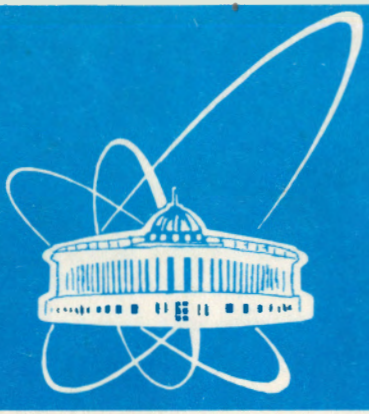

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EXACT EQUATIONS FOR LARGE BIPOLARONS IN THE STRONG-COUPLING LIMIT

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I. INTRODUCTION

Two identical charged particles (electrons), being placed in a polar or ionic crystal, interact with the lattice vibrations which results in attractive forces between them. Under certain conditions a bound state can exist which is constituted of two electrons surrounded by a common cloud of virtual phonons. Such a quasiparticle is referred to as a *bipolaron*. The interest in the bipolaron properties is renewed by a possibility of a *bipolaron mechanism of high T_c superconductivity*. It was supposed that bipolarons could act as charge boson undergoing the Bose-Einstein condensation in a real space. For large bipolarons such a mechanism was studied by Vinetskii and Pashitskii[1] and then significantly developed by Emin and Hillery[2]. For the recent discussions see also papers by Verbist, Peeters and Devreese[3] and by Gataudella, Iadonisi and Ninno[4].

The prerequisite of such theories is the very existence of bipolarons. As is known, the problem of bipolaron formation is studied attentively. People investigate various bipolaron characteristics such as its ground-state energy, effective mass, radius, number of virtual phonons in a cloud (for the references see a review article[5]). The main conclusion of the majority of the published papers is that bipolarons can exist at some critical values of coupling constants of the competing interactions: both electron-phonon attractive and Coulomb repulsive forces. It is clear that to let the bipolaron to be formed, the repulsive forces should be weak enough while the electron-phonon interaction has to be sufficiently strong to overcome that repulsion.

To calculate the critical values of the coupling constants authors used as a rule different versions of variational upper estimates for the bipolaron energy. The advantages of such an approach are obvious: these methods lead to estimates of the bipolaron characteristics for the whole range of values of the electron-phonon coupling constant, especially for its intermediate values. Polaron effects are important for many polar dielectrics and semiconductors of the $A^{III}B^{V}$ and the $A^{II}B^{VI}$ groups. Indeed, the small and intermediate values of the electron-phonon coupling constant are usual for these materials. But the investigation of the bipolaron characteristics in the limiting cases of the weak- and strong-coupling regimes is of use to prove the effectiveness of the approximations being made.

Besides, there exist systems with anomaly high values of the electron-phonon coupling constant. Between those should be mentioned protein globules and solvated electrons in liquids (see, e.g., papers by Pushchino group[6]). Another reason is the existence of the excited states of the bipolaron which are not taken into account by variational calculations. The exact equation for single polaron led to the detailed

investigation of such states (see e.g.[7]). The analogous equations for the bipolaron could reveal also the richness of this system. The formation of the bipolaron and the existence of excited states of polarons and bipolarons is important in processes of electron transfer of excitations in a broad variety of condensed matter.

The goal of the present paper is to derive the exact equations for the bipolaron in the strong-coupling limit. The same limit for the single polaron was investigated in early papers[8] by Pekar, Landau and Pekar, Bogolubov and Tyablikov. Numerical calculations for 3D (bulk) polarons have been performed by Miyake[9] and for 2D (flat) polarons - by Wu, Peeters and Devreese[10]. In a recent paper by Bogolubov[11] the procedure of deriving the strong-coupling equations was simplified. Here we generalize it to the case of the bipolaron and improve this approach to avoid divergencies.

The modern art of creating new materials such as thin films and quantum wires makes it possible to confine moving electrons in one or two dimensions. That is why we consider bipolarons in a space with arbitrary number D of dimensions. Note, that at $D = 2$ the polaron effects are enlarged[12–14].

The present paper is organized as follows. In Sec. 2 we derive the exact equations for the bipolaron characteristics in the strong-coupling limit. In Sec. 3 we study the equation for the bipolaron ground-state energy and effective mass. Sec. 4 is devoted to the reduction of the results obtained to the one-dimensional case.

II. BASIC EQUATIONS

The Fröhlich Hamiltonian for two electrons interacting with phonon field is written as follows

$$H = \frac{\vec{p}_1^{\,2}}{2m} + \frac{\vec{p}_2^{\,2}}{2m} + \sum_{\vec{k}} \hbar\omega_{\vec{k}}\, a_{\vec{k}}^{\dagger} a_{\vec{k}} + U(\mid \vec{r}_1 - \vec{r}_2 \mid) + \sum_{\vec{k}} \left[a_{\vec{k}} V_{\vec{k}} \left(e^{i\vec{k}\cdot\vec{r}_1} + e^{i\vec{k}\cdot\vec{r}_2} \right) + a_{\vec{k}}^{\dagger} V_{\vec{k}}^{*} \left(e^{-i\vec{k}\cdot\vec{r}_1} + e^{-i\vec{k}\cdot\vec{r}_2} \right) \right], \tag{2.1}$$

where $\vec{r}_i(\vec{p}_i)$ are the positions (momenta) operators of the i-th electron, m is the electron band mass, $a_{\vec{k}}^{\dagger}$ ($a_{\vec{k}}$) are the creation (annihilation) operators of phonons with the wave vector $\vec{k}$ and the frequency $\omega_{\vec{k}}$. The potential $U(\mid \vec{r}_1 - \vec{r}_2 \mid)$ stands for the direct (Coulomb) interaction between electrons, the quantities $V_{\vec{k}}$ are the Fourier transforms of the electron-phonon interaction. The total momentum of the system is conserved: one can readily verify that the operator

