Large bipolarons in two and three dimensions

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Feynman path-integral techniques are used to study the large bipolaron system. A new trial action is introduced, which takes into account a nonzero average distance between the electrons. With this trial action, variational expressions are derived for the free energy for arbitrary electron-phonon interactions and spatial dimensions. For large interelectronic repulsions (twice) the Feynman upper bound for a single polaron is reobtained. Therefore it is possible to discuss the single-polaron–bipolaron transition within the same physical picture for both bipolarons and single polarons. Numerical results are presented for the case of LO-phonon interaction and a Coulombic repulsion between the electrons. For this system a scaling relation between the free energies in two (2D) and three dimensions (3D) is obtained. Bipolaron formation is only possible above a critical value for the coupling constant α_c, which is lower in two than in three dimensions (in 2D: $\alpha_c \approx 2.9$ and in 3D: $\alpha_c \approx 6.8$). This indicates more favorable conditions for bipolaron formation in two dimensions, which might be of relevance for the bipolaron model of high-T_c superconductivity. The single-polaron–bipolaron transition behaves much like a first-order phase transition.

I. INTRODUCTION

Bipolaron formation has been put forward as a possible pairing mechanism for superconductivity.[1] Bipolarons are a generalization of the polaron concept to the case where two electrons (instead of one) interact with the surrounding lattice of the solid and with each other. In the literature, one distinguishes between the so-called *small* and *large* bipolarons, depending on whether the single polarons would have a localized state (small polaron) or an extended state (large polaron). Recently, Emin[2] proposed Bose-Einstein condensation of large bipolarons into a superfluid as a possible mechanism for superconductivity in the new high-temperature superconductors.[3]

In this paper we will study the large bipolaron. Early studies,[4] within the Hamiltonian formalism, indicated quite large regions in which bipolaron formation would be possible. The ground-state energy for single-polaron formation, however, was taken within the proposed models and poorly compared to existing path-integral studies.[5,6] Adamowski[7] introduced a singlet ground state and performed a numerical minimization of the ground-state energy. He found a very narrow region where bipolaron formation is possible. His formulation is restricted to the zero-temperature case and it does not give a value for the effective mass of the bipolaron. Another drawback of this operator formulation is that it does not permit us to study the single-polaron–bipolaron transition since the estimations of the single-polaron energies are poor compared to path-integral calculations. Adamowski resolved this by comparing his bipolaron ground-state energy with path-integral results for the (single) polaron ground-state energy. Recently Bassani *et al.*[8] extended the work of Adamowski and introduced a translational invariant trial wave function. They found that large bipolarons can be mobile and that bipolaron formation is easier in two dimensions than in three dimensions. Mitra[9] gives a simple criterion on $\epsilon_0/\epsilon_\infty$ for bipolaron formation. Hiramoto and Toyozawa[10] have treated the problem with path integrals. Their system includes a Coulombic repulsion between the electrons together with an interaction between the electrons and two types of phonons (longitudinal optical and acoustical). Their results apply to a three-dimensional (3D) system.

In this paper we will apply the path-integral method which allows for an *exact* elimination of the phonon coordinates. The electrons are treated as distinguishable particles and their spin degrees of freedom are neglected. The electron-lattice interaction is included in the form proposed by Fröhlich.[11] It is well known that, even in the single-polaron case, this problem cannot be solved exactly. Our approach, therefore, relies on the path-integral technique in conjunction with the Feynman-Jensen inequality, which will provide us with an upper bound to the exact ground state. This upper bound will be derived for the case of a general electron-phonon interaction and for an arbitrary electron-electron interaction. In general, we find an attraction between the electrons as a result of the electron-phonon interaction. The competition between this mechanism and the (repulsive) electron-electron interaction determines whether or not bipolarons can exist. For large repulsive forces between the electrons, we reobtain Feynman's expression for the ground-state energy of two single polarons.

Although our treatment of the problem is valid for arbitrary temperature, we limit our numerical results to the important case of zero temperature. Only the interaction with the longitudinal-optical (LO) phonons is considered and the interaction between the electrons is taken as

purely Coulombic. The proposed trial action is a generalization of Hiramoto and Toyozawa's. Furthermore, our trial action is translational invariant which ensures conservation of the total linear momentum. Hiromato and Toyozawa's results are, analytically, obtained as a limiting case. Our numerical minimization also leads to these limits. We also find a *scaling relation* between the 3D and 2D results. Two relevant parameters determine the bipolaron formation: (a) the electron-phonon coupling constant α, which measures the attractive part, and (b) the strength U of the Coulomb repulsion. Since both parameters are related to the static and high-frequency dielectric constants of the crystal (ϵ_0 and ϵ_∞, respectively), only the part $U \geq \sqrt{2}\alpha$ of the (α, U) space has physical significance. We find (a) that the nonphysical region is entirely bipolaronic, and (b) that below a critical value α_c, the bipolaron-single-polaron transition is continuous and occurs at $U=\sqrt{2}\alpha$. For $\alpha > \alpha_c$, bipolaron formation is discontinuous, analogous to a first-order phase transition, and occurs in the physical region of the (α, U) space. Thus, for $\alpha > \alpha_c$, bipolarons start to exist in physical space and the transition becomes discontinuous in the derivative of the energy.

II. THE BIPOLARON SYSTEM

The bipolaron system consists of two electrons in interaction with a phonon field and is described by the following Hamiltonian:

$$H=\sum_{j=1,2}\left[\frac{\mathbf{p}_j^2}{2m}+\sum_{\mathbf{k}}(V_{\mathbf{k}}a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}_j}+V_{\mathbf{k}}^{*}a_{\mathbf{k}}^{\dagger}e^{-i\mathbf{k}\cdot\mathbf{r}_j})\right]+\sum_{\mathbf{k}}\hbar\omega_{\mathbf{k}}a_{\mathbf{k}}a_{\mathbf{k}}^{\dagger}+U(\mathbf{r}_1-\mathbf{r}_2)\,, \tag{1}$$

where we neglected the spin degrees of freedom of the electrons. $\mathbf{r}_j$ ($\mathbf{p}_j$) is the position (momentum) operator of the jth electron ($j=1,2$), m is the electron band mass, $U(\mathbf{r})$ is the repulsive potential between the electrons, $a_{\mathbf{k}}^{\dagger}$ ($a_{\mathbf{k}}$) is the creation (annihilation) operator for a phonon with wave vector $\mathbf{k}$ and frequency $\omega_{\mathbf{k}}$, $V_{\mathbf{k}}$ is the electron-phonon interaction coefficient, and the crystal volume will be denoted by V. The general formalism will be constructed without any reference to the specific $\mathbf{k}$ dependence of $\omega_{\mathbf{k}}$ and $V_{\mathbf{k}}$ or form of $U(\mathbf{r})$. Furthermore, the number of spatial dimensions will be taken as general and denoted by d.

