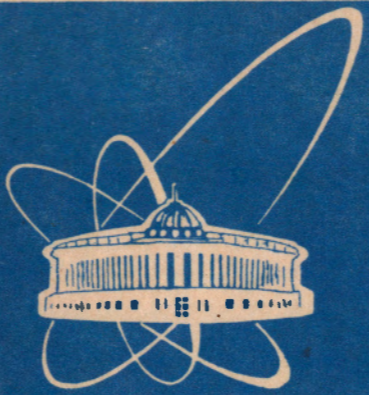

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EQUIVALENCE OF TWO APPROACHES TO BIPOLARONS IN THE STRONG-COUPLING LIMIT

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Эквивалентность двух подходов к проблеме биполяронов в пределе сильной связи

Для описания сильного взаимодействия двух нерелятивистских частиц со скалярным квантованным полем используются два подхода. Более распространен метод, основанный на вариационной технике, где должным образом выбранная пробная волновая функция приводит к точному решению в пределе сильной связи. Другой подход опирается на идеи Боголюбова и Тябликова и учитывает прямым образом трансляционную инвариантность системы. Мы показываем, что оба подхода приводят к одинаковым уравнениям для лидирующего порядка разложения сильной связи. Применение обоих методов продемонстрировано для случая биполяронов.

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Equivalence of Two Approaches to Bipolarons in the Strong-Coupling Limit

Two different approaches are used to describe two non-relativistic particles strongly interacting with a scalar quantum field. A more conventional technique is based on variational trial wave vectors that give exact solutions in the strong-coupling limit. Another approach based on ideas of Bogoliubov and of Tyablikov exploits, in a direct way, the translation invariance of a system. We demonstrate that both approaches result, to leading order, in the same equations. These concepts are applied to the case of bipolarons.

The investigation has been performed at the University of Antwerp (UIA), Belgium and N.N.Bogoliubov Laboratory of Theoretical Physics, JINR.

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I. INTRODUCTION

Two identical charge particles (electrons), placed in a polar medium, interact with the lattice vibrations which results in attractive forces between them. There are conditions when these forces can overcome the direct Coulomb repulsion and a bound state can be formed with two electrons as constituents and a common cloud of virtual phonons around them. Such a quasi-particle is called a *bipolaron*. Possible applications, especially to the hypothetical bipolaron mechanism of high-T_c superconductivity, renewed interest in this problem of two particles strongly interacting with a quantum field. Besides concrete goals such as to calculate characteristics of bipolarons (ground-state energy, effective mass etc.) this system is used also as a tool to clarify more general problems. Among them is the problem of underlying symmetries. In the most popular bipolaron type models one imposes translation-invariance which is to be taken into account before one proceeds further to various approximations. The same type of Hamiltonians was used not only to describe bipolarons but also to study different models of particle and nuclear physics.

Sometimes there arises a misunderstanding in the interpretation of different approaches to the two-particle problem. When one faces an interaction of the type $\hat{V}(\vec{r}_1 - \vec{r}_2)$, one can be sure of the translation-invariance. But this is not the case for bipolaron type systems where the interaction of particles with a field can be represented as a *sum* of terms which depend on coordinates of one particle only: $\hat{V}(\vec{r}_1) + \hat{V}(\vec{r}_2)$. This interaction evidently *would not* be translation-invariant *if* there is no quantum field interacting with both particles. In the presence of a field its quanta take away some part of the total (conserving) momentum so that the latter *is not* a conjugate momentum corresponding to the (particles) center of mass (cms) coordinate $\vec{R} = (\vec{r}_1 + \vec{r}_2)/2$. Applying variational methods to such systems one can take a trial wave vector : $|\psi\rangle = |\vec{R}, \vec{r}, q_{\vec{k}}\rangle$, where $\vec{r} = \vec{r}_1 - \vec{r}_2$ is a relative coordinate and $q_{\vec{k}}$ are field coordinates. A wave vectro $|\psi\rangle$ can be "located" at some point $\vec{R}_c$ in the space. But this does not necessarily mean that the translation-invariance disappeared in such an approximation. If one takes a trial wave vector $|\vec{R} - \vec{R}_0, \vec{r}, q_{\vec{k}}\rangle$ "located" at another point and if this wave vector happens to lead to the same energy, this degeneracy is just another way for the translation-invariance to reveal itself.