$$\hat{\vec{P}} = -i\hbar\nabla_{\vec{r}_1} - i\hbar\nabla_{\vec{r}_2} + \sum_{\vec{k}} \hbar\vec{k}\, a_{\vec{k}}^{\dagger} a_{\vec{k}} \tag{2.2}$$

commutes with the Hamiltonian (2.1). So we can consider states with the total conserving momentum being a c-number $\vec{\mathcal{P}}$. To realize this we use a Lagrange factor $\vec{v}$ in a conventional manner. Let us take instead of (2.1) a new Hamiltonian of the form

$$H(\vec{v}) = H - \vec{v}\cdot(\vec{p}_1 + \vec{p}_2 + \sum_{\vec{k}} \hbar\vec{k}\, a_{\vec{k}}^{\dagger} a_{\vec{k}} - \vec{\mathcal{P}}). \tag{2.3}$$

The physical meaning of the Lagrange factor $\vec{v}$ is quite obvious from the relation $\partial H(\vec{v})/\partial\vec{\mathcal{P}} = \vec{v}$, so $\vec{v}$ is the average velocity of the system. Then at small velocities one may define a bipolaron effective mass m^* as usual

$$\vec{\mathcal{P}} = m^*\,\vec{v} + O(\vec{v}^{\,2}). \tag{2.4}$$

The first step to treat the Hamiltonian (2.3) is to apply the unitary transformation:

$$U_1 = \exp\left[-i\frac{\vec{r}_1 + \vec{r}_2}{2\hbar}\cdot\left(2m\vec{v} - a\sum_{\vec{k}} \hbar\vec{k}\, a_{\vec{k}}^{\dagger} a_{\vec{k}} \right) \right];$$
$$H'(\vec{v}) = U_1\, H(\vec{v})\, U_1^{-1}. \tag{2.5}$$

The operator (2.2) of the total momentum is transformed then as follows:

$$\hat{\vec{P}}' = U_1\,\hat{\vec{P}}\,U_1^{-1} = \vec{p}_1 + \vec{p}_2 + 2m\vec{v} + (1-a)\sum_{\vec{k}} \hbar\vec{k}\, a_{\vec{k}}^{\dagger} a_{\vec{k}}. \tag{2.6}$$

The goal of the transformation (2.5) is 1) to reveal the motion of the center of mass of two electrons (which is not the same as *the bipolaron center of mass*) and 2) to take into account the recoil effects. The idea to use for this a parameter a was suggested in Ref.[15] When $a = 1$ this part of the transformation generalizes the well-known Lee-Low-Pines transformation by using the c.m. coordinate of two electrons instead of a single electron coordinate, which makes it possible to work with the total momenta as with a c-number.

With this transformation the Hamiltonian takes the form:

$$H'(\vec{v}) = \frac{\vec{p}_1^{\,2}}{2m} + \frac{\vec{p}_2^{\,2}}{2m} + U(\mid \vec{r}_1 - \vec{r}_2 \mid) - m\vec{v}^{\,2} + \vec{v}\cdot\vec{\mathcal{P}} + \sum_{\vec{k}} a_{\vec{k}}^{\dagger} a_{\vec{k}} \left[\hbar\omega_{\vec{k}} - \hbar\vec{k}\cdot\vec{v} - \frac{a}{2m}\hbar\vec{k}\cdot(\vec{p}_1 + \vec{p}_2) \right] + \frac{a^2}{4m}\left(\sum_{\vec{k}} \hbar\vec{k}\, a_{\vec{k}}^{\dagger} a_{\vec{k}} \right)^2 + \sum_{\vec{k}} \left[a_{\vec{k}} V_{\vec{k}}\, e^{-ia\vec{k}\cdot\frac{\vec{r}_1+\vec{r}_2}{2}} \left(e^{i\vec{k}\cdot\vec{r}_1} + e^{i\vec{k}\cdot\vec{r}_2} \right) + \text{h.c.} \right]. \tag{2.7}$$

Now we use the transformation

$$U_2 = \exp\left[\sum_{\vec{k}} \left(c^*_{\vec{k}}(\vec{v})a_{\vec{k}} - c_{\vec{k}}(\vec{v})a^\dagger_{\vec{k}}\right)\right],$$
$$H''(\vec{v}) = U_2\, H'(\vec{v})\, U_2^{-1} \tag{2.8}$$

to shift the phonon field operators $a_{\vec{k}} \to a_{\vec{k}} + c_{\vec{k}}(\vec{v})$ by c-numbers $c_{\vec{k}}(\vec{v})$. By this shifting one can describe a polaron in a strong coupling limit as an electron captured by a potential well generated by a large classical component of a phonon field. The resulting Hamiltonian can be splitted then into two parts: $H''(\vec{v}) = H_0(\vec{v}) + H_{int}(\vec{v})$. One of them contains the energy of the free phonon field and the energy of electrons moving in an effective potential:

$$H_0(\vec{v}) = \frac{\vec{p}_1^{\,2}}{2m} + \frac{\vec{p}_2^{\,2}}{2m} + U(\mid \vec{r}_1 - \vec{r}_2 \mid) - m\vec{v}^{\,2} + \vec{v}\cdot\vec{\mathcal{P}} +$$
$$\sum_{\vec{k}} |c_{\vec{k}}(\vec{v})|^2 \left[\hbar\omega_{\vec{k}} + \frac{a^2}{4m}(\hbar\vec{k})^2 - \hbar\vec{k}\cdot\left(\vec{v} + \frac{a}{2m}(\vec{p}_1+\vec{p}_2) - \frac{a^2}{4m}\sum_{\vec{l}}\hbar\vec{l}\,|c_{\vec{l}}(\vec{v})|^2\right)\right] +$$
$$\sum_{\vec{k}} a^\dagger_{\vec{k}}a_{\vec{k}} \left[\hbar\omega_{\vec{k}} + \frac{a^2}{4m}(\hbar\vec{k})^2 - \hbar\vec{k}\cdot\left(\vec{v} + \frac{a}{2m}(\vec{p}_1+\vec{p}_2) - \frac{a^2}{2m}\sum_{\vec{l}}\hbar\vec{l}\,|c_{\vec{l}}(\vec{v})|^2\right)\right] +$$
$$\sum_{\vec{k}} \left[c_{\vec{k}}(\vec{v})\, V_{\vec{k}}\, e^{-ia\vec{k}\cdot\frac{\vec{r}_1+\vec{r}_2}{2}}\left(e^{i\vec{k}\cdot\vec{r}_1} + e^{i\vec{k}\cdot\vec{r}_2}\right) + \text{h.c.}\right]. \tag{2.9}$$

The other part H_{int} of the Hamiltonian (2.3) can be written in a normally ordered form and contains terms playing no role in what follows.

Up to now $c_{\vec{k}}(\vec{v})$ are arbitrary c-numbers. To fix them we average $H(\vec{v}) = H_0(\vec{v}) + H_{int}(\vec{v})$ with $H_0(\vec{v})$ defined by Eq. (2.9) over a trial wave vector

$$\mid \Phi_{\vec{v}}\rangle = \phi_{\vec{v}}(\vec{r}_1, \vec{r}_2)\ \mid 0\rangle .$$

The average $< H_{int}(\vec{v}) >= 0$ is equal to zero so we consider the variational problem with the energy functional of the form

$$E[\phi_{\vec{v}}] = \langle H_0(\vec{v})\rangle - E\,(\langle\Phi_{\vec{v}} \mid \Phi_{\vec{v}}\rangle - 1) = \langle\frac{\vec{p}_1^{\,2}}{2m}\rangle + \langle\frac{\vec{p}_2^{\,2}}{2m}\rangle + \langle U(\mid \vec{r}_1 - \vec{r}_2 \mid)\rangle +$$
$$\langle\phi_{\vec{v}} \mid \phi_{\vec{v}}\rangle\left(\vec{v}\cdot\vec{\mathcal{P}} - m\vec{v}^{\,2}\right) - \frac{a}{2m}\langle\vec{p}_1+\vec{p}_2\rangle\cdot\sum_{\vec{k}}\hbar\vec{k}\,|c_{\vec{k}}(\vec{v})|^2 +$$
$$\langle\phi_{\vec{v}} \mid \phi_{\vec{v}}\rangle\sum_{\vec{k}}|c_{\vec{k}}(\vec{v})|^2\left(\hbar\omega_{\vec{k}} + \frac{a^2}{4m}(\hbar\vec{k})^2 - \hbar\vec{k}\cdot\vec{v} + \frac{a^2}{4m}\hbar\vec{k}\cdot\sum_{\vec{l}}\hbar\vec{l}\,|c_{\vec{l}}(\vec{v})|^2\right) +$$

$$2\sum_{\vec{k}}\left[V_{\vec{k}}\, c_{\vec{k}}(\vec{v})\,\rho_{\vec{k}}(a) + V^*_{\vec{k}}\, c^*_{\vec{k}}(\vec{v})\,\rho^*_{\vec{k}}(a)\right] + E\,(\langle\phi_{\vec{v}} \mid \phi_{\vec{v}}\rangle - 1), \tag{2.10}$$

where the notations are used

$$\rho_{\vec{k}}(a) = \frac{1}{2}\int d\vec{r}_1 d\vec{r}_2\, e^{-ia\vec{k}\cdot\frac{\vec{r}_1+\vec{r}_2}{2}}\left(e^{i\vec{k}\cdot\vec{r}_1} + e^{i\vec{k}\cdot\vec{r}_2}\right)\phi^*_{\vec{v}}(\vec{r}_1, \vec{r}_2)\ \phi_{\vec{v}}(\vec{r}_1, \vec{r}_2)\,. \tag{2.11}$$

A parameter E in Eq. (2.10) is a Lagrange factor. A variation over E gives us the conventional normalization of the wave function:

$$\langle\phi_{\vec{v}} \mid \phi_{\vec{v}}\rangle = \int d\vec{r}_1 d\vec{r}_2\ \phi^*_{\vec{v}}(\vec{r}_1, \vec{r}_2)\ \phi_{\vec{v}}(\vec{r}_1, \vec{r}_2)\ = 1\,. \tag{2.12}$$

Note that the Hamiltonian (2.3) is symmetrical under permutations the places of the electrons. So the wave functions should be either symmetrical (para-bipolaron) or antisymmetrical (ortho-bipolaron): $\phi_{\vec{v}}(\vec{r}_1, \vec{r}_2) = \pm\phi_{\vec{v}}(\vec{r}_2, \vec{r}_1)$.

