reached in real materials. Emin [3] has suggested that additional interaction mechanisms like electron–acoustical-phonon scattering may help to stabilize the optical bipolaron and may increase the bipolaron stability region to a region in parameter space which may be more easily found in real materials. In the present paper, we consider only the acoustical polaron problem and

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neglect the interaction with optical phonons. We determine the parameter space in which bipolarons can exist.

In [7, 8], it was found that the acoustical polaron exhibits a transition from the quasi-free state to the self-trapped state, for some critical coupling constant α_c, which depends on the value of the cut-off (k_0) in phonon wavevector space. This transition can be continuous ($k_0 < 18$) or discontinuous ($k_0 > 18$), i.e. first order. Here, we generalize this work to the case of two electrons. Using the technique of path integration the ground-state properties of the system of two electrons which interact with each other via the Coulomb force and indirectly through acoustical phonons is investigated in the limit of zero temperature. The state of the system is determined by the strength of the electron–phonon coupling constant α, the strength $U(\boldsymbol{r}_1-\boldsymbol{r}_2)$ of the Coulomb repulsion and the phonon cut-off (k_0) wavevector. We found three different states: (i) two quasi-free electrons infinitely separated; (ii) two self-trapped polarons infinitely separated; and (iii) the bipolaron state where two electrons are self-trapped around the same position. In section 2, we present the Fröhlich Hamiltonian and give the bipolaron action which is needed in a path integral description of the problem after elimination of the phonons. In section 3, the Feynman bipolaron model is described. We then use the Feynman variational principle to derive an upper bound to the exact ground-state energy of the bipolaron. Explicit analytic results are obtained in limiting cases of α and k_0. The numerical results are presented in section 4. In the last section we present our conclusions.

2. The bipolaron Hamiltonian and bipolaron model

In this section, we present the Hamiltonian which describes two electrons interacting with the vibrational modes of a crystal and pave the way to a Feynman-type approach to the bipolaron problem, which we describe in the next section. The Hamiltonian is given by

$$H = \sum_{j=1,2} \frac{\boldsymbol{p}_j^2}{2m} + \sum_{\boldsymbol{k}} \hbar\omega_{\boldsymbol{k}}(a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + \tfrac{1}{2}) + H_I + U(\boldsymbol{r}_1 - \boldsymbol{r}_2) \tag{1}$$

with the electron–phonon interaction

$$H_I = \sum_{j=1,2} \sum_{\boldsymbol{k}} \left(V_{\boldsymbol{k}} a_{\boldsymbol{k}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_j} + V_{\boldsymbol{k}}^* a_{\boldsymbol{k}}^\dagger \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_j} \right) \tag{2}$$

where $\boldsymbol{r}_j$ ($\boldsymbol{p}_j$) are the position (momenta) operators of the jth electron, m is the electron band mass, $a_{\boldsymbol{k}}^\dagger$ ($a_{\boldsymbol{k}}$) are the creation (annihilation) operators for phonons with wavevector $\boldsymbol{k}$, and frequency $\omega_{\boldsymbol{k}}$, and $U(\boldsymbol{r}_1 - \boldsymbol{r}_2) = e^2/\epsilon_0|\boldsymbol{r}_1 - \boldsymbol{r}_2|$ is the Coulomb potential between the two electrons. For longitudinal acoustic phonons we have $\omega_{\boldsymbol{k}} = s|\boldsymbol{k}|$ and $V_{\boldsymbol{k}}$, the Fourier transform of the electron–phonon interaction, takes the form

$$V_{\boldsymbol{k}} = (4\pi\alpha/V)^{1/2}\hbar k^{1/2}/m$$

with s the velocity of sound, V the volume of the crystal and $\alpha = D^2m^2/8\pi\rho\hbar^3 s$ 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 wavevectors $\sum_{\boldsymbol{k}}$ will be replaced by the integral $(V/(2\pi)^3)\int \mathrm{d}\boldsymbol{k}$, which is cut off at k_0, the boundary of the first Brillouin zone. Next we will use dimensionless units and express the energy in units of ms^2 and the length in units of $\hbar/ms$.