All thermodynamic quantities are known if we can calculate the partition sum $Z=\mathrm{Tr}(e^{-\beta H})$, where $\beta=1/k_B T$ is the inverse temperature. Within the framework of Feynman path integrals, the phonon degrees of freedom can be eliminated exactly[5] $Z=Z_{\mathrm{ph}}Z_{\mathrm{bip}}$, where

$$Z_{\mathrm{ph}}=\prod_{\mathbf{k}}[2\sinh(\hbar\omega_{\mathbf{k}}\beta/2)]^{-d}$$

is the partition sum of the free-phonon system. The *bipolaron* partition sum Z_{bip} is a path integral in only the electron coordinates

$$Z_{\mathrm{bip}}=\prod_{j=1,2}\left[\int d\mathbf{x}_j\iint_{\mathbf{r}_j(0)=\mathbf{x}_j}^{\mathbf{r}_j(\beta)=\mathbf{x}_j}\mathcal{D}\mathbf{r}_j(t)\right]e^{S[\mathbf{r}_1(t),\mathbf{r}_2(t)]}\,. \tag{2}$$

Formally, the electrons undergo interactions nonlocal in time, governed by the action

$$S[\mathbf{r}_1(t),\mathbf{r}_2(t)]=-\int_0^\beta dt\{\tfrac{1}{2}m\dot{\mathbf{r}}_1(t)^2+\tfrac{1}{2}m\dot{\mathbf{r}}_2(t)^2+U[\mathbf{r}_1(t)-\mathbf{r}_2(t)]\}+\sum_{j,l=1,2}\sum_{\mathbf{k}}|V_{\mathbf{k}}|^2\int_0^\beta dt\int_0^\beta ds\,G_{\omega_{\mathbf{k}}}(t-s)e^{i\mathbf{k}\cdot[\mathbf{r}_j(t)-\mathbf{r}_l(s)]} \tag{3}$$

with the phonon Green's function

$$G_\Omega(u)=\cosh[\hbar\Omega(\beta/2-|u|)]/2\sinh(\hbar\Omega\beta/2)\,.$$

In Eq. (3) there is a competition between the direct interelectronic repulsion and a retarded attraction, which stems from the elimination of the phonon coordinates.

The resulting path integral of Eq. (2) cannot be solved analytically. Therefore, the Feynman variational principle[5] is used. This gives an upper bound to the free energy $F_{\mathrm{bip}}=-\ln(Z_{\mathrm{bip}})/\beta$ in terms of an arbitrary trial action S_t

$$F_{\mathrm{bip}}\leq F_t-\frac{1}{\beta}\langle S-S_t\rangle\,, \tag{4}$$

where F_t ($Z_t=e^{-\beta F_t}$) is the free energy (partition function) corresponding to the trial action S_t, and $\langle\cdots\rangle$ denotes an average with weight e^{S_t} defined as

$$\langle A\rangle=\frac{1}{Z_t}\prod_{j=1,2}\left[\int d\mathbf{x}_j\iint_{\mathbf{r}_j(0)=\mathbf{x}_j}^{\mathbf{r}_j(\beta)=\mathbf{x}_j}\mathcal{D}\mathbf{r}_j(t)\right]Ae^{S_t[\mathbf{r}_1(t),\mathbf{r}_2(t)]}\,. \tag{5}$$

III. THE MODEL SYSTEM AND THE CORRESPONDING TRIAL ACTION

We propose a four-particle model to simulate the bipolaron system. The trial action S_t will be obtained after the elimination of extra oscillator variables from S_m. In analogy with the Feynman model for a free polaron,[5] each electron interacts quadratically with a fictitious particle of mass M and oscillator strength κ. Furthermore, we also allow for a quadratic interaction, with an oscillator strength κ', between each electron and the oscillator of the other electron. The two electrons fluctuate around a mean distance $\mathbf{a}$ from each other. The Coulomb repulsion between the electrons is approximated by a quadratic repulsion with strength K. Thus, the model is determined by the parameters M, κ, κ', K, and the vector $\mathbf{a}$.

The Hamiltonian describing this model is

$$H_m=\sum_{j=1,2}\left[\frac{\mathbf{p}_j^2}{2m}+\frac{\mathbf{P}_j^2}{2M}+\frac{\kappa}{2}(\mathbf{r}_j-\mathbf{R}_j)^2\right]+\frac{\kappa'}{2}[(\mathbf{r}_1-\mathbf{R}_2-\mathbf{a})^2+(\mathbf{R}_1-\mathbf{r}_2-\mathbf{a})^2]-\frac{K}{2}(\mathbf{r}_1-\mathbf{r}_2-\mathbf{a})^2\ , \tag{6}$$

which is translational invariant and quadratic. The latter implies that it can be solved exactly. The center-of-mass motion is free and after a normal-mode analysis we find three eigenfrequencies which are associated with the internal degrees of freedom

$$\begin{aligned}\Omega_1^2&=\frac{M+m}{Mm}(\kappa+\kappa')\ ,\\ \Omega_{2,3}^2&=\frac{1}{2}\left\{\frac{M+m}{Mm}(\kappa+\kappa')-\frac{2K}{m}\pm\left[\left[\frac{M-m}{Mm}(\kappa+\kappa')-\frac{2K}{m}\right]^2+\frac{4}{Mm}(\kappa-\kappa')^2\right]^{1/2}\right\}.\end{aligned} \tag{7}$$

These eigenfrequencies satisfy the following inequalities: $\Omega_1^2\geq\Omega_2^2+\Omega_3^2$ and $\Omega_2\geq\nu\geq\Omega_3\geq 0$, where $\nu=[(\kappa+\kappa')/M]^{1/2}$ is the frequency of the free oscillator (analogous to the Feynman parameter w in the single-polaron problem). The partition sum $Z_m=\mathrm{Tr}(e^{-\beta H_m})$ of this model system can easily be derived and we found

$$Z_m=V\left[\frac{2m(\Omega_1/\nu)^2}{2\pi\hbar^2\beta}\right]^{d/2}\prod_{j=1}^{3}\left[2\sinh\left[\frac{\hbar\Omega_j\beta}{2}\right]\right]^{-d}. \tag{8}$$

The total mass of the model is given by $2(M+m)=2m(\Omega_1^2/\nu^2)$. Note that the eigenfrequencies and the partition sum Z_m do not depend on the average separation $\mathbf{a}$ between the electrons.

The action S_m corresponding to the model Hamiltonian H_m is

$$\begin{aligned}S_m[\mathbf{R}_1(t),\mathbf{R}_2(t),\mathbf{r}_1(t),\mathbf{r}_2(t)]=\int_0^\beta dt\Bigg[&\sum_{j=1,2}\left[\frac{m}{2}\dot{\mathbf{r}}_j(t)^2+\frac{m}{2}\dot{\mathbf{R}}_j(t)^2+\frac{\kappa}{2}[\mathbf{r}_j(t)-\mathbf{R}_j(t)]^2\right]\\&+\frac{\kappa'}{2}\{[\mathbf{r}_1(t)-\mathbf{R}_2(t)-\mathbf{a}]^2+[\mathbf{R}_1(t)-\mathbf{r}_2(t)-\mathbf{a}]^2\}-\frac{K}{2}[\mathbf{r}_1(t)-\mathbf{r}_2(t)-\mathbf{a}]^2\Bigg]\ .\end{aligned} \tag{9}$$

In analogy with the elimination of the phonon variables, the oscillator coordinates $\mathbf{R}_j$ can be eliminated to construct the trial action S_t in the following way:

$$\prod_{j=1,2}\left[\int d\mathbf{X}_j\iint_{\mathbf{R}_j(0)=\mathbf{X}_j}^{\mathbf{R}_j(\beta)=\mathbf{X}_j}\mathcal{D}\mathbf{R}_j(t)\right]e^{S_m[\mathbf{R}_1(t),\mathbf{R}_2(t),\mathbf{r}_1(t),\mathbf{r}_2(t)]}=Z_{\mathrm{osc}}e^{S_t[\mathbf{r}_1(t),\mathbf{r}_2(t)]} \tag{10}$$

with $Z_{\mathrm{osc}}=[2\sinh(\hbar\nu\beta/2)]^{-2d}$ denoting the partition sum of the free oscillators. Such a construction leads to the trial action

$$\begin{aligned}S_t[\mathbf{r}_1(t),\mathbf{r}_2(t)]=&-\int_0^\beta dt\{\tfrac{1}{2}m\dot{\mathbf{r}}_1(t)^2+\tfrac{1}{2}m\dot{\mathbf{r}}_2(t)^2-\tfrac{1}{2}K[\mathbf{r}_1(t)-\mathbf{r}_2(t)-\mathbf{a}]^2\}\\&-\int_0^\beta dt\int_0^\beta ds\,G_\nu(t-s)\left[\frac{\hbar(\kappa^2+\kappa'^2)}{4M\nu}\sum_{j=1,2}[\mathbf{r}_j(t)-\mathbf{r}_j(s)]^2+\frac{\hbar\kappa\kappa'}{M\nu}[\mathbf{r}_1(t)-\mathbf{r}_2(s)-\mathbf{a}]^2\right],\end{aligned} \tag{11}$$

where the electrons now exhibit a quadratic attractive self-interaction. The electrons are bound together at an average distance $|\mathbf{a}|$ if the retarded interaction is larger than the direct quadratic repulsion, which is governed by the constant K.