The variations of the functional $E[\phi_{\vec{v}}]$ of Eq. (2.10) over $c_{\vec{k}}(\vec{v})$ and $c^*_{\vec{k}}(\vec{v})$ lead to the solutions for these c-numbers:

$$c_{\vec{k}}(\vec{v}) = -\frac{2\,V^*_{\vec{k}}\,\rho^*_{\vec{k}}(a)}{\hbar\omega_{\vec{k}} - \hbar\vec{k}\cdot\vec{v} - \frac{a}{2m}\hbar\vec{k}\cdot(\vec{p}_1+\vec{p}_2) + \frac{a^2}{4m}\left[2\hbar\vec{k}\cdot\sum_{\vec{l}}\hbar\vec{l}\,|c_{\vec{l}}(\vec{v})|^2 + (\hbar\vec{k})^2\right]}. \tag{2.13}$$

The variation of the functional $E[\phi_{\vec{v}}]$ of Eq. (2.10) over $\vec{v}$ leads to a link of the average velocity with the total bipolaron momentum:

$$\vec{\mathcal{P}} = 2m\vec{v} + \sum_{\vec{k}}\hbar\vec{k}\,|c_{\vec{k}}(\vec{v})|^2. \tag{2.14}$$

On the other hand, the averaging of the operator $\hat{\vec{P}}'' = U_2\hat{\vec{P}}'U_2^{-1}$ with $\hat{\vec{P}}'$ and U_2 being defined by Eq. (2.6) and Eq. (2.8), respectively gives us the result

$$\langle\hat{\vec{P}}''\rangle = <\vec{p}_1 + \vec{p}_2> + 2m\vec{v} + (1-a)\sum_{\vec{k}}\hbar\vec{k}\,|c_{\vec{k}}(\vec{v})|^2. \tag{2.15}$$

Comparing Eq. (2.14) and (2.15) we arrive at the relation

$$<\vec{p}_1 + \vec{p}_2> = a\sum_{\vec{k}}\hbar\vec{k}\,|c_{\vec{k}}(\vec{v})|^2, \tag{2.16}$$

which simplifies the expression for the coefficients $c_{\vec{k}}(\vec{v})$:

$$c_{\vec{k}}(\vec{v}) = -\frac{2\,V^*_{\vec{k}}\,\rho^*_{\vec{k}}(a)}{\hbar\omega_{\vec{k}} - \hbar\vec{k}\cdot\vec{v} + (a^2/4m)\,(\hbar\vec{k})^2} \tag{2.17}$$

and the expression (2.10) for the functional $E[\phi_{\vec{v}}]$.

Introducing the notation $M = 2m/a^2$ we may represent the denominator of the expression (2.17) as follows:

$$\hbar\omega_{\vec{k}} - \hbar\vec{k}\cdot\vec{v} + \frac{(\hbar\vec{k})^2}{2M} = \hbar\omega_{\vec{k}} + \frac{(M\vec{v} - \hbar\vec{k})^2}{2M} - \frac{M\vec{v}^2}{2}, \tag{2.18}$$

which describes the transition between a free moving particle with the momenta $M\vec{v}$ and a state with one emitted phonon with the momenta $\hbar\vec{k}$. Thus, the parameter M should be close to the bipolaron effective mass m^* which is large in the strong coupling limit. That is, the parameter a is small in this limit, but if one takes $a = 0$ one arrives at the expression for $c_{\vec{k}}(\vec{v})$ whose denominator can be equal to zero no matter how small value takes the velocity $\vec{v}$. In theories without a cut-off this leads to divergencies which is the main theoretical disadvantage of the approach[11]. With an electron recoil energy being taken into account we avoid this difficulty. The equation for the parameter a can be obtained by the variation of Eq. (2.10). The last of the variational equations $\delta E[\phi_{\vec{v}}]/\delta\phi^*_{\vec{v}} = 0$ leads to the Schrödinger equation for the wave function $\phi_{\vec{v}}(\vec{r}_1, \vec{r}_2)$ where the Lagrange factor E plays the role of the ground-state energy of the system. These two equations will be presented in the next Section.

III. BIPOLARON GROUND STATE ENERGY AND EFFECTIVE MASS

To come to the ground state energy and the effective mass one has to consider the limit of slowly moving bipolaron. At first we concentrate on the bipolaron effective mass. When $\vec{v}$ tends to zero one may to neglect terms of the order of $o(\vec{v}^{\,2})$. We denote by ϕ_0 the wave function $\phi_{\vec{v}}$ at $\vec{v} = 0$ and all averages should be now performed over ϕ_0 rather than over $\phi_{\vec{v}}$. Expanding $c_{\vec{k}}(\vec{v})$ of Eq. (2.17) in powers of $\vec{v}$ and substituting it into Eq. (2.14) we arrive at the equation for the bipolaron effective mass

$$m^* = 2m + 8\sum_{\vec{k}} (\vec{n}\cdot\hbar\vec{k})^2 \frac{|\,V_{\vec{k}}\,|^2\,|\,\rho_{\vec{k}}(a)\,|^2}{[\hbar\omega_{\vec{k}} + (a^2/4m)(\hbar\vec{k})^2]^3}, \tag{3.1}$$

where $\vec{n}$ is a vector of unit length in a direction of the total momentum $\vec{\mathcal{P}}$ (or the average velocity $\vec{v}$). For the isotropic electron-phonon interaction one may replace $(\vec{n}\cdot\vec{k})^2$ by $\vec{k}^{\,2}/D$ where D is the number of space dimensions. In this case Eq. (3.1) is simplified:

$$m^* = 2m + \frac{8}{D}\sum_{\vec{k}} (\hbar\vec{k})^2 \frac{|\,V_{\vec{k}}\,|^2\,|\,\rho_{\vec{k}}(a)\,|^2}{[\hbar\omega_{\vec{k}} + (a^2/4m)(\hbar\vec{k})^2]^3}. \tag{3.2}$$