In using the techniques of path integration we first have to compute the Lagrangian corresponding to the Hamiltonian (1). The action is defined as the time integral over the Lagrangian of this dynamical system [9]. For our purposes we want to calculate the partition function and therefore we introduce imaginary times $\tau = -\mathrm{i}t = \beta$ (t is real), with $\beta^{-1} = Tk_B$ where T is the temperature of the system and k_B the Boltzmann constant. After eliminating the field variables [2, 10], we obtain the action $S[\boldsymbol{r}_1(t), \boldsymbol{r}_2(t)]$ (see also [4])

$$S[\boldsymbol{r}_1(t), \boldsymbol{r}_2(t)] = -\int_0^\beta \mathrm{d}t \left[\sum_{j=1}^{2} \frac{1}{2m}\dot{\boldsymbol{r}}_j(t)^2 + U(\boldsymbol{r}_1(t) - \boldsymbol{r}_2(t))\right] + \sum_{j,l=1,2}\sum_{\boldsymbol{k}} |V_k|^2 \int_0^\beta \mathrm{d}t \int_0^\beta \mathrm{d}s\; G_{\omega_k}(t-s)\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot[\boldsymbol{r}_j(t)-\boldsymbol{r}_l(s)]} \tag{3}$$

with

$$G_\Omega(u) = \frac{1}{2}n(\Omega)(\mathrm{e}^{\Omega|u|} + \mathrm{e}^{\Omega(\beta-|u|)}) \tag{4}$$

the phonon Green's function, where $n(\Omega) = 1/(\mathrm{e}^{\beta\hbar\Omega} - 1)$ is the occupation number of phonons with frequency Ω.

In Feynman's polaron model one replaces the virtual phonon cloud surrounding the electron by a fictitious particle which is bound to the electron through a spring. In a bipolaron system we have two electrons each with their own phonon cloud, and consequently the Feynman bipolaron model consists of four particles, described by the following Hamiltonian:

$$H_F = \sum_{j=1,2}\left[\frac{\boldsymbol{p}_j^2}{2m} + \frac{\boldsymbol{P}_j^2}{2M} + \frac{\kappa}{2}(\boldsymbol{r}_j - \boldsymbol{R}_j)^2\right] + \frac{\kappa'}{2}\left[(\boldsymbol{r}_1 - \boldsymbol{R}_2)^2 + (\boldsymbol{R}_1 - \boldsymbol{r}_2)^2\right] - \frac{K}{2}(\boldsymbol{r}_1 - \boldsymbol{r}_2)^2 \tag{5}$$

where $(\boldsymbol{r}_j, \boldsymbol{p}_j)$ are the electron coordinates with mass m and which interact with a second particle, called the fictitious particle, with coordinates $(\boldsymbol{R}_j, \boldsymbol{P}_j)$ of mass M. κ, κ' are the oscillator strengths with which each electron interacts with the fictitious particles. The Coulomb repulsion between the electrons is approximated by a quadratic repulsion with strength K. The resulting bipolaron model is illustrated in figure 1. Note that the model is determined by the four parameters M, κ, κ' and K. The action corresponding to the Hamiltonian (5) in which we have eliminated the coordinates of the fictitious particle is given by

$$S_t[\boldsymbol{r}_1(t), \boldsymbol{r}_2(t)] = -\int_0^\beta \mathrm{d}t \left[\sum_{j=1}^{2} \frac{m}{2}\dot{\boldsymbol{r}}_j(t)^2 - \frac{K}{2}[\boldsymbol{r}_1(t) - \boldsymbol{r}_2(t)]^2\right] - \int_0^\beta \mathrm{d}t \int_0^\beta \mathrm{d}s\; G_w(t-s)\left[\frac{\hbar(\kappa^2+\kappa'^2)}{4Mw}\sum_{j=1,2}[\boldsymbol{r}_j(t) - \boldsymbol{r}_j(s)]^2 + \frac{\hbar\kappa\kappa'}{Mw}[\boldsymbol{r}_1(t) - \boldsymbol{r}_2(s)]^2\right]. \tag{6}$$

3. The bipolaron ground-state energy

The ground-state energy of the bipolaron system is calculated using the Feynman variational principle which provides an upper bound to the exact bipolaron ground-state energy E_{bip}.