In Eq. (4) we need the partition sum Z_t of the trial action which is found to be equal to

$$\begin{aligned}Z_t&=\prod_{j=1,2}\left[\int d\mathbf{x}_j\iint_{\mathbf{r}_j(0)=\mathbf{x}_j}^{\mathbf{r}_j(\beta)=\mathbf{x}_j}\mathcal{D}\mathbf{r}_j(t)\right]e^{S_t[\mathbf{r}_1(t),\mathbf{r}_2(t)]}\\&=\frac{Z_m}{Z_{\mathrm{osc}}}=V\left[\frac{2m(\Omega_1/\nu)^2}{2\pi\hbar^2\beta}\right]^{d/2}[2\sinh(\hbar\nu\beta/2)]^{+2d}\\&\quad\times\prod_{j=1}^{3}\left[2\sinh\left[\frac{\hbar\Omega_j\beta}{2}\right]\right]^{-d}.\end{aligned} \tag{12}$$

A central quantity needed in the evaluation of $\langle S\rangle_t$ in Eq. (4) is the correlation function

$$\langle e^{i\mathbf{k}\cdot[\mathbf{r}_j(t)-\mathbf{r}_l(s)]}\rangle_t\ ,$$

which is the Fourier transform of the position correlation function of electron j at time t and electron l at time s

$$\begin{aligned}\langle e^{i\mathbf{k}\cdot[\mathbf{r}_1(t)-\mathbf{r}_1(s)]}\rangle&=\langle e^{i\mathbf{k}\cdot[\mathbf{r}_2(t)-\mathbf{r}_2(s)]}\rangle=e^{-\mathbf{k}^2D_{11}(|t-s|)}\ ,\\ \langle e^{i\mathbf{k}\cdot[\mathbf{r}_1(t)-\mathbf{r}_2(s)]}\rangle&=\langle e^{i\mathbf{k}\cdot[\mathbf{r}_2(t)-\mathbf{r}_1(s)]}\rangle^*=e^{i\mathbf{k}\cdot\mathbf{a}}e^{-\mathbf{k}^2D_{12}(|t-s|)}\ .\end{aligned} \tag{13}$$

We found the following expressions for the D functions:

$$D_{11}(u)=\frac{\hbar}{2m}\left[\frac{\nu^2}{\Omega_1^2}\hbar\frac{u}{2}\left[1-\frac{u}{\beta}\right]+\frac{\Omega_1^2-\nu^2}{\Omega_1^2}E(\Omega_1,\beta,u)+\frac{\Omega_2^2-\nu^2}{\Omega_2^2-\Omega_3^2}E(\Omega_2,\beta,u)+\frac{\nu^2-\Omega_3^2}{\Omega_2^2-\Omega_3^2}E(\Omega_3,\beta,u)\right],$$

$$D_{12}(u)=\frac{\hbar}{2m}\left[\frac{\nu^2}{\Omega_1^2}\hbar\frac{u}{2}\left[1-\frac{u}{\beta}\right]+\frac{\Omega_1^2-\nu^2}{\Omega_1^2}E(\Omega_1,\beta,u)+\frac{\Omega_2^2-\nu^2}{\Omega_2^2-\Omega_3^2}F(\Omega_2,\beta,u)+\frac{\nu^2-\Omega_3^2}{\Omega_2^2-\Omega_3^2}F(\Omega_3,\beta,u)\right], \tag{14}$$

where we defined the auxiliary functions

$$E(\Omega,\beta,u)=\frac{1}{\Omega}\sinh\left[\frac{\hbar\Omega u}{2}\right]\sinh\left[\frac{\hbar\Omega(\beta-u)}{2}\right]\Big/\sinh\left[\frac{\hbar\Omega\beta}{2}\right], \tag{15}$$

$$F(\Omega,\beta,u)=\frac{1}{\Omega}\cosh\left[\frac{\hbar\Omega u}{2}\right]\cosh\left[\frac{\hbar\Omega(\beta-u)}{2}\right]\Big/\sinh\left[\frac{\hbar\Omega\beta}{2}\right].$$

The mean-square separation r_{12} between the electrons is given by

$$r_{12}^2=\langle[\mathbf{r}_1(t)-\mathbf{r}_2(t)]^2\rangle=\mathbf{a}^2+2dD_{12}(0)=\mathbf{a}^2+\frac{d\hbar}{m\Omega_2}\frac{\Omega_2^2-\nu^2}{\Omega_2^2-\Omega_3^2}\coth\left[\frac{\hbar\Omega_2}{2}\beta\right]+\frac{d\hbar}{m\Omega_3}\frac{\nu^2-\Omega_3^2}{\Omega_2^2-\Omega_3^2}\coth\left[\frac{\hbar\Omega_3}{2}\beta\right]. \tag{16}$$

Note also that the average electron separation $\langle\mathbf{r}_1(t)-\mathbf{r}_2(t)\rangle=\mathbf{a}$, which can be nonzero in contrast to the model used in Ref. 10, which has $\langle\mathbf{r}_1(t)-\mathbf{r}_2(t)\rangle=\mathbf{0}$.

IV. AN UPPER BOUND TO THE FREE ENERGY

The Feynman variational principle is used to derive an upper bound to the exact free energy $F_{\rm bip}$ of the bipolaron:

$$F_{\rm bip}\le F_t-\frac{1}{\beta}\langle S-S_t\rangle .$$

In the previous section, the trial action S_t, Eq. (11), and the corresponding free energy F_t were introduced. Since $S-S_t$ involves no derivatives of $\mathbf{r}_j(t)$, the average $\langle S-S_t\rangle$ can be entirely expressed in terms of

$$\langle e^{i\mathbf{k}\cdot[\mathbf{r}_j(t)-\mathbf{r}_l(s)]}\rangle ,$$

Eq. (13), after making the suitable Fourier transformations.