The goal of the present paper is to compare two different approaches to the bipolaron type Hamiltonians which conserve translation-invariance. One of these approaches allows us to take into account the translation-invariance from the very beginning, before any approximation is made. Another approach is based on properly

chosen trial wave vectors so that solutions obtained are asymptotically exact in the strong-coupling limit. We demonstrate the equivalence of both approaches.

II. BOGOLIUBOV-TYABLIKOV ADIABATIC THEORY

The conventional Hamiltonian to describe two nonrelativistic particles interacting with a scalar quantum field is given by

$$H = \frac{\vec{p}_1^{\,2}}{2m} + \frac{\vec{p}_2^{\,2}}{2m} + U(|\vec{r}_1 - \vec{r}_2|) + \frac{1}{2}\sum_{\vec{k}} \hbar\omega_{\vec{k}} \left(a_{\vec{k}}^\dagger a_{\vec{k}} + a_{\vec{k}} a_{\vec{k}}^\dagger\right) + \sum_{\vec{k}} |V_{\vec{k}}| \left(e^{i\vec{k}\cdot\vec{r}_1} + e^{i\vec{k}\cdot\vec{r}_2}\right)\left(a_{\vec{k}} + a_{-\vec{k}}^\dagger\right), \tag{2.1}$$

where $\vec{r}_i(\vec{p}_i)$ are the positions (momenta) operators of the i-th particle, m is the particle (bare) mass, $a_{\vec{k}}^\dagger$ ($a_{\vec{k}}$) are the creation (annihilation) operators of the field quantum with wave vector $\vec{k}$ and the frequency $\omega_{\vec{k}}$. The coefficients $V_{\vec{k}}$ are the Fourier transform of the particle-field interaction and $U(r)$ stands for the direct interaction between the particles.

The Hamiltonian (2.1) can be used for different physical systems, in particular, for bipolarons. In this case particles are electrons, m is their band mass, field quanta are phonons whose frequencies obey the Einstein law $\omega_{\vec{k}} = \omega_{\rm LO}$ and coefficients $V_{\vec{k}}$ are specified as follows

$$|V_{\vec{k}}| = \hbar\omega_{\rm LO} \left(\frac{4\pi\alpha}{Vk^2}\sqrt{\frac{\hbar}{2m\omega_{\rm LO}}}\right)^{1/2}. \tag{2.2}$$

The dimensionless electron-phonon coupling constant is defined in the standard way

$$\alpha = \frac{1}{\hbar\omega_{\rm LO}}\frac{e^2}{\sqrt{2}}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)\sqrt{\frac{m\omega_{\rm LO}}{\hbar}}, \tag{2.3}$$

and depends on the static (ϵ_0) and high-frequency (ϵ_∞) dielectric constants. The direct inter-particle interaction is the Coulomb repulsion $U(r) = e^2/\epsilon_\infty r$. When introducing the ratio of the dielectric constants $\eta = \epsilon_\infty/\epsilon_0$, the Coulomb repulsion can be written as follows

$$U(r) = \hbar\omega_{\rm LO}\frac{\sqrt{2}\,\alpha}{1-\eta}\frac{\sqrt{h/m\omega_{\rm LO}}}{r}. \tag{2.4}$$