This variational principle states that

$$F_{bip} \leqslant F_t - \frac{1}{\beta}\langle S - S_t\rangle_t \tag{7}$$

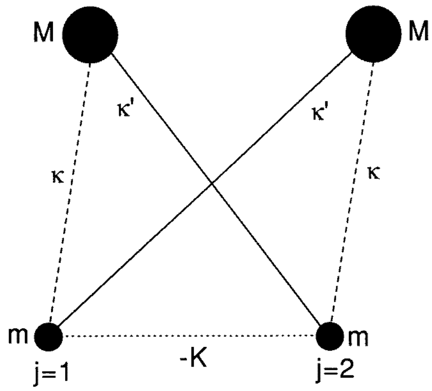

Figure 1. Graphical representation of the Feynman bipolaron model.

where F_t is the free energy of some trial action S_t. $\langle \ldots \rangle_t$ is a path integral average with weight e^{S_t}. For the trial action S_t we choose the one corresponding to the Feynman bipolaron model (6). The partition sum $Z_t = e^{\beta F_t}$ of the trial action can be evaluated explicitly [4]:

$$Z_t = V \frac{2m(\Omega_1/w)^2}{2\pi\hbar^2\beta} \left[2\sinh\left(\frac{\hbar w\beta}{2}\right)\right] \prod_{j=1}^{3} \left[2\sinh\left(\frac{\hbar\Omega_j\beta}{2}\right)\right] \qquad j = 1, 3 \tag{8}$$

where

$$\Omega_1^2 = \frac{M+m}{Mm}(\kappa + \kappa') \tag{9}$$

and

$$\Omega_{2,3}^2 = \frac{1}{2}\left\{\Omega_1^2 - \frac{2K}{m} \pm \left[\left[\frac{M-m}{Mm}(\kappa+\kappa') - \frac{2K}{m}\right]^2 + \frac{4}{Mm}(\kappa-\kappa')^2\right]^{1/2}\right\} \tag{10}$$

are the eigenfrequencies of the Feynman bipolaron model. The total mass of the composite system is $\Omega_1^2/w^2 = (M+m)/m$, where $w^2 = (\kappa+\kappa')/M$ is the frequency of the free oscillator. These eigenfrequencies satisfy the following inequalities: $\Omega_1^2 \geqslant \Omega_2^2 + \Omega_3^2$ and $\Omega_2 \geqslant w \geqslant \Omega_3 \geqslant 0$. Recently, the present authors [11] obtained the eigenfrequencies of the Feynman bipolaron model in the presence of a magnetic field. Such a field couples the polaron motion in the two directions perpendicular to the magnetic field, which leads to seven eigenfrequencies of the diagonalized bipolaron model.

The bipolaron ground-state energy, E_{bip}, is obtained as the zero-temperature limit of the free energy (7). We found the following result:

$$E_{bip} = \frac{3}{2}\sum_{j=1}^{3}\Omega_j - 3w - \frac{3}{4}\left(\Omega_1\frac{\Omega_1^2 - w^2}{\Omega_1^2} + \Omega_2\frac{\Omega_2^2 - w^2}{\Omega_2^2 - \Omega_3^2} + \Omega_3\frac{w^2 - \Omega_3^2}{\Omega_2^2 - \Omega_3^2}\right)$$
$$-A + \frac{U}{\sqrt{\pi D_{12}(0)}} \tag{11a}$$

where

$$A = \frac{4\alpha}{\pi}\int_0^\infty \mathrm{d}t \int_0^{k_0} k^3 \,\mathrm{d}k\; e^{-kt}\left(e^{-k^2 D_{11}(t)} + e^{-k^2 D_{12}(t)}\right) \tag{11b}$$