After a tedious calculation, we obtain the following expression:

$$F_{\rm bip}\le\frac{d}{\beta}\sum_{j=1}^{3}\ln\left[2\sinh\left[\frac{\hbar\Omega_j\beta}{2}\right]\right]-\frac{2d}{\beta}\ln\left[2\sinh\left[\frac{\hbar\nu\beta}{2}\right]\right]-\frac{1}{\beta}\ln\left[V\left[\frac{2m(\Omega_1^2/\nu^2)}{2\pi\hbar^2\beta}\right]^{d/2}\right]$$
$$-\frac{d}{2}\left\{\frac{\Omega_1^2-\nu^2}{\Omega_1^2}\frac{\hbar\Omega_1}{2}\left[\coth\left[\frac{\hbar\Omega_1\beta}{2}\right]-\frac{2}{\hbar\Omega_1\beta}\right]+\frac{\Omega_2^2-\nu^2}{\Omega_2^2-\Omega_3^2}\frac{\hbar\Omega_2}{2}\coth\left[\frac{\hbar\Omega_2\beta}{2}\right]+\frac{\nu^2-\Omega_3^2}{\Omega_2^2-\Omega_3^2}\frac{\hbar\Omega_3}{2}\coth\left[\frac{\hbar\Omega_3\beta}{2}\right]\right\}$$
$$-2\int_0^\beta du\sum_{\mathbf{k}}|V_{\mathbf{k}}|^2G_{\omega_{\mathbf{k}}}(u)(e^{-\mathbf{k}^2D_{11}(u)}+e^{i\mathbf{k}\cdot\mathbf{a}}e^{-\mathbf{k}^2D_{12}(u)})+\sum_{\mathbf{k}}U_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{a}}e^{-\mathbf{k}^2D_{12}(0)}, \tag{17}$$

where the Fourier transform for the direct electron-electron repulsion is introduced $U(\mathbf{r})=\sum_{\mathbf{k}}U_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}$.

V. CALCULATIONS FOR LO PHONONS AND A COULOMB REPULSION

In this section we will limit ourselves to the specific case with only longitudinal optical phonons in three dimensions. The phonon frequencies are taken as dispersionless $\omega_{\mathbf{k}}=\omega_{\rm LO}$, and the interaction coefficients are

$$V_{\mathbf{k}}=-i\hbar\omega_{\rm LO}\left[\frac{4\pi\alpha}{k^2V}\left[\frac{\hbar}{2m\omega_{\rm LO}}\right]^{1/2}\right]^{1/2}$$

with

$$\alpha=\frac{1}{\hbar\omega_{\rm LO}}\frac{e^2}{2}\left[\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right]\left[\frac{2m\omega_{\rm LO}}{\hbar}\right]^{1/2}$$

the dimensionless Fröhlich coupling constant which depends on the static (ϵ_0) and high-frequency (ϵ_∞) dielectric constants. The interelectronic repulsion is taken to be an unscreened Coulomb potential $U(\mathbf{r})=U/r$, where $U>0$ is a measure for the strength of the repulsion. If no screening is taken into account, U is directly related to the dielectric constant ϵ_∞: $U=e^2/\epsilon_\infty$. In fact, a classical approximation to the LO-phonon interaction will replace $U=e^2/\epsilon_\infty$ by $U=e^2/\epsilon_0$ and is unable to give bipolarons. Here we will solve the problem more exactly and incorporate quantum mechanical corrections.

The exact action S of the bipolaron system, Eq. (3), takes now the form

$$S[\mathbf{r}_1(t),\mathbf{r}_2(t)]=-\int_0^\beta dt \sum_{j=1,2}\left[\frac{m}{2}\dot{\mathbf{r}}_j(t)^2-\alpha\int_0^\beta ds\frac{G_{\omega_{\rm LO}}(t-s)}{|\mathbf{r}_j(t)-\mathbf{r}_j(s)|}\right]+\int_0^\beta dt\left[\sqrt{2}\alpha\int_0^\beta ds\frac{G_{\omega_{\rm LO}}(t-s)}{|\mathbf{r}_1(t)-\mathbf{r}_2(s)|}-\frac{U}{|\mathbf{r}_1(t)-\mathbf{r}_2(t)|}\right], \tag{18}$$

where we use units $k_B=\hbar=m=\omega_{\rm LO}=1$ for convenience. We see that the attractive and the repulsive part have the same $1/r$ dependence as a function of the interelectronic distance.

The expression for the free energy, Eq. (17), now reduces to

$$\begin{aligned}F_{\rm bip}\le{}&\frac{3}{\beta}\sum_{j=1}^{3}\ln\left[2\sinh\left[\frac{\Omega_j\beta}{2}\right]\right]-\frac{6}{\beta}\ln\left[2\sinh\left[\frac{\nu\beta}{2}\right]\right]-\frac{1}{\beta}\ln\left[V\left[\frac{2(\Omega_1^2/\nu^2)}{2\pi\beta}\right]^{3/2}\right]\\&-\frac{3}{2}\left\{\frac{\Omega_1^2-\nu^2}{\Omega_1^2}\frac{\Omega_1}{2}\left[\coth\left[\frac{\Omega_1\beta}{2}\right]-\frac{2}{\beta\Omega_1}\right]+\frac{\Omega_2^2-\nu^2}{\Omega_2^2-\Omega_3^2}\frac{\Omega_2}{2}\coth\left[\frac{\Omega_2\beta}{2}\right]+\frac{\nu^2-\Omega_3^2}{\Omega_2^2-\Omega_3^2}\frac{\Omega_3}{2}\coth\left[\frac{\Omega_3\beta}{2}\right]\right\}\\&-\alpha\sqrt{2/\pi}\int_0^\beta du\,G_1(u)\left[\frac{1}{\sqrt{D_{11}(u)}}+\frac{1}{\sqrt{D_{12}(u)}}\chi\left[\frac{a}{2\sqrt{D_{12}(u)}}\right]\right]+\frac{U}{\sqrt{\pi D_{12}(0)}}\chi\left[\frac{a}{2\sqrt{D_{12}(0)}}\right],\end{aligned} \tag{19}$$

where the function $\chi(x)$ is defined as

$$\chi(x)=\frac{1}{x}\int_0^x dy\,e^{-y^2}=\frac{\sqrt{\pi}}{2x}\mathrm{erf}(x)\ , \tag{20}$$

which has the following limiting behavior:

$$\chi(x=0)=1$$

and (21)

$$\chi(x\to+\infty)\to 0\ .$$

An inspection of Eq. (19) reveals that, in the limit of infinite separation $|\mathbf{a}|\to\infty$, all terms representing the attraction as well as the repulsion between the electrons vanish. In this case, two independent single polarons are obtained. Hence, only an upper bound to (twice) the single-polaron ground-state energy will be found. The same limit is studied if the function $D_{12}(u)$ becomes infinitely large, we will comment on this in Sec. VII.

VI. A SCALING RELATION BETWEEN THE FREE ENERGIES OF 2D AND 3D BIPOLARONS

Because of the specific nature of the electron-phonon interaction introduced in the previous section, it was found[12] that, within the Feynman approximation, the 2D free energy of a *single polaron* can be obtained from the 3D result by scaling the electron-phonon coupling constant. In this section we will prove a similar scaling relation for the bipolaron system. The electron-phonon interaction coefficients in 2D are

$$V_k=-i\hbar\omega_{\rm LO}\left[\frac{2\pi\alpha}{Ak}\left[\frac{\hbar}{2m\omega_{\rm LO}}\right]^{1/2}\right]^{1/2},$$

where A is the crystal area. The repulsion between the electrons, however, remains of the 3D Coulombic type $U(\mathbf{r})=U/r$. Substitution of this expression in Eq. (17) leads to the following upper bound to the free energy:

$$\begin{aligned}F_{\rm bip}\le{}&\frac{2}{\beta}\sum_{j=1}^{3}\ln\left[2\sinh\left[\frac{\Omega_j\beta}{2}\right]\right]-\frac{4}{\beta}\ln\left[2\sinh\left[\frac{\nu\beta}{2}\right]\right]-\frac{1}{\beta}\ln\left[A\left[\frac{2(\Omega_1^2/\nu^2)}{2\pi\beta}\right]\right]\\&-\left\{\frac{\Omega_1^2-\nu^2}{\Omega_1^2}\frac{\Omega_1}{2}\left[\coth\left[\frac{\Omega_1\beta}{2}\right]-\frac{2}{\beta\Omega_1}\right]+\frac{\Omega_2^2-\nu^2}{\Omega_2^2-\Omega_3^2}\frac{\Omega_2}{2}\coth\left[\frac{\Omega_2\beta}{2}\right]+\frac{\nu^2-\Omega_3^2}{\Omega_2^2-\Omega_3^2}\frac{\Omega_3}{2}\coth\left[\frac{\Omega_3\beta}{2}\right]\right\}\\&-\alpha\sqrt{\pi/2}\int_0^\beta du\,G_1(u)\left[\frac{1}{\sqrt{D_{11}(u)}}+\frac{1}{\sqrt{D_{12}(u)}}\chi_{2D}\left[\frac{a}{\sqrt{8D_{12}(u)}}\right]\right]+\frac{\sqrt{\pi}}{2}\frac{U}{\sqrt{D_{12}(0)}}\chi_{2D}\left[\frac{a}{\sqrt{8D_{12}(0)}}\right],\end{aligned} \tag{22}$$

where the function $\chi_{2D}(x)$ is defined as

$$\chi_{2D}(x)=e^{-x^2}I_0(x^2)\ , \tag{23}$$

with $I_0(x)$ the modified Bessel function of the first kind and zeroth order. The function χ_{2D} has the following limiting behavior:

$$\chi_{2D}(x=0)=1$$

and (24)

$$\chi_{2D}(x\to+\infty)\to 0\ .$$

An inspection of Eq. (19) reveals that, in the limit of

infinite separation $|\mathbf{a}|\to\infty$, all terms which describe the interaction between the electrons approach zero and, consequently, a model system of noninteracting electrons is described in this limit.

In the important case, where $\mathbf{a}=\mathbf{0}$, a scaling relation can be derived for our results of the free energy between different dimensions. Denoting the upper bounds to the exact free energy by F_{2D} (F_{3D}) in two (respectively, three) dimensions, one notices the following relationship:

$$F_{2D}(\alpha,U,\beta)=\tfrac{2}{3}F_{3D}\left[\frac{3\pi}{4}\alpha,\frac{3\pi}{4}U,\beta\right]. \tag{25}$$

From now on we will discard the trivial volume- (area) dependent term.

This means that the (upper bound to the exact) free energy in two dimensions can be calculated from the (upper bound to the exact) free energy in three dimensions simply by scaling the coupling constant α as well as the repulsion strength U with a factor $3\pi/4$. Since the calculation of this upper bound requires the numerical minimalization of a four-parameter expression, Eq. (16), which includes a numerical integration, this scaling relation is found to be quite useful in practice.

VII. NUMERICAL RESULTS AND DISCUSSION

In this section numerical results are presented for the case of zero temperature, where the free energy equals the ground-state energy. A bipolaron is formed when our estimation for the bipolaron ground-state energy is lower than twice the ground-state energy for a single polaron.

The lowest free energies for single polarons are obtained within the general path-integral formalism by Adamowski *et al.*[13] They used an iterative procedure, starting from the Feynman expression.[5] These estimations were calculated for zero temperature and introduced small corrections ($\leq 1\%$) to the original estimations.

In this paper our main concern is to give a consistent description of the single polaron as well as the bipolaron within the same physical picture. Since it is possible to obtain the Feynman expression for the single-polaron free energy within our formalism, we will use this expression as our estimate for the single-polaron free energy. This procedure has the advantage that it is also applicable to nonzero temperatures. Therefore, we will first show how the Feynman expression for the single-polaron free energy can be obtained from Eq. (19). Then we discuss the estimate for the bipolaron free energy and the single-polaron–bipolaron transition.

Single polarons will occur if the repulsion U is large enough to inhibit bipolaron formation. If the limit $U\to\infty$ is taken, the upper bounds in Eqs. (19) and (22) will remain finite only if either $D_{12}(u=0)\to\infty$ or the function χ approaches zero. From Eq. (21), we find $\chi=0$ if its argument is infinite. This means $|\mathbf{a}|\to\infty$ or $D_{12}(u=0)=0$. The latter possibility is ruled out because of the inequality $\Omega_2\geq\nu\geq\Omega_3$. Let us now consider the case $D_{12}(u=0)\to\infty$, which is the only possibility when $\mathbf{a}=\mathbf{0}$. From Eq. (14) and in view of the inequalities for Ω_j and ν, we find that Ω_3 must be zero. This also follows from our physical model. If the bipolaron model represents two single polarons, there is translational invariance not only for the center of mass of the whole bipolaron system, but for each polaron separately. Consequently, the lowest bipolaron eigenfrequency (Ω_3) must be zero. Note that, in both cases, the mean-square separation r_{12} becomes infinity.

Numerically we found for large values of U that (i) $|\mathbf{a}|\to\infty$, (ii) $\Omega_1\to\Omega_2$, and (iii) $\Omega_3\to 0$. Comparing with the Feynman expression we note $\Omega_1=\Omega_2=v$ and $\nu=w$, where v and w are the Feynman variation parameters for the single-polaron free energy. Rewriting Eq. (19) with these values, one finds (twice) the Feynman upper bound to the free energy. This result verifies the correctness of our numerical procedures since it can also be imposed by putting the force constants K and κ' equal to zero in our model Hamiltonian. Note that, in this case, we have $\Omega_3=0$ and, hence, the parameter $\mathbf{a}$ is of no relevance. Numerically, however, the minimum upper bound to the free energy was obtained much faster if $\mathbf{a}$ was included as a variation parameter.

In units $\hbar=m=\omega_{LO}=k_B=1$, the coupling constant α and the repulsion U are given by

$$\alpha=\frac{e^2}{\sqrt{2}}\left[\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right] \tag{26}$$

and

$$U=\frac{e^2}{\epsilon_\infty}.$$

Because ϵ_0 is a positive quantity, we must demand $U\geq\sqrt{2}\alpha$ in order to have a physically meaningful model.

For small values of the coupling constant α, no bipolaron formation was found for $U\geq\sqrt{2}\alpha$. We also minimized the upper bound in the hypothetical region $U\leq\sqrt{2}\alpha$. Bipolaron formation was found to occur for the whole region $0\leq U\leq\sqrt{2}\alpha$. Thus, $U=\sqrt{2}\alpha$ is the

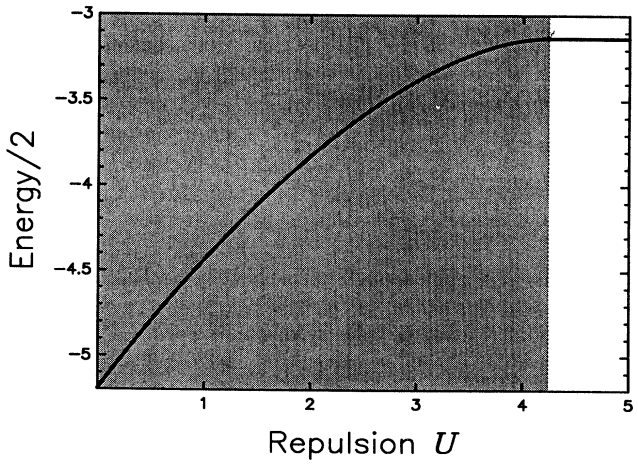

FIG. 1. The upper bound to the ground-state energy (3D) is plotted as a function of the repulsion U for a relatively weak coupling $\alpha=3$. Bipolaron formation is only possible in the nonphysical region $U\leq\sqrt{2}\alpha$ (shaded area).