Now we turn at the bipolaron ground state energy. At $\vec{v} = 0$ we obtain from Eq. (2.10) the energy functional

$$E[\phi_0] = \langle\frac{\vec{p}_1^{\,2}}{2m}\rangle + \langle\frac{\vec{p}_2^{\,2}}{2m}\rangle + \langle U(|\,\vec{r}_1 - \vec{r}_2\,|)\rangle +$$
$$\langle\phi_0\,|\,\phi_0\rangle \sum_{\vec{k}} |c_{\vec{k}}|^2 \left[\hbar\omega_{\vec{k}} + \frac{a^2}{4m}(\hbar\vec{k})^2\right] +$$
$$2\sum_{\vec{k}} \left[V_{\vec{k}}\, c_{\vec{k}}\, \rho_{\vec{k}}(a) + V^*_{\vec{k}}\, c^*_{\vec{k}}\, \rho^*_{\vec{k}}(a)\right] + E\left(\langle\phi_0\,|\,\phi_0\rangle - 1\right), \tag{3.3}$$

where it follows from Eq. (2.13) the expression for the coefficients $c_{\vec{k}}$:

$$c_{\vec{k}} = c_{\vec{k}}(0) = -\frac{2\,V^*_{\vec{k}}\,\rho^*_{\vec{k}}(a)}{\hbar\omega_{\vec{k}} + (a^2/4m)(\hbar\vec{k})^2}. \tag{3.4}$$

The equation for the parameter a takes the form

$$\frac{\partial}{\partial a}\left[\sum_{\vec{k}} \frac{|\,V_{\vec{k}}\,|^2\,|\,\rho_{\vec{k}}(a)\,|^2}{\hbar\omega_{\vec{k}} + (a^2/4m)(\hbar\vec{k})^2}\right] = 0. \tag{3.5}$$

Variating the functional $E[\phi_0]$ over ϕ^*_0 we arrive at the Schrödinger equation for the bipolaron at rest:

$$\left[\frac{\vec{p}_1^{\,2}}{2m} + \frac{\vec{p}_2^{\,2}}{2m} + U(\vec{r}_1, \vec{r}_2; \phi_0)\right]\phi_0(\vec{r}_1, \vec{r}_2) = E_0\,\phi_0(\vec{r}_1, \vec{r}_2) \tag{3.6}$$

with the effective potential

$$U(\vec{r}_1, \vec{r}_2; \phi_0) = U(|\,\vec{r}_1 - \vec{r}_2\,|) + 4\sum_{\vec{k}} \frac{|\,V_{\vec{k}}\,|^2\,|\,\rho_{\vec{k}}(a)\,|^2}{\hbar\omega_{\vec{k}} + (a^2/4m)(\hbar\vec{k})^2} -$$
$$-2\sum_{\vec{k}} \frac{|\,V_{\vec{k}}\,|^2}{\hbar\omega_{\vec{k}} + (a^2/4m)(\hbar\vec{k})^2}\left[\rho^*_{\vec{k}}(a)\, e^{-i\vec{a}\frac{\vec{r}_1+\vec{r}_2}{2}}\left(e^{i\vec{k}\cdot\vec{r}_1} + e^{i\vec{k}\cdot\vec{r}_2}\right) + \text{c.c.}\right]. \tag{3.7}$$

Note the translation degeneracy of Eq. (3.6): if $\phi_0(\vec{r}_1, \vec{r}_2)$ is a solution then $\phi_0(\vec{r}_1 + \vec{r}_0, \vec{r}_2 + \vec{r}_0)$ is also a solution to the same equation and the same energy with any vector $\vec{r}_0$. Choosing some of these solution means to fix a point somewhere in a space. Afterwards Eq. (3.6) and its solutions are completely determined.

The equations derived can be formulated as the variational problem which is useful in numerical calculations. Really, the ground-state energy E_0 can be defined as minimum of the functional $E[\phi_0]$ of Eq. (3.3). The average kinetic energies of both electrons are equal due to the symmetry so one arrives at the functional

$$E[\phi_0] = \bar{T} + \bar{U},$$

$$\bar{T} = \frac{\hbar^2}{m} \int d\vec{r}_1 d\vec{r}_2 \, |\vec{\nabla}_1 \, \phi_0(\vec{r}_1, \vec{r}_2)|^2,$$

$$\bar{U} = -4 \sum_{\vec{k}} \frac{|\, V_{\vec{k}} \,|^2 \, |\, \rho_{\vec{k}}(a) \,|^2}{\hbar\omega_{\vec{k}} + (a^2/4m)(\hbar\vec{k})^2} + \int d\vec{r}_1 d\vec{r}_2 \, U(|\, \vec{r}_1 - \vec{r}_2 \,|) \, |\phi_0(\vec{r}_1, \vec{r}_2)|^2. \quad (3.8)$$

Now we specify the electron-phonon interaction for the case of the Pekar-Fröhlich optical polarons for which the phonon frequency does not depend on the wave vector: $\omega_{\vec{k}} = \omega_D$. According to the paper by Peeters, Wu and Devreese[16] one has in D-dimensional space

$$V_{\vec{k}} = -i\hbar\omega_D \left(\frac{\alpha_D}{V k^{D-1}} \sqrt{\frac{\hbar}{2m\omega_D}} (2\sqrt{\pi})^{D-1} \, \Gamma(\frac{D-1}{2}) \right)^{1/2}, \quad (3.9)$$

where V is the volume of a D-dimensional "crystal". The indices D are introduced in the notations for the electron-phonon coupling constant α_D and LO-phonon frequency ω_D. At $D = 3$ one arrives at the standard electron-phonon interaction with conventional phonon frequency $\omega_{3D} = \omega_{LO}$ and dimensionless electron-phonon coupling constant

$$\alpha_{3D} = \alpha = \frac{e^2}{\hbar} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right) \sqrt{\frac{m}{2\hbar\omega_{LO}}}.$$

Here e is the electron charge and ϵ_∞ (ϵ_0) are the high frequency (static) dielectric constants.