with $U = e^2/\hbar\epsilon_0 s$ and where dimensionless units have been used. In equation (11*b*) we introduced the functions

$$D_{1j}(t) = \frac{w^2}{\Omega_1^2}\frac{t}{4} + \frac{\Omega_1^2 - w^2}{\Omega_1^2}\frac{1-\mathrm{e}^{-\Omega_1 t}}{4\Omega_1} + \frac{\Omega_2^2 - w^2}{\Omega_2^2 - \Omega_3^2}\frac{1+(-1)^j\mathrm{e}^{-\Omega_2 t}}{4\Omega_2}$$
$$+\frac{w^2 - \Omega_3^2}{\Omega_2^2 - \Omega_3^2}\frac{1+(-1)^j\mathrm{e}^{-\Omega_3 t}}{4\Omega_3} \qquad j = 1, 2. \tag{12}$$

In general the integral in equation (11*a*) has to be calculated numerically, and subsequently E_{bip} has to be minimized with respect to the four variational parameters $(w, \Omega_1, \Omega_2, \Omega_3)$.

In previous work by Hiramoto and Toyozawa [12] the above system was studied in the case in which the electron interacted with both acoustical and optical phonons. Here, we are interested in the limiting case of pure acoustical phonon interaction. As it turns out, this allows us to pinpoint the driving mechanism for bipolaron formation and to present explicit analytic expressions for the polaron–bipolaron phase boundary which were not present in [12].

In the strong-coupling limit it is possible to obtain the analytic behaviour of equation (11*a*). In this limit we have $\Omega_1/w \gg 1$, $\Omega_2 \approx \Omega_1$ and $\Omega_3 \approx w$, and consequently $D_{11}(t) = D_{12} \approx 1/2\Omega_1$. After a variational calculation one finds

$$\Omega_1 \approx \sqrt{\frac{8\alpha k_0^5}{15\pi}}\left(1 - \frac{U}{3\sqrt{2\pi}}\left(\frac{15\pi}{8\alpha k_0^5}\right)^{1/4}\right) \tag{13}$$

which leads to in the ground-state energy

$$E_{bip} \approx -\frac{8\alpha k_0^3}{3\pi} + 2\left(\frac{2\alpha k_0^5}{15\pi^3}\right)^{1/4} U + \frac{2}{5}\sqrt{\frac{30\alpha k_0^5}{\pi}}. \tag{14}$$

In order to calculate the bipolaron transition we have to compare the bipolaron energy with the energy of two separate polarons which are infinitely far apart. This limit is contained in equation (11*a*) and is obtained by choosing $\kappa' = K = 0$ and $U = 0$. Now only two variational parameters, Ω_1 and w, are left. The resulting upper bound E_{pol} to the ground-state energy [8] is given by

$$E_{pol} = \frac{3(\Omega_1 - w)^2}{4\Omega_1} - \frac{2\alpha}{\pi}\int_0^\infty \mathrm{d}t \int_0^{k_0} \mathrm{d}k\; k^3\mathrm{e}^{-kt}\mathrm{e}^{-k^2 D(t)} \tag{15}$$

where

$$D(t) = \frac{w^2}{2\Omega_1^2}t + \frac{\Omega_1^2 - w^2}{2v^3}(1 - \mathrm{e}^{-\Omega_1 t}). \tag{16}$$

In [8] it was shown that in the weak-coupling limit $\Omega_1/w \to 1$, the polaron self-energy can be obtained from equation (15):

$$E_{pol} \approx -\frac{2\alpha}{\pi}\left[k_0^2 - 4k_0 + 8\ln\left[1 + \frac{k_0}{2}\right]\right]. \tag{17}$$

In the strong-coupling limit one has $\Omega_1 \gg w$ which leads to the results

$$E_{pol} \approx -\frac{2\alpha}{3\pi}k_0^3 + \left[\frac{3\alpha}{5\pi}\right]^{1/2} k_0^{5/2}. \tag{18}$$