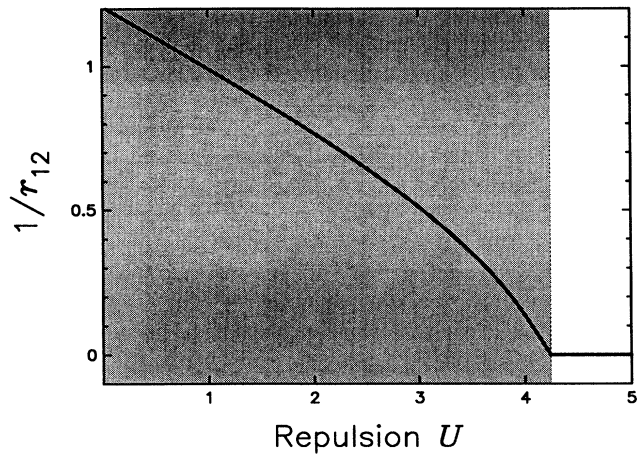

FIG. 2. The inverse mean-square distance $1/r_{12}$, as a function of the repulsion U for $\alpha=3$. The mean-square separation r_{12} is infinite throughout the entire physical space $U \geq \sqrt{2}\alpha$, where *single* polarons are more stable than bipolarons.

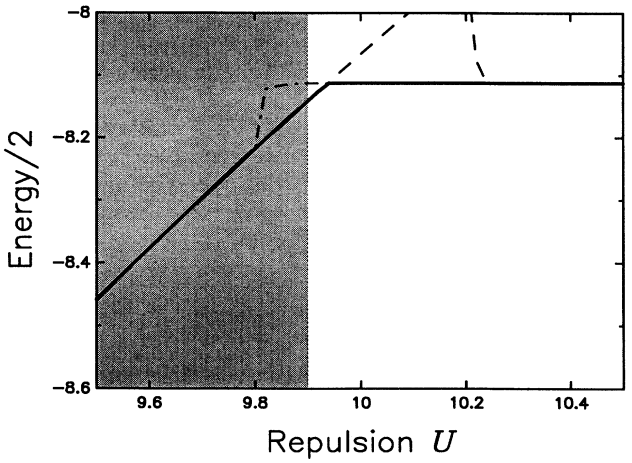

FIG. 4. The ground-state energy as a function of the repulsion U for a typical strong-coupling case: $\alpha=7$. Bipolaron formation is possible in the physical region (nonshaded area) below a critical value U_c.

critical value below which bipolarons can exist. As a typical value we will discuss $\alpha=3$. In Fig. 1, half the ground-state energy in units $\hbar\omega_{\mathrm{LO}}$ is plotted as a function of the repulsion U (while the coupling constant is kept fixed at $\alpha=3$). The shaded area represents the nonphysical region $U \leq \sqrt{2}\alpha$. In this region we find bipolaron formation since the energy is lower than the Feynman upper bound. In the physical region, however, the energy is equal to the Feynman upper bound and hence, no bipolaron is formed. Figure 2 shows, for the same values of U and α as in Fig. 1, the inverse of the mean-square separation $1/r_{12}$ in units of $\sqrt{m\omega_{\mathrm{LO}}/\hbar}$. As expected, r_{12} approaches infinity in the single-polaron region. When a bipolaron is formed, r_{12} has a finite value. We did not plot the separation $|\mathbf{a}|$ because its value was found to be zero when bipolaron formation occurs. In the single-polaron region, we have $\Omega_3=0$ and, hence, the parameter $\mathbf{a}$ is of no relevance. We plotted (half) the total mass $m+M$ of the model system in Fig. 3. Note how all three quantities, E, r_{12}, and $m+M$, are smooth functions of U, even at the critical value $U=\sqrt{2}\alpha$.

The latter is no longer true in the case of strong coupling. We will focus on $\alpha=7$ as a typical example. We find that bipolarons occur throughout the nonphysical region $U \leq \sqrt{2}\alpha$ and in the physical region below a certain value U_c. Two different local minima are found in the four-dimensional parameter space. One of them corresponds to the single-polaron case and is characterized by $\Omega_3=0$. The other minimum corresponds to the bipolaron

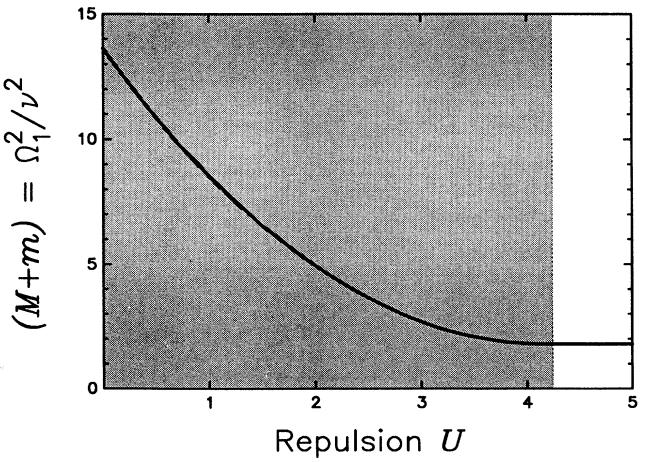

FIG. 3. The model bipolaron mass as a function of the repulsion U at fixed coupling constant $\alpha=3$. In the nonphysical region $U \leq \sqrt{2}\alpha$ (shaded area), the mass is enhanced because of bipolaron formation.

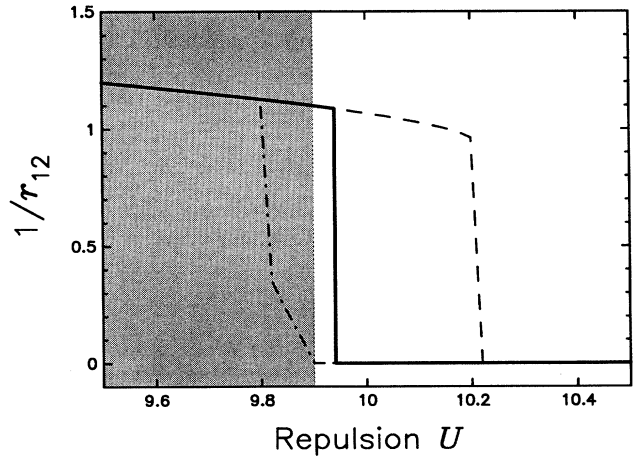

FIG. 5. The inverse mean-square distance $1/r_{12}$ as a function of the repulsion U for the strong-coupling value $\alpha=7$. The mean-square separation r_{12} remains finite for $U \leq U_c$ and jumps discontinuously to infinity at U_c where bipolaron formation is no longer energetically favorable.

state. Again it is characterized by $\mathbf{a}=\mathbf{0}$. In order to minimize the energy, only the lowest of the two minima has to be kept. This global minimum was found to jump from one local minimum to the other at a certain value U_c. As a consequence, the variation parameters exhibit abrupt changes. Because the different local minima represent physically different situations (single-polaron–bipolaron), a possible occurrence of discontinuous changes in certain physical quantities is to be expected. In order to compare this situation to the smooth behavior in the weak-coupling regime, we plot in Figs. 4–6 the same quantities as in Figs. 1–3. Throughout these three figures, dashed and dash-dotted curves are used to represent the quantities corresponding to the different local minima which represent metastable states. A solid curve is drawn for the global minimum. Whereas the energy (Fig. 4) itself is a continuous function of the repulsion U, its first derivative will be discontinuous. The mean-square separation r_{12} (Fig. 5) exhibits a sudden change from its finite value (in the bipolaron region) to infinity when entering the single-polaron region. Figure 6 shows an increase for the mass by almost a factor 3 for this choice of α.