Introducing center of mass and relative coordinates

$$\vec{r} = \vec{r}_1 - \vec{r}_2, \quad \vec{R} = \frac{\vec{r}_1 + \vec{r}_2}{2}, \tag{2.5}$$

and using complex field coordinates $q_{\vec{k}}$, ($q_{\vec{k}}^\dagger = q_{-\vec{k}}$) instead of creation (annihilation) operators

$$q_{\vec{k}} = \frac{a_{\vec{k}} + a_{-\vec{k}}^\dagger}{\sqrt{2}}, \qquad \frac{\partial}{\partial q_{\vec{k}}} = \frac{a_{-\vec{k}} - a_{\vec{k}}^\dagger}{\sqrt{2}}, \tag{2.6}$$

we write the Hamiltonian (2.1) as follows

$$H = -\frac{\hbar^2}{4m}\nabla_R^2 - \frac{\hbar^2}{m}\nabla_r^2 + U(r) + \frac{1}{2}\sum_{\vec{k}} \hbar\omega_{\vec{k}} q_{-\vec{k}} q_{\vec{k}} + 2\sqrt{2}\sum_{\vec{k}} |V_{\vec{k}}|\, q_{\vec{k}} \cos\frac{\vec{k}\cdot\vec{r}}{2}\, e^{i\vec{k}\cdot\vec{R}} - \frac{1}{2}\sum_{\vec{k}} \hbar\omega_{\vec{k}} \frac{\partial}{\partial q_{-\vec{k}}}\frac{\partial}{\partial q_{\vec{k}}}. \tag{2.7}$$

The idea of Bogoliubov[1] and of Tyablikov[2] developed initially for a single particle interacting with a quantum field is based on an elegant physical picture of the particle motion. The system is translation-invariant, and the symmetry group is defined by

$$\vec{R} \to \vec{R} + \vec{R}_0, \quad q_{\vec{k}} \to q_{\vec{k}} e^{-i\vec{k}\cdot\vec{R}_0}. \tag{2.8}$$

Correspondingly, the total momentum

$$\vec{P} = -i\hbar\nabla_R + \hbar\sum_{\vec{k}} \vec{k}\, a_{\vec{k}}^\dagger a_{\vec{k}} = -i\hbar\nabla_R - \hbar\sum_{\vec{k}} \vec{k}\, q_{\vec{k}}\frac{\partial}{\partial q_{\vec{k}}}. \tag{2.9}$$

is conserved. Bogoliubov and Tyablikov suggested to split up the particle coordinate operator into a translation-invariant part responsible for the momentum conservation and an internal quantum vibrational part. Applied to the two-particle problem this idea can be realized with the transformations

$$\vec{R} = \vec{q} + \vec{\lambda}, \quad q_{\vec{k}} = G_{\vec{k}} e^{-i\vec{k}\cdot\vec{q}}, \tag{2.10}$$

where $G_{\vec{k}}$ are new field coordinate operators. Then the group defined by Eq. (2.8) can be considered as corresponding to the transformation $\vec{q} \to \vec{q} + \vec{R}_0$ of the translation-invariant operator only, while the quantum vibrational coordinate operator $\vec{\lambda}$ and the field coordinate operators $G_{\vec{k}}$ are not influenced.

Because the relative coordinate operator is not involved in the transformations (2.10), the corresponding mathematics is just the same as was developed in Ref. 1, 2

for the one-particle problem. To find details, we refer also to the German translation of these papers in Ref. 3. In what follows we present only the main ideas and results of the Bogoliubov-Tyablikov adiabatic theory.

If the field kinetic energy [the last term in the Hamiltonian (2.7)] were absent, the field coordinate operators would commute with the Hamiltonian and could be considered as c-numbers which would take some definite values. Thus, the authors of Ref. 1, 2 suggested to introduce new field operators $Q_{\vec{k}}$ related to $G_{\vec{k}}$ as follows

$$G_{\vec{k}} = u_{\vec{k}} + Q_{\vec{k}}, \quad u^*_{\vec{k}} = u_{-\vec{k}}, \quad Q^\dagger_{\vec{k}} = Q_{-\vec{k}}, \tag{2.11}$$

where $u_{\vec{k}}$ are c-numbers to be determined later on. This allows us to extract the classical part of the field coordinates which form a well to confine constituent particles. After that $Q_{\vec{k}}$-dependent parts of the Hamiltonian (2.7) are treated as perturbations. Because the resulting Bogoliubov-Tyablikov transformations