The bipolaron transition occurs when $E_{bip} = 2E_{pol}$. In the strong-coupling limit, and when the polarons are self-trapped we find from equations (14) and (18) the approximate condition for the bipolaron transition:

$$U_c \approx \frac{2\alpha k_0^2}{3}\left(\frac{15}{2\pi\alpha k_0}\right)^{1/4} + k_0\left(1-\sqrt{2}\right)\left(\frac{27}{10}\pi\alpha k_0\right)^{1/4}. \tag{19}$$

For fixed k_0 this leads to a non-linear relation between the Coulomb repulsion U and the electron–phonon coupling strength α. When the bipolaron transition occurs from two polarons which are in the quasi-free state we have to compare equations (14) and (17). For large k_0, this leads to the following equation:

$$\alpha \approx 2.121\frac{1}{k_0} + (1.456U + 6.362)\frac{1}{k_0^2} + (3.276U + 14.314)\frac{1}{k_0^3} + \mathrm{O}\left(\frac{1}{k_0^4}\right). \tag{20}$$

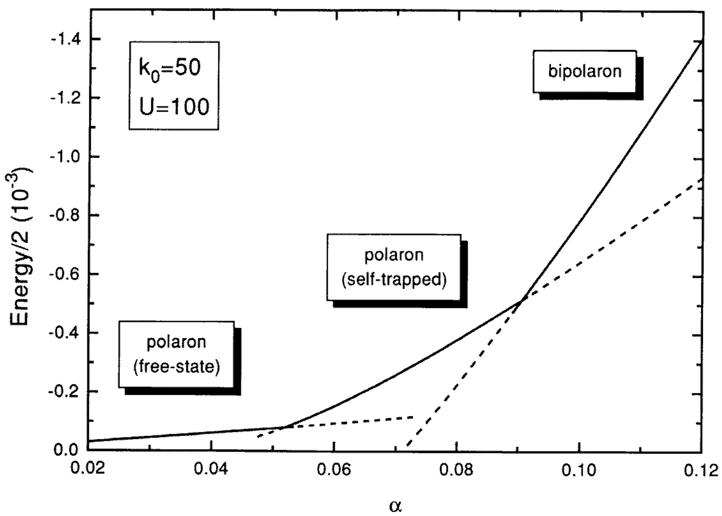

Figure 2. The ground-state energy as a function of the electron–phonon coupling constant α for a cut-off $k_0 = 50$ and Coulomb repulsion $U = 100$.

4. Numerical results

In this section we calculate the bipolaron and polaron energy numerically and perform a numerical minimization in order to find the optimal polaron and bipolaron energy. A typical result for the energy per polaron as a function of α is shown in figure 2 for $k_0 = 50$ and fixed repulsion $U = 100$. The corresponding one-polaron mass is plotted in figure 3. Note that there are two transition points. For small α we have two separate quasi-free polarons each with an effective mass which is slightly larger than 1, i.e. the free-electron mass. With increasing α, we notice that for $\alpha = 0.052$ the self-trapped polaron has a lower energy and the stable state consists of two heavy polarons which are infinitely far apart. Within the present Feynman type of approach the self-trapped polaron is still mobile and has an effective mass which is more than two orders of magnitude larger than the bare electron mass. When we further increase α, the polaron self-energy increases continuously until $\alpha = 0.091$ at which point the bipolaron state has lower energy and consequently is the