With the parametrization (3.9) one has

$$\sum_{\vec{k}} \frac{|\, V_{\vec{k}} \,|^2}{\hbar\omega_{\vec{k}} + (a^2/4m)(\hbar\vec{k})^2} e^{i\vec{k}\cdot\vec{r}} = \hbar\omega_D \, \frac{\alpha_D\sqrt{2}}{a} \, J\left(\frac{\vec{r}}{a} \sqrt{\frac{m\omega_D}{\hbar}} \right),$$

$$J(\vec{r}) = \int_0^1 dx \, [1 - x^2]^{(D-3)/2} \exp(-2x \, |\vec{r}\,|). \quad (3.10)$$

The function $J(\vec{r})$ can be expressed as a sum of modified Bessel and Struve functions:

$$J(\vec{r}) = \frac{\sqrt{\pi}}{2} \, \Gamma\left(\frac{D-1}{2} \right) \left(-\frac{1}{r} \right)^{\frac{D}{2}-1} \left[I_{\frac{D}{2}-1}(-2r) + \mathbf{L}_{\frac{D}{2}-1}(-2r) \right]. \quad (3.11)$$

To describe the direct interaction of electrons we choose the Coulomb type potential

$$U(|\, \vec{r}_1 - \vec{r}_2 \,|) = \hbar\omega_D \frac{U_D}{|\, \vec{r}_1 - \vec{r}_2 \,|} \sqrt{\frac{\hbar}{m\omega_D}}. \quad (3.12)$$

At $D = 3$ the dimensionless Coulomb coupling constant takes the form

$$U_{3D} = \frac{e^2}{\hbar\omega_{LO}\epsilon_\infty} \sqrt{\frac{m\omega_{LO}}{\hbar}} = \frac{\sqrt{2}\alpha}{1 - \epsilon_\infty/\epsilon_0}.$$

From Eq. (3.10), (3.12) it follows then the concrete realization of the Eq. (3.8) for the average potential energy of large bipolaron:

$$\bar{U} = \hbar\omega_D \left\{ -\frac{4\sqrt{2}\alpha_D}{a} \int d\vec{r}_1 d\vec{r}_2 d\vec{r}\,'_1 d\vec{r}\,'_2 \, |\phi_0(\vec{r}_1, \vec{r}_2)|^2 \, |\phi_0(\vec{r}\,'_1, \vec{r}\,'_2)|^2 \times \right.$$
$$J\left[\sqrt{\frac{m\omega_D}{\hbar}} \left(\frac{\vec{r}_1 - \vec{r}\,'_1}{a} - \frac{\vec{r}_1 + \vec{r}_2 - \vec{r}\,'_1 - \vec{r}\,'_2}{2} \right) \right] +$$
$$\left. U_D \sqrt{\frac{\hbar}{m\omega_D}} \int d\vec{r}_1 d\vec{r}_2 \, \frac{|\phi_0(\vec{r}_1, \vec{r}_2)|^2}{|\, \vec{r}_1 - \vec{r}_2 \,|} \right\}, \quad (3.13)$$

where we took into account the symmetry of the wave functions.

Note that at $a \to 0$ we have from Eq. (3.10)

$$\lim_{a \to 0} \frac{1}{a} J\left(\frac{\vec{r}}{a} \right) = \frac{1}{2|\vec{r}|}, \quad (3.14)$$

where from we obtain instead of Eq. (3.13) the average potential energy

$$\bar{U}_0 = \hbar\omega_D \sqrt{\frac{\hbar}{m\omega_D}} \left\{ -2\sqrt{2}\alpha_D \int d\vec{r}_1 d\vec{r}_2 d\vec{r}\,'_1 d\vec{r}\,'_2 \, \frac{|\phi_0(\vec{r}_1, \vec{r}_2)|^2 \, |\phi_0(\vec{r}\,'_1, \vec{r}\,'_2)|^2}{|\vec{r}_1 - \vec{r}\,'_1|} + \right.$$
$$\left. U_D \int d\vec{r}_1 d\vec{r}_2 \, \frac{|\phi_0(\vec{r}_1, \vec{r}_2)|^2}{|\, \vec{r}_1 - \vec{r}_2 \,|} \right\}. \quad (3.15)$$

The energy functional (3.8) for $3D$-bipolarons with the potential energy given by Eq. (3.15) appeared at first in the pioneering paper by Pekar and Ol'ga Tomasevich[17] as a starting point for the Pekar's adiabatic approach to the bipolaron problem. The very name *bipolaron* have been given to this quasiparticle in the cited paper albeit the authors made a wrong conclusion on a bipolaron *unstability*. Here we start from the Fröhlich type Hamiltonian and find the same functional as the leading approximation as is shown in the next Section.

IV. APPLICATIONS TO 1D-BIPOLARONS

In what follows we shall use a scaled electron-phonon coupling constant

$$\alpha'_D = \alpha_D \sqrt{\pi} \frac{\Gamma[(D-1)/2]}{2\Gamma(D/2)}. \quad (4.1)$$

In a similar way we define a scaled Coulomb coupling constant U'_D so that the ratio $U_D/\alpha_D = U'_D/\alpha'_D$ remains the same. At $D = 3$ we have $\alpha'_{3D} = \alpha_{3D}$ and $U'_{3D} = U_{3D}$, but the renormalization (4.1) of the electron-phonon coupling constant is necessary to obtain finite results when $D \to 1$ (see Ref.[18]). To derive the equation for the strong-coupling limit in its final form it is convenient to perform a scaling

$$\vec{r}_i \to \frac{\vec{r}_i}{\alpha'_D}\sqrt{\frac{\hbar}{m\omega_D}}, \qquad a = \frac{b}{\alpha'^2_D},$$