$$\vec{R} = \vec{q} + \vec{\lambda}, \quad q_{\vec{k}} = (u_{\vec{k}} + Q_{\vec{k}})e^{-i\vec{k}\cdot\vec{q}} \tag{2.12}$$

introduce an additional dynamical vector variable, one has to add three independent constraints to the operators $Q_{\vec{k}}$. They are chosen as follows

$$\sum_{\vec{k}} \vec{k}\, v^*_{\vec{k}} Q_{\vec{k}} = 0, \tag{2.13}$$

where $v_{\vec{k}}$ are arbitrary complex numbers which satisfy the same relations $v^*_{\vec{k}} = v_{-\vec{k}}$ as field coordinates. Further, to simplify calculations, these numbers are chosen to satisfy an orthogonality condition (without loss of generality, as was shown in Ref. 1, 2)

$$\sum_{\vec{k}} k_i k_j v^*_{\vec{k}} u_{\vec{k}} = \delta_{i,j}, \tag{2.14}$$

Here k_i, k_j are components of the vector $\vec{k}$. With the constraints (2.13) one obtains the same number of independent dynamical variables as in the initial Hamiltonian.

The transformed Hamiltonian depends on the translation-invariant variable $\vec{q}$ via the gradient operator $\partial/\partial\vec{q}$ only. One can prove[1,2] that

$$\frac{\partial}{\partial\vec{q}} = \nabla_R - i\sum_{\vec{k}} \vec{k}\, q_{\vec{k}} \frac{\partial}{\partial q_{\vec{k}}}, \tag{2.15}$$

that is $-i\hbar\nabla_q$ coincides with the total conserved momentum (2.9) of the system, as it should be due to the translation invariance. It can be replaced by a c-number vector

$\vec{P}$. Thus, the translation-invariant coordinates $\vec{q}$ describe a position of the center of mass of a bipolaron. In this way, the translation-invariance of the considered system is taken into account explicitly, and we can proceed further to make approximations.

To take into account the fact that field quanta contribute also to the (non-zero) total momentum $\vec{P}$, we perform a transformation of the wave function

$$\Psi = \exp\left(i\sum_{\vec{k}} s_{\vec{k}} Q_{\vec{k}}\right)\Phi, \tag{2.16}$$

where $s_{\vec{k}}$ are complex c-numbers which satisfy the familiar condition $s^*_{\vec{k}} = s_{-\vec{k}}$ and (again without loss of generality) a constraint

$$\sum_{\vec{k}} \vec{k} u_{\vec{k}} s_{\vec{k}} = 0. \tag{2.17}$$

The transformation (2.16) replaces operators $-i\partial/\partial Q_{\vec{k}}$ by $s_{\vec{k}} - i\partial/\partial Q_{\vec{k}}$. This allows us to extract a classical part of the field contribution to the total momentum too.

Once derivatives are calculated, one arrives at the results[1,2]

$$\begin{aligned} &\frac{\partial}{\partial\vec{R}} = \frac{\partial}{\partial\vec{\lambda}}, \\ &q_{\vec{k}} = u_{\vec{k}} e^{-i\vec{k}\cdot\vec{q}} + O(Q_{\vec{k}}), \\ &\frac{\partial}{\partial q_{\vec{k}}} = ie^{i\vec{k}\cdot\vec{q}}\left(s_{\vec{k}} + i\frac{v_{\vec{k}}}{h}\vec{k}\cdot\vec{P}\right) + O(Q_{\vec{k}}). \end{aligned} \tag{2.18}$$