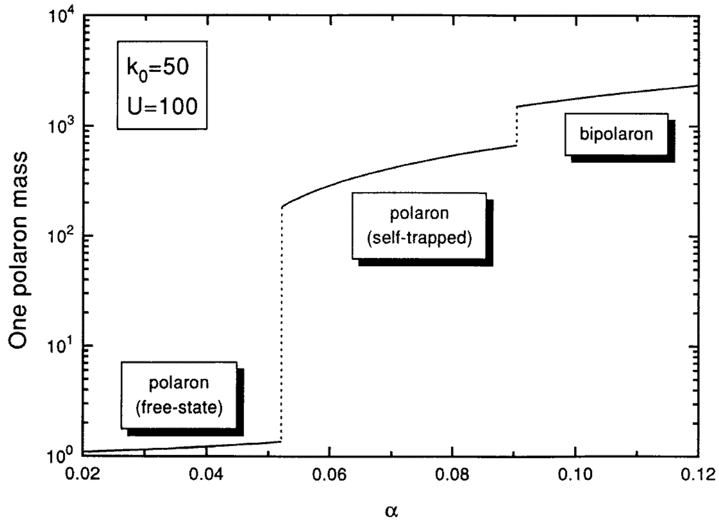

Figure 3. The one-polaron mass, $\frac{1}{2}\Omega_1^2/w^2 = (M+m)/2m$, of the electron–phonon coupling constant α for cut-off $k_0 = 50$ and $U = 100$.

stable state. From figure 3 we note that the *one*-polaron mass increases by almost a factor of two when the two polarons form the bipolaron state. Also in this case the bipolaron system is still mobile but with a very large mass. We would like to point out that the three energy curves in figure 2 are results from the minimization of only one expression, namely equation (11*a*). The dashed curves in figure 2 indicate the metastable states. Note that the first derivative of the energy as a function of α is discontinuous at both transition points, and consequently they are of first order.

In figure 4 we present the phase diagram for the two-electron–acoustical-polaron problem in three dimensions for a fixed value of the cut-off $k_0 = 50$. The phase diagram exhibits three possible states for this system. The constant curve ($\alpha = 0.052$) separates the single-polaron regions where the acoustical polaron is in the quasi-free state, $\alpha < 0.052$, and in the self-trapped state, $\alpha > 0.052$. The self-trapping transition of the acoustical polaron occurs when the polaron ground-state energy in the self-trapped state becomes equal to the ground-state energy in the quasi-free state. In this phase diagram, there is also a second transition, which is connected to the bipolaron state. Note the remarkable result that for sufficiently small U, i.e. $U < 50.05$, bipolaron formation can occur before the individual polarons are self-trapped. Thus for $U < 50.05$ the bipolaron state is formed out of two quasi-free polarons.

Next let us investigate the k_0-dependence of the phase diagram. We consider the extreme case in which there is no Coulomb repulsion between the electrons, i.e. $U = 0$. In the optical bipolaron case [4] it was found that for such a system the bipolaron state is always the most stable state, irrespective of the value of α. For the present system under study this is not the case as is illustrated in figure 5, where we plot the phase diagram for bipolaron formation in the $(1/k_0, \alpha)$ parameter space. Notice that for every k_0-value there is a critical α_c such that bipolarons will only be stable when $\alpha > \alpha_c$. This critical value α_c decreases with increasing k_0. Notice also that the bipolaron region is always bounded by the quasi-free-polarons region and consequently, in the absence of any Coulomb repulsion, in the present two-electron system the one-polaron self-trapping transition will not occur. This is

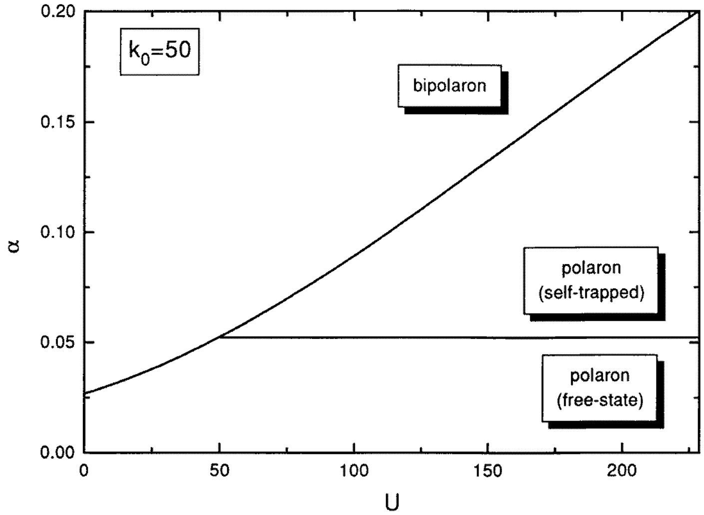

Figure 4. A phase diagram for the self-trapping transition of the acoustical-polaron–bipolaron with $k_0 = 50$.