To preserve the normalization of the wave function one has to perform as well the scaling

$$\phi_0\left(\frac{\vec{r}_1}{\alpha'_D}\sqrt{\frac{\hbar}{m\omega_D}}, \frac{\vec{r}_2}{\alpha'_D}\sqrt{\frac{\hbar}{m\omega_D}}\right) \to \left(\alpha'_D\sqrt{\frac{m\omega_D}{\hbar}}\right)^D \phi_0(\vec{r}_1\,,\vec{r}_2)\,.$$

The effective potential transforms then as follows:

$$U(\vec{r}_1,\vec{r}_2;\,\phi_0) \to \hbar\omega_D\alpha'^2_D\,U(\vec{r}_1,\vec{r}_2;\,\phi_0)\,.$$

As the result one arrives instead of the Eq. (3.6) at the Schrödinger equation ($\vec{p}_i = -i\vec{\nabla}_i$):

$$\left[\frac{\vec{p}_1^{\,2}}{2} + \frac{\vec{p}_2^{\,2}}{2} + U(\vec{r}_1\,,\vec{r}_2\,;\phi_0)\right]\phi_0(\vec{r}_1\,,\vec{r}_2) = \epsilon_0\,\phi_0(\vec{r}_1\,,\vec{r}_2)\,,$$
$$\epsilon_0 = \frac{E_0}{\hbar\omega_D\alpha'^2_D}\,, \tag{4.2}$$

where the potential of Eq. (3.7) takes now the form

$$U(\vec{r}_1\,,\vec{r}_2\,;\phi_0) = \frac{2\Gamma(D/2)}{\sqrt{\pi}\Gamma[(D-1)/2]}\left\{\frac{U'_D}{\alpha'_D}\frac{1}{|\vec{r}_1-\vec{r}_2|} + \right.$$
$$4\sqrt{2}\,\frac{\alpha'_D}{b}\int d\vec{r}_1 d\vec{r}_2 d\vec{r}\,'_1 d\vec{r}\,'_2\,|\phi_0(\vec{r}_1\,,\vec{r}_2)|^2\,|\phi_0(\vec{r}\,'_1\,,\vec{r}\,'_2)|^2\,\times$$
$$J\left(\alpha'_D\frac{\vec{r}_1-\vec{r}\,'_1}{b} - \frac{\vec{r}_1+\vec{r}_2-\vec{r}\,'_1-\vec{r}\,'_2}{2\alpha'_D}\right) -$$
$$4\sqrt{2}\,\frac{\alpha'_D}{b}\int d\vec{r}\,'_1 d\vec{r}\,'_2\,|\phi_0(\vec{r}\,'_1\,,\vec{r}\,'_2)|^2\,\left[J\left(\alpha'_D\frac{\vec{r}_1-\vec{r}\,'_1}{b} - \frac{\vec{r}_1+\vec{r}_2-\vec{r}\,'_1-\vec{r}\,'_2}{2\alpha'_D}\right) + \right.$$
$$\left.\left. J\left(\alpha'_D\frac{\vec{r}_2-\vec{r}\,'_1}{b} - \frac{\vec{r}_1+\vec{r}_2-\vec{r}\,'_1-\vec{r}\,'_2}{2\alpha'_D}\right)\right]\right\} \tag{4.3}$$

and the average potential energy is as follows

$$\bar{U} = \frac{2\Gamma(D/2)}{\sqrt{\pi}\Gamma[(D-1)/2]}\left\{\frac{U'_D}{\alpha'_D}\int d\vec{r}_1 d\vec{r}_2\,\frac{|\phi_0(\vec{r}_1\,,\vec{r}_2)|^2}{|\vec{r}_1-\vec{r}_2|} - \right.$$
$$4\sqrt{2}\,\frac{\alpha'_D}{b}\int d\vec{r}_1 d\vec{r}_2 d\vec{r}\,'_1 d\vec{r}\,'_2\,|\phi_0(\vec{r}_1\,,\vec{r}_2)|^2\,|\phi_0(\vec{r}\,'_1\,,\vec{r}\,'_2)|^2\,\times$$
$$\left. J\left(\alpha'_D\frac{\vec{r}_1-\vec{r}\,'_1}{b} - \frac{\vec{r}_1+\vec{r}_2-\vec{r}\,'_1-\vec{r}\,'_2}{2\alpha'_D}\right)\right\}. \tag{4.4}$$

The average kinetic energy is the same as in Eq. (3.8) except of the factor $\hbar^2/m$.

Eq. (3.2) for the bipolaron effective mass together with Eq. (3.9) and the same strong-coupling scaling leads at the expression

$$\frac{m^*}{m} = 2 + \alpha'^4\,\frac{4\sqrt{2}}{D}\,\frac{\Gamma(D/2)}{\pi^{1+D/2}}\int\frac{d\vec{k}}{k^{D-1}}\,\frac{k^2\,|\rho_{\vec{k}}(b/\alpha'^2_D)|^2}{[1+(b/4\alpha'^2_D\,k^2]^3}. \tag{4.5}$$

To apply the equations derived to $1D$-bipolarons one has to use the relation

$$\lim_{D\to 1}\frac{\Gamma(D/2)}{\sqrt{\pi}\Gamma[(D-1)/2]}\,\frac{1}{|\vec{r}|} = \delta(z)\,, \tag{4.6}$$

where $\vec{r}$ is a D-dimensional vector and z is its component along the direction of the easy motion of the bipolaron. Besides it follows from Eq. (3.11) the expression

$$\lim_{D\to 1}\frac{\Gamma(D/2)}{\sqrt{\pi}\Gamma[(D-1)/2]}\,J(\vec{r}) = \frac{1}{2}\,e^{-2|z|}. \tag{4.7}$$