Here $O(Q_{\vec{k}})$ symbolically stand to show that some terms are omitted. They contribute to the parts of the Hamiltonians considered as *perturbations* in the adiabatic theory. Inserting Eq. (2.18) into the Hamiltonian (2.7) we arrive at the "unperturbed" Hamiltonian which gives the solution to the two-particle problem to leading order of the strong-coupling limit

$$\begin{aligned} H_0 = &-\frac{h^2}{4m}\nabla^2_\lambda - \frac{h^2}{m}\nabla^2_r + U(r) + \frac{1}{2}\sum_{\vec{k}} h\omega_{\vec{k}} u_{-\vec{k}} u_{\vec{k}} \\ &+2\sqrt{2}\sum_{\vec{k}} |V_{\vec{k}}|\, u_{\vec{k}} \cos\frac{\vec{k}\cdot\vec{r}}{2} e^{i\vec{k}\cdot\vec{\lambda}} - \frac{1}{2}\sum_{\vec{k}} h\omega_{\vec{k}} \left|s_{\vec{k}} + i\frac{v_{\vec{k}}}{h}\vec{k}\cdot\vec{P}\right|^2. \end{aligned} \tag{2.19}$$

Note that despite of the translation invariance which allowed us to remove the dependence on the translation-invariant variable $\vec{q}$, the unperturbed Hamiltonian remains essentially the two-particle one. It depends on the relative coordinate operator $\vec{r}$ and on the quantum vibrational coordinate $\vec{\lambda}$. One can then be back to "one-particle coordinate operators" $\vec{\lambda}_1$, $\vec{\lambda}_2$ where

$$\vec{\lambda}_{1(2)} = \vec{\lambda} \pm \frac{\vec{r}}{2}. \tag{2.20}$$

Then the Hamiltonian (2.19) takes the form

$$H_0 = -\frac{\hbar^2}{2m}\nabla^2_{\lambda_1} - \frac{\hbar^2}{2m}\nabla^2_{\lambda_2} + U(|\vec{\lambda}_1 - \vec{\lambda}_2|) + \frac{1}{2}\sum_{\vec{k}} h\omega_{\vec{k}} u_{-\vec{k}} u_{\vec{k}}$$
$$+\sqrt{2}\sum_{\vec{k}} |V_{\vec{k}}|\, u_{\vec{k}} \left(e^{i\vec{k}\cdot\vec{\lambda}_1} + e^{i\vec{k}\cdot\vec{\lambda}_2}\right) + \frac{1}{2}\sum_{\vec{k}} h\omega_{\vec{k}} \left| s_{\vec{k}} + i\frac{v_{\vec{k}}}{\hbar}\vec{k}\cdot\vec{P}\right|^2. \tag{2.21}$$

It follows then that H_0 does not depend on the field operators $Q_{\vec{k}}$ so that the wave function to leading order takes the form $\Phi = \phi(\vec{\lambda}_1, \vec{\lambda}_2)\theta(Q_{\vec{k}})$, where a function θ is undefined while dealing with the unperturbed Hamiltonian H_0.

The first "correction" H_1 to the Hamiltonian H_0 (which is not displayed here) is linear in the operators $Q_{\vec{k}}$, $\partial/\partial Q_{\vec{k}}$. Therefore, following arguments by Bogoliubov and Tyablikov, its average $\langle\phi|H_1|\phi\rangle$ over $\phi(\vec{\lambda}_1, \vec{\lambda}_2)$ equals zero. This provides solutions for the parameters $s_{\vec{k}}$ and $u_{\vec{k}}$, unspecified before. For instance

$$s_{\vec{k}} = -i\frac{v^*_{\vec{k}}}{\hbar}\vec{k}\cdot\vec{P} + i\frac{u^*_{\vec{k}}}{\omega_{\vec{k}}}\vec{k}\cdot\vec{V}, \tag{2.22}$$

where $\vec{V}$ is a mean velocity of a system as a whole. Inserting $s_{\vec{k}}$ from Eq. (2.22) into the constraint (2.17) and using the condition (2.14) one obtains a relation of $\vec{V}$ to the total momentum $\vec{P}$:

$$\vec{P} = h\sum_{\vec{k}} \vec{k}\frac{\vec{k}\cdot\vec{V}}{\omega_{\vec{k}}} u_{-\vec{k}} u_{\vec{k}}. \tag{2.23}$$