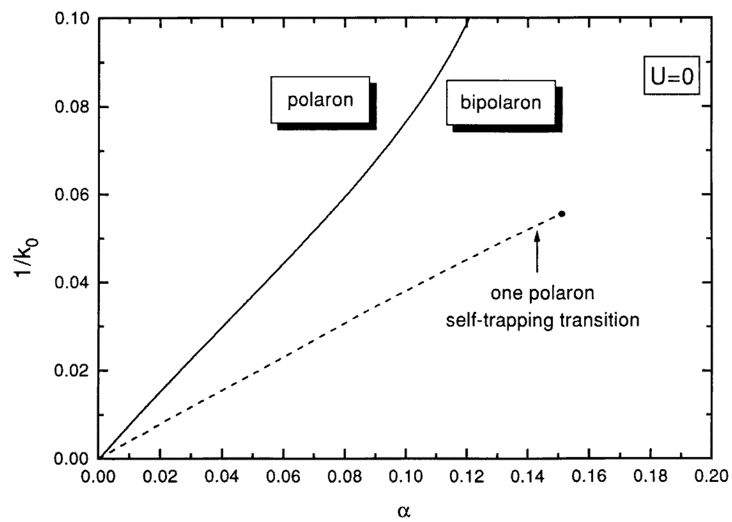

Figure 5. A phase diagram for the self-trapping transition of the acoustical-polaron–bipolaron as a function of α, in the absence of Coulomb repulsion.

also illustrated in figure 6 where we show the ground-state energy as a function of α for the case where $k_0 = 15$ and $U = 0$. In this case there is no discontinuous one-polaron self-trapping transition and we observe only the discontinuous bipolaron transition. In the inset of figure 6 the effective mass is plotted; it exhibits a jump at the bipolaron transition point.

Figure 7 illustrates the decrease of the bipolaron region in the $(1/k_0, \alpha)$ plane with increasing U. Note also that the one–polaron region becomes more interesting with

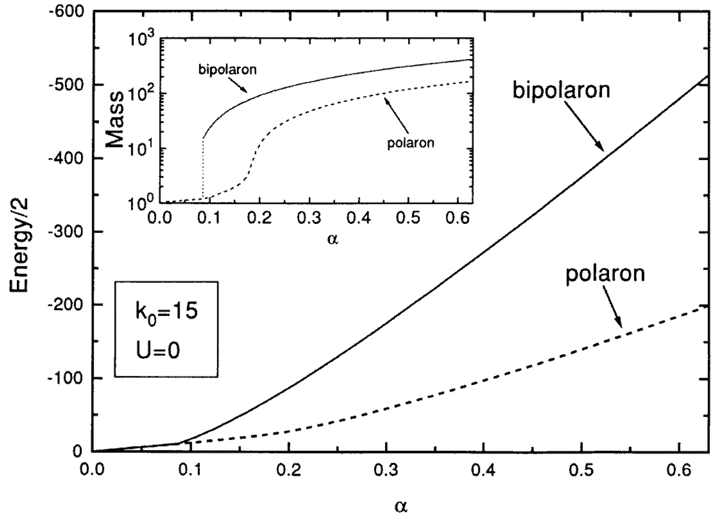

Figure 6. The ground-state energy as a function of the electron–phonon coupling constant α for cut-off $k_0 = 15$ and Coulomb repulsion $U = 0$. In the inset we show the corresponding one-polaron mass.