With Eq. (4.6), (4.7) being inserted into Eq. (4.4) one arrives at the corresponding relations for the average potential energy in a 1D-space

$$\bar{U} = 2\,\frac{U'_{1D}}{\alpha'_{1D}}\int dz_1\,|\phi_0(z_1\,,z_1)|^2 -$$
$$4\sqrt{2}\,\frac{\alpha'_{1D}}{b}\int dz_1 dz_2 dz\,'_1 dz\,'_2\,|\phi_0(z_1\,,z_2)|^2\,|\phi_0(z\,'_1\,,z\,'_2)|^2\,\times$$
$$\exp\left(-\left|2\alpha'_{1D}\frac{z_1-z\,'_1}{b} - \frac{z_1+z_2-z\,'_1-z\,'_2}{\alpha'_{1D}}\right|\right). \tag{4.8}$$

Performing in succession changes of variables in the second term of Eq. (4.8)

$$z\,'_1 \to z\,'_1 + z_1, \quad z\,'_1 \to z\,'_1\frac{b/2\alpha'_{1D}}{1-b/2\alpha'^2_{1D}}, \quad z\,'_1 \to z\,'_1 + \frac{z\,'_2-z_2}{\alpha'_{1D}} \tag{4.9}$$

we arrive at the following representation for $\bar{U}$

$$\bar{U} = 2\,\frac{U'_{1D}}{\alpha'_{1D}}\int dz_1\,|\phi_0(z_1\,,z_1)|^2 - \frac{2\sqrt{2}}{1-b/2\alpha'^2_{1D}}\int dz_1 dz_2 dz\,'_1 dz\,'_2\,e^{|z\,'_1|}\,|\phi_0(z_1\,,z_2)|^2\,\times$$
$$\left|\phi_0\left(z_1 + z\,'_1\frac{b/2\alpha'_{1D}}{1-b/2\alpha'^2_{1D}} + (z\,'_2-z_2)\frac{b/2\alpha'^2_{1D}}{1-b/2\alpha'^2_{1D}}\,,z\,'_2\right)\right|^2. \tag{4.10}$$

Taking the limit $\alpha'_{1D} \to \infty$ in Eq. (4.10) we obtain a strong coupling expansion

$$\bar{U} = \bar{U}_0 + \frac{1}{\alpha'^2_{1D}}\bar{U}_1 + o\left(\frac{1}{\alpha'^2_{1D}}\right), \tag{4.11}$$

where the linear term dissapeared because of the integration over z'_1 and $\bar{U}_0$, $\bar{U}_1$ are given by equations

$$\bar{U}_0 = 2\frac{U'_{1D}}{\alpha'_{1D}}\int dz_1\,|\phi_0(z_1\,,z_1)|^2 - 4\sqrt{2}\int dz_1 dz_2 dz'_1\,|\phi_0(z_1\,,z_2)|^2\,|\phi_0(z_1\,,z'_2)|^2 \tag{4.12}$$

and

$$\bar{U}_1 = \sqrt{2}\,b^2\int dz_1 dz_2 dz'_2\left[\frac{\partial}{\partial z_1}|\phi_0(z_1\,,z_2)|^2\right]\left[\frac{\partial}{\partial z_1}|\phi_0(z_1\,,z'_2)|^2\right] -$$

$$2\sqrt{2}\,b\int dz_1 dz_2 dz'_2|\phi_0(z_1\,,z_2)|^2\left[|\phi_0(z_1\,,z'_2)|^2 + (z'_2 - z_2)\frac{\partial}{\partial z_1}|\phi_0(z_1\,,z'_2)|^2\right]. \tag{4.13}$$

Minimum of the potential energy is reached at some finite value of b as it follows from Eq. (4.13). Thus, the parameter M in Eq. (2.18) behaves at large α'_{1D} as $M \approx \mathcal{O}(\alpha'^4_{1D})$. To calcuate the leading term of the strong coupling expansion we may deal only with $\bar{U}_0$. The corresponding effective potential obtained in the same manner from Eq. (3.6) is of the form

$$U(z_1\,,z_2\,;\phi_0) = 4\sqrt{2}\int dz_1 dz_2 dz'_2\,\phi_0^2(z_1\,,z_2)\,\phi_0^2(z_1\,,z'_2) -$$

$$4\sqrt{2}\int dz'_1\,\left[\phi_0^2(z_1\,,z'_1) + \phi_0^2(z_2\,,z'_1)\right] + 2\frac{U'_{1D}}{\alpha'_{1D}}\,\delta(z_1 - z_2). \tag{4.14}$$

The same limit $D \to 1$ for the effective mass of Eq. (4.5) creates no problems. Using the symmetry of the wave-function $\phi_0(z_1\,,z_2)$ it can be written as follows:

$$\frac{m^*}{m} = 2 + 8\sqrt{2}\alpha'^4_{1D}\int dz_1 dz_2 dz'_2\left[\frac{\partial}{\partial z_1}|\phi_0(z_1\,,z_2)|^2\right]\left[\frac{\partial}{\partial z_1}|\phi_0(z_1\,,z'_2)|^2\right]. \tag{4.15}$$

We convince ourselves that the bipolaron effective mass and the parameter M are both proportional to α'^4_{1D}, that is, M indeed is close to m^*. It is not equivalent to m^* because we calculate the bipolaron energy only to a leading term of the strong coupling expansion. The same is valid for the spaces of dimensionalities $D = 2,\ 3$. For instance, at $D = 3$ we have from Eq. (3.10)

$$J(\vec{r}) = \frac{1}{2r}(1 - e^{-2r}). \tag{4.16}$$

At large α_{3D} the second term will not contribute and we arrive at the conventional potential energy (3.15).

V. CONCLUSION

To conclude we presented the systematic study of the equations describing large bipolarons in a strong coupling regime in spaces of arbitrary dimensionality. Some of these equations were used previously for $3D$ case. The numerical results for $1D$ case obtained with these equations will be published elsewhere.

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