The expression for the coefficients $u_{\vec{k}}$ which follows from the equation $\langle\phi|H_1|\phi\rangle = 0$ can be determined also by minimizing the average $\langle\phi|H_0|\phi\rangle$ with respect to $u_{\vec{k}}$. Taking into account Eq. (2.22) one obtains in this way

$$u_{\vec{k}} = -2\sqrt{2}\frac{\omega_{\vec{k}} V^*_{\vec{k}} \rho^*_{\vec{k}}}{h\omega^2_{\vec{k}} - (\vec{k}\cdot\vec{V})^2} \tag{2.24}$$

with the notation

$$\rho_{\vec{k}} = \frac{1}{2}\int d\vec{\lambda}_1 d\vec{\lambda}_2 \,|\phi(\vec{\lambda}_1, \vec{\lambda}_2)|^2 \left(e^{i\vec{k}\cdot\vec{\lambda}_1} + e^{i\vec{k}\cdot\vec{\lambda}_2}\right). \tag{2.25}$$

With these parameters $s_{\vec{k}}$, $u_{\vec{k}}$ taken at $\vec{V} = 0$ and after inserting into the Hamiltonian (2.21) one arrives finally at the Hamiltonian H_{00} which describes a bipolaron at rest to leading order of the "adiabatic" limit

$$H_{00} = -\frac{\hbar^2}{2m}\nabla^2_{\lambda_1} - \frac{\hbar^2}{2m}\nabla^2_{\lambda_2} + V_{eff}(\vec{\lambda}_1, \vec{\lambda}_2; \phi),$$
$$V_{eff} = U(|\vec{\lambda}_1 - \vec{\lambda}_2|) + 4\sum_{\vec{k}} \frac{|V_{\vec{k}}|^2}{h\omega_{\vec{k}}} |\rho_{\vec{k}}|^2 - 4\sum_{\vec{k}} \frac{|V_{\vec{k}}|^2}{h\omega_{\vec{k}}} \rho^*_{\vec{k}} \left(e^{i\vec{k}\cdot\vec{\lambda}_1} + e^{i\vec{k}\cdot\vec{\lambda}_2}\right). \tag{2.26}$$

Denote $\phi(\vec{\lambda}_1, \vec{\lambda}_2)$ as the ground-state wave function. It is obtained as a solution to the Schrödinger equation $(H_{00} - E)\phi = 0$.

The last term in the Hamiltonian (2.21) together with the expansion of $u_{\vec{k}}$ in powers of $\vec{V}$ lead to the expression for the bipolaron effective mass within the same approximation. It is given by

$$M = \frac{8}{3}\sum_{\vec{k}} (\hbar\vec{k})^2 \frac{|V_{\vec{k}}|^2 |\rho_{\vec{k}}|^2}{(h\omega_{\vec{k}})^3}. \tag{2.27}$$

Relations (2.26),(2.27) complete the solution to leading order of the adiabatic limit for slowly moving bipolarons.

III. COMPARISON OF RESULTS

Let us turn now to another approach to the same two-particle problem as considered in Ref. 4. For simplicity we consider now the case of zero total momentum. Then the scheme is as follows: canonical transformations are used to shift the creation (annihilation) operators by c-numbers $a_{\vec{k}} \to c_{\vec{k}} + a_{\vec{k}}$. This means that the classical part of the field is extracted in this scheme too (and $c_{\vec{k}}$ differs from $u_{\vec{k}}$ by a constant factor only). Subsequently a trial wave vector is chosen in the form $|\Phi\rangle = \phi(\vec{r}_1, \vec{r}_2)|0\rangle$. The coefficients $c_{\vec{k}}$ are found by minimizing the average energy $\langle\Phi|H|\Phi\rangle$. Because $u_{\vec{k}}$ can be thus determined too, one finally arrives at the same Hamiltonian (2.26) with the only (formal) difference that we deal with variables $\vec{r}_1$, $\vec{r}_2$ instead of their quantum vibrational parts $\vec{\lambda}_1$, $\vec{\lambda}_2$. The expression for the bipolaron effective mass derived in this scheme coincides also with Eq. (2.27).