Finally, we present the phase diagram for bipolaron formation in Fig. 7. As in Figs. 1–6, the shaded area represents the nonphysical part $U \leq \sqrt{2}\alpha$ of the (α, U) space. Below the solid curve, bipolaron formation will occur in *three* dimensions. The dashed curve separates the region of single polarons from the region of bipolarons in *two* dimensions. The solid circles indicate where the phase separation starts to deviate from the line $U=\sqrt{2}\alpha$. These points are given by $\alpha_c=6.8$ (3D) and $\alpha_c=2.9$ (2D). The 2D curve was calculated from the 3D curve by application of the scaling law, presented in Sec. VI. In the neighborhood of α_c, both curves are linear $U \approx 1.63\alpha + C$, where the constant C depends on the dimension; in 3D, $C=1.49$ and in 2D, $C=0.63$, For larger values of α, U deviates slightly from this linear behavior. It is found that the bipolaron region is much larger in two dimensions than in three. Perhaps it is even more important that, in two dimensions, bipolaron formation might occur at *lower* values of the coupling constant α.

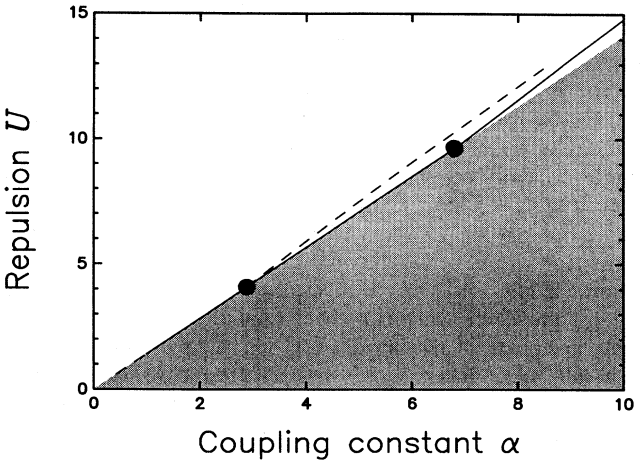

FIG. 7. The phase diagram for bipolaron formation in two (dashed curve) and three dimensions (solid curve) is presented. Bipolarons are formed below the curves. The nonphysical part $U \leq \sqrt{2}\alpha$ of the (α, U) space is shaded.

A comparison with the work of Adamowski[7] for a 3D bipolaron shows that his onset of bipolaron formation ($\alpha_c=7.3$) is close to our estimate $\alpha_c=6.8$ in 3D. For higher values of the coupling constant α, he finds a slightly larger stability region for bipolaron formation, e.g., at $\alpha=9$ he obtained $U_c=13.48$ where our result is $U_c=13.21$. Bassani *et al.*[8] found $\alpha_c \approx 6$ in 3D and $\alpha_c \approx 2$ in 2D, but his bipolaron energies are larger than ours. Because the results of Ref. 8 and ours are upper bounds to the exact energy, the present result is closest to the exact result.

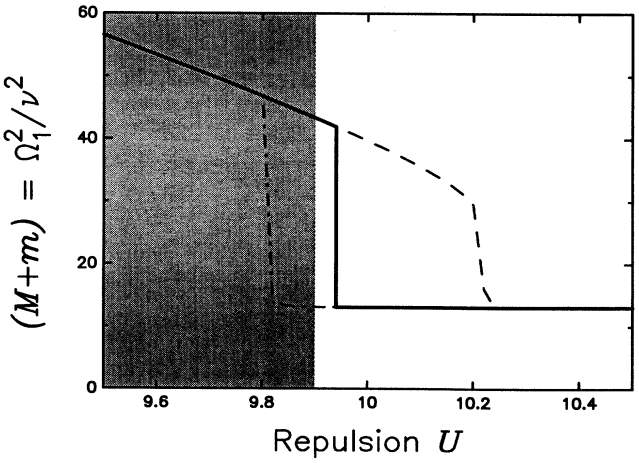

FIG. 6. The model bipolaron mass as a function of the repulsion U at a fixed coupling constant $\alpha=7$.

VIII. CONCLUSION

We have studied the bipolaron system and single-polaron–bipolaron transition for an arbitrary number of spacial dimensions. An upper bound to the free energy of a bipolaron in the case of a general electron-phonon coupling in different dimensions, Eq. (19), was obtained using the path-integral formalism. This upper bound was derived using a new trial action, Eq. (8), in which the electrons are separated spatially by a vector $\mathbf{a}$.

For the numerical work, we restricted ourselves to an interaction with LO phonons and a Coulomb repulsion between the electrons at zero temperature. The physical parameters are the electron-phonon coupling constant α and the interelectron repulsion strength U. The region of physically realizable materials had to satisfy $U \leq \sqrt{2}\alpha$. In the case of large repulsions, (twice) the Feynman result for the single-polaron ground-state energy was obtained. Therefore, bipolarons and single polarons, as well as their transition, could be studied within the *same* physical model. For this choice of interaction, a *scaling* relation

was derived. This permits us to deduce 2D results from our 3D analysis simply by scaling the coupling constant α and the repulsion U.

Our numerical results showed a different behavior at weak coupling as compared to strong coupling. Below a critical value α_c, no bipolarons exist for $U \geq \sqrt{2}\alpha$. The single-polaron–bipolaron is a continuous transition and occurs at $U = \sqrt{2}\alpha$. Only when $\alpha \geq \alpha_c$ do bipolarons exist in the physical region. The single-polaron–bipolaron transition, however, behaves like a first-order phase transition. This leads to a discontinuous behavior of the mean-square separation r_{12} between the electrons and of the total mass of the model system. Our estimations are $\alpha_c \approx 6.8$ in 3D and $\alpha_c \approx 2.9$ in 2D. Bipolaron formation is found to be more favorable in two dimensions and might be an important mechanism in the high-temperature superconductors.

In the present paper we showed that the interaction of the electrons with LO-phonons is already able to stabilize the bipolaron state. From Ref. 10 we know that the integration of electrons with acoustical phonons will enlarge the bipolaron region in the phase diagram of Fig. 7. But it is known[14] that strong acoustical phonon interaction strongly reduces the polaron mobility and it is expected that this will also be the case for the bipolaron. Therefore, a strong acoustical phonon interaction will tend to localize the bipolaron, which is unfavorable for a possible superconducting state.

Note added. While revising our manuscript, it was brought to our attention that a trial action similar to Hiramoto and Toyozawa's[10] and ours, Eq. (11), has been introduced by Kochetov *et al.*[15] They obtained analytical results in the strong-coupling region which were found to agree with our numerical results for large values of α.

ACKNOWLEDGMENTS

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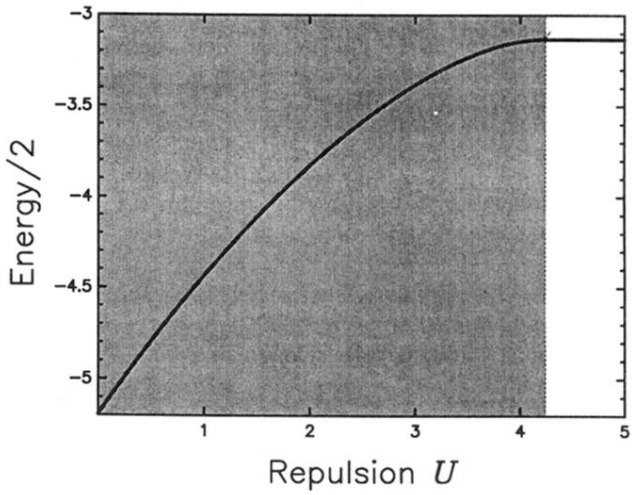


FIG. 1. The upper bound to the ground-state energy (3D) is plotted as a function of the repulsion U for a relatively weak coupling $\alpha=3$. Bipolaron formation is only possible in the non-physical region $U \leq \sqrt{2}\alpha$ (shaded area).