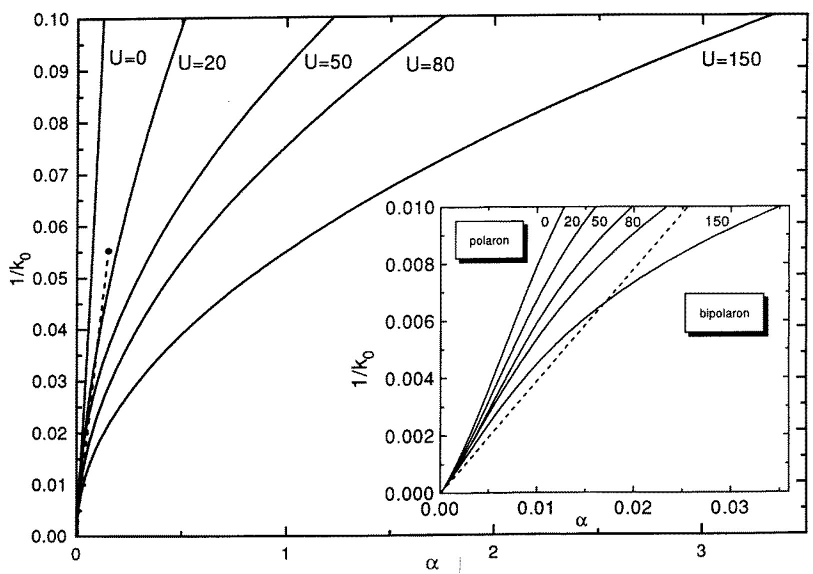

Figure 7. A phase diagram for the self-trapping $(1/k_0, \alpha)$ transition of the acoustical-polaron–bipolaron as function of α, for different values of the Coulomb repulsion U.

increasing U because it now exhibits a one-polaron self-trapping transition. The region for small α is enlarged in the inset of figure 7. The portion of the solid curves above the dashed curve, i.e. the one-polaron self-trapping transition, is well described by equation (20).

5. Conclusion

In the present work we used the Feynman path integral method to study the ground-state properties of the system of two electrons moving in three dimensions which interact with each other via the Coulomb force and through acoustical phonons. We determined the phase diagram for bipolaron formation and found it to be much richer than the equivalent case of optical bipolarons. In the present case there is an interesting interplay between quasi-free polarons, self-trapped polarons and bipolarons which is absent in the optical case.

We investigated the possibility of acoustical bipolaron formation in two different systems. For the La_2CuO_4 system it was found [4] that the optical three-dimensional bipolaron did not exist. In order to determine the relevant parameters for the acoustical interaction we used $m = 23m_e$, $s = 5.6 \times 10^5$ m s^{-1}, $\rho = 5.8$ g cm^{-3}, and $\epsilon_0 = 50$ [13]. Consequently, the coupling constant $\alpha = 1.18$ and the cut-off in units of $\hbar/ms$ is $k_0 = 5.24$. When we insert the relevant quantities $\alpha k_0 = 6.18$ and $U = 7.82$ into equation (19) we find that *single* bipolarons in La_2CuO_4 can exist. Of course, other effects like many-particle effects, screening, and quasi-two-dimensional behaviour of the carriers, which are present in a real material and which were not included in the present analysis, may change this conclusion.

For the alkali halides, as an example we took NaCl, which has a lattice constant of $a = 5.6$ Å; the energy unit is $ms^2 = 0.57$ meV, and the length unit is $\hbar/ms = 556$ Å. Moreover, $k_0 = 310$, $\alpha = 7.7 \times 10^{-4}$ and $U = 83.33$. Consequently the product $\alpha U = 0.064$ is too small for there to be bipolarons. In [8] it was found that for NaCl the product $\alpha k_0 = 0.24$ was too small for there to be self-trapping of electrons. However, the holes in some alkali halides are found experimentally to be self-trapped. This can be explained by the fact that the effective mass of holes is a factor of 3–4 times larger than those of the electrons which gives the result $\alpha = 6.95 \times 10^{-3}$. Consequently the product $\alpha k_0 = 2.15$ is sufficiently large to have self-trapping of *single* polarons. Using equation (19) we found that hole bipolarons are not stable.

Acknowledgments

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