We describe this "variational" scheme very briefly now. There are peculiarities which are not so important for the moment. Details can be found in Ref. 4. Use is made in this scheme of a trial wave vector which leads some authors to think that the translation-invariance is broken in this approach. This is not the case, however, despite the fact that the final effective potential in Eq. (2.26) *does not* depend solely on the relative coordinates $\vec{r}$. The classical parts of the field operators depend on the wave function $\phi(\vec{\lambda}_1, \vec{\lambda}_2)$ too. Let us shift the reference point by a vector $\vec{R}_0$. When one takes a wave function $\phi(\vec{\lambda}_1 - \vec{R}_0, \vec{\lambda}_2 - \vec{R}_0)$ "localized" at another point, the only

change is that $\rho_{\vec{k}} \to \rho_{\vec{k}} \exp(i\vec{k}\cdot\vec{R}_0)$. Because the modulus of $\rho_{\vec{k}}$ is not changed, this leads to the same effective potential which is just translated by the vector $\vec{R}_0$: $V_{eff}(\vec{\lambda}_1,\vec{\lambda}_2;\phi) \to V_{eff}(\vec{\lambda}_1-\vec{R}_0,\vec{\lambda}_2-\vec{R}_0;\phi)$. Thus, the effective potential follows a shift of a wave function and the bipolaron energy evidently is not influenced by this translation. This means that even on the level of the effective Schrödinger equation the translation-invariance of the system is still preserved.

It is important to mention that both schemes lead to the same energy functional

$$E = -\frac{\hbar^2}{2m}\langle\nabla^2_{\lambda_1}\rangle - \frac{\hbar^2}{2m}\langle\nabla^2_{\lambda_2}\rangle + \langle U(|\vec{\lambda}_1-\vec{\lambda}_2|)\rangle - 4\sum_{\vec{k}}\frac{|V_{\vec{k}}|^2}{\hbar\omega_{\vec{k}}}|\rho_{\vec{k}}|^2. \qquad (3.1)$$

Applied to bipolarons with Eq. (2.2), (2.4) it takes the form

$$E = \frac{\hbar^2}{m}\int d\vec{\lambda}_1 d\vec{\lambda}_2\,|\nabla_{\lambda_1}\phi(\vec{\lambda}_1,\vec{\lambda}_2)|^2 + \hbar\omega_{\rm LO}\,\frac{\sqrt{2}\alpha}{1-\eta}\sqrt{\frac{\hbar}{m\omega_{\rm LO}}}\int d\vec{\lambda}_1 d\vec{\lambda}_2\,\frac{|\phi(\vec{\lambda}_1,\vec{\lambda}_2)|^2}{|\vec{\lambda}_1-\vec{\lambda}_2|}$$

$$-\hbar\omega_{\rm LO}\,2\sqrt{2}\alpha\sqrt{\frac{\hbar}{m\omega_{\rm LO}}}\int d\vec{\lambda}_1 d\vec{\lambda}_2 d\vec{\lambda}'_1 d\vec{\lambda}'_2\,\frac{|\phi(\vec{\lambda}_1,\vec{\lambda}_2)|^2\,|\phi(\vec{\lambda}'_1,\vec{\lambda}'_2)|^2}{|\vec{\lambda}_1-\vec{\lambda}'_1|}. \qquad (3.2)$$

While deriving (3.2), symmetry properties of the wave function with respect to particles permutations were taken into account. The energy functional (3.2) which should be minimized with respect to ϕ appeared first in the pioneering paper by Pekar and Tomasevich[5] and was used by many authors afterwards (for references see the review paper[6]). We demonstrated for both approaches: 1) the coincidence of the "unperturbed" Hamiltonians, energies and effective masses and 2) the fact that the "variational" approach preserves the translation-invariance too. Thus, both schemes are equivalent.

It should be noted also that the Bogoliubov-Tyablikov approach was applied to the two-particle problem already in Ref. 7. The authors splitted up both the cms and the relative-coordinates operators. This made the scheme much more complicated. We see no reasons to split up the relative coordinate operator, that is not related to the symmetry group (2.8).