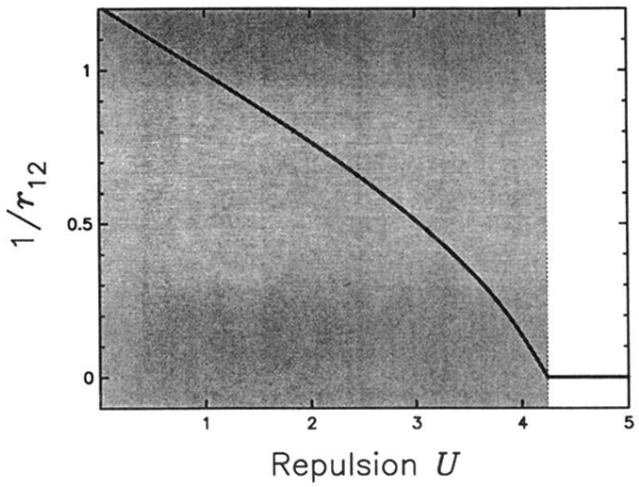


FIG. 2. The inverse mean-square distance $1/r_{12}$, as a function of the repulsion U for $\alpha=3$. The mean-square separation r_{12} is infinite throughout the entire physical space $U \geq \sqrt{2}\alpha$, where *single* polarons are more stable than bipolarons.

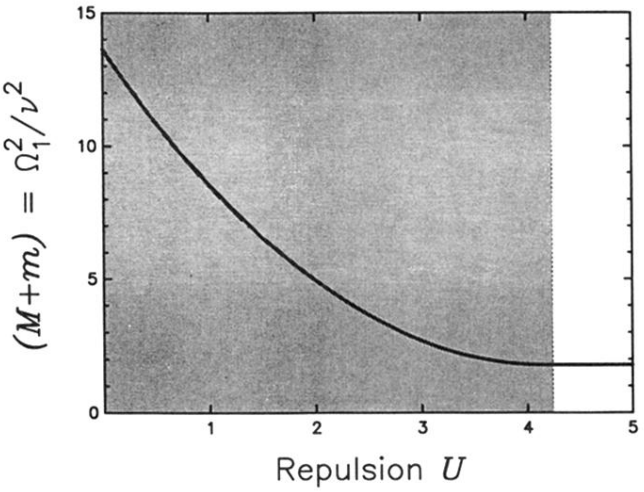


FIG. 3. The model bipolaron mass as a function of the repulsion U at fixed coupling constant $\alpha=3$. In the nonphysical region $U \leq \sqrt{2}\alpha$ (shaded area), the mass is enhanced because of bipolaron formation.

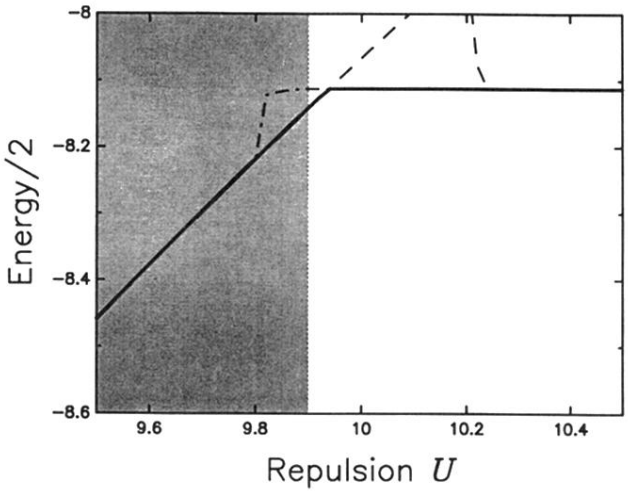
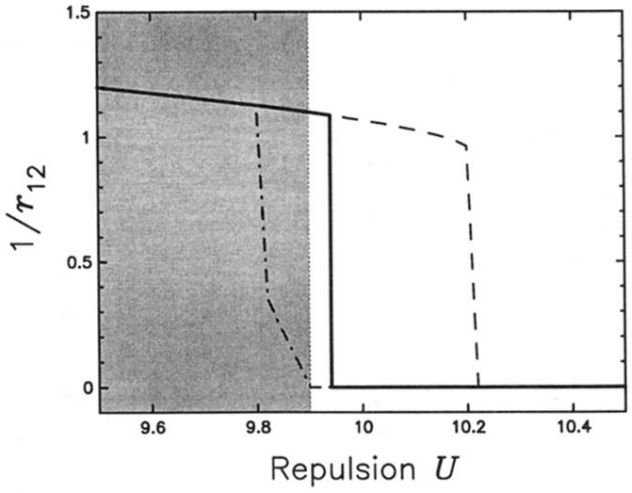


FIG. 4. The ground-state energy as a function of the repulsion U for a typical strong-coupling case: $\alpha=7$. Bipolaron formation is possible in the physical region (nonshaded area) below a critical value U_c.



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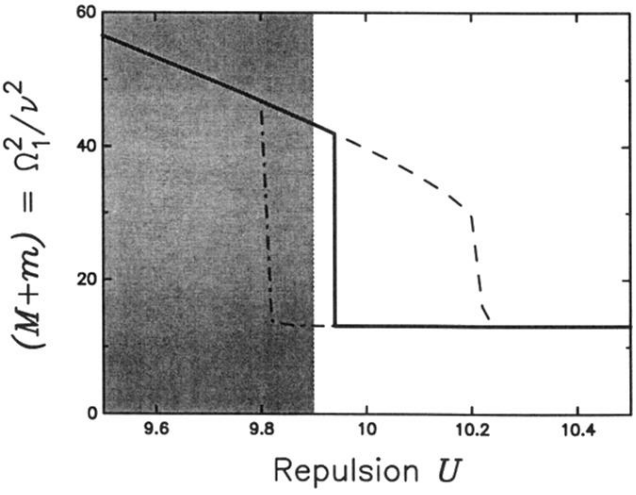

FIG. 6. The model bipolaron mass as a function of the repulsion U at a fixed coupling constant $\alpha=7$.

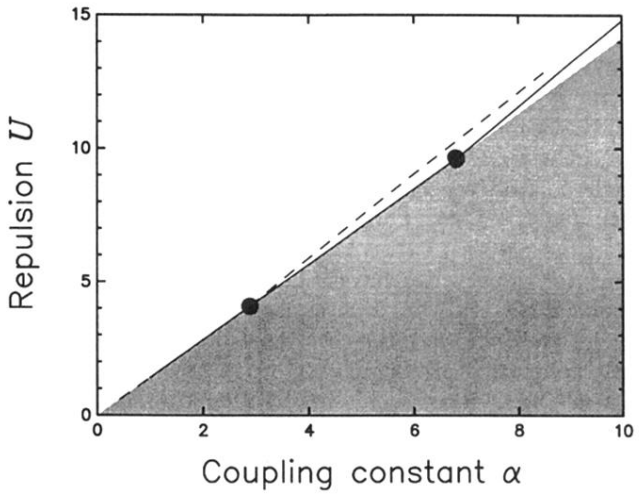

FIG. 7. The phase diagram for bipolaron formation in two (dashed curve) and three dimensions (solid curve) is presented. Bipolarons are formed below the curves. The nonphysical part $U \leq \sqrt{2}\alpha$ of the (α, U) space is shaded.