An attempt to exploit the Bogoliubov-Tyablikov technique for the two-particle problem was undertaken recently by V. D. Lakhno. The author applied his model to bipolarons[8–10], to deuterons[11] and to binucleons[12]. Unfortunately, all his results are not reliable. The main reason is that he splitted up the cms-coordinate operator in an inconsistent way, so that the dependence on the quantum vibrational coordinate $\vec{\lambda}$ disappeared from the interaction term [namely, the exponent $\exp(i\vec{k}\cdot\vec{\lambda})$ is not present in his version of the Hamiltonian (2.19)]. This resulted essentially in a one-particle

Hamiltonian which can be obtained if one sets $\vec{R}_i = 0$ in the initial Hamiltonian (2.7). Thus, the author of Ref. 8 allows the system to be at the bottom of the effective potential corresponding to the motion of the system as a whole. This leads to a significant decrease of the bipolaron energy. Critical comments on this paper are given in Ref. 13. Note also that the technique of Ref. 8 applied to a single polaron would lead to the Hamiltonian

$$H_s = \frac{\vec{p}^2}{2m} + \sum_{\vec{k}}\hbar\omega_{\vec{k}}\,a^\dagger_{\vec{k}}a_{\vec{k}} + \sum_{\vec{k}}|V_{\vec{k}}|(a_{\vec{k}}+a^\dagger_{\vec{k}}). \qquad (3.3)$$

Then, the problem can be solved explicitly; but this Hamiltonian results in the ground-state energy

$$E_s = -\sum_{\vec{k}}\frac{|V_{\vec{k}}|^2}{\hbar\omega_{\vec{k}}} = -\hbar\omega_{\rm LO}\alpha\frac{\sqrt{\hbar/2m\omega_{\rm LO}}}{r_C}, \qquad (3.4)$$

where a cut-off r_C of the effective Coulomb potential is introduced at small r. Thus, this energy tends to (negative) infinity when $r_C \to 0$. This demonstrates that the scheme of Ref. 8 indeed corresponds to energies which are significantly lower in comparison with the correct quantum results.

To conclude, we analyzed two (seemingly different) approaches to the problem of two interacting particles and proved their equivalence to leading order of the adiabatic limit.

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REFERENCES

[1] N. N. Bogoliubov, Ukrainski Mat. Zh. **2**, 3 (1950);

[2] S. V. Tyablikov, JETP **21**, 377 (1951).

[3] *Polaronen*, ed. G. Höhler, Akademie-Verlag, Berlin, 1961, pp. 1-22, 23-36.

[4] P. Vansant, M. A. Smondyrev, F. M. Peeters, and J. T. Devreese, J. Phys. A: Math. Gen. **27**, 7925 (1994).

[5] S. I. Pekar and O. F. Tomasevich, JETP **21**, 1218 (1951).

[6] M. A. Smondyrev and V. M. Fomin. *Pekar-Fröhlich Bipolarons*. In: 'Polarons & Applications', ed. V. D. Lakhno, J. Wiley, NY, 1994, pp. 13-71.

[7] E. P. Solodovnikova and A. N. Tavkhelidze, Teor. Mat. Fiz. **21**, 13 (1974).

[8] V. D. Lakhno, Phys. Rev. B **51**, 3512 (1995).

[9] V. D. Lakhno and G. N. Chuev, Physics: uspekhi (1995) (to be published).

[10] V. D. Lakhno. "*Adiabatic Theory of Bipolarons*". In: Proceedings of the N. N. Bogoliubov International Symposium "Fundamental Problems in Theoretical & Mathematical Physics", August 1994, Dubna, Russia.

[11] V. D. Lakhno, Teor. Mat. Fiz. **100**, 219 (1994).

[12] I. V. Amirkhanov, I. V. Puzynin, T. P. Puzynina, T. A. Strizh, and V. D. Lakhno. "*Quantum Field Theory of Binucleons*". Talk given at the International Conference "Deuteron-95", July 1995, Dubna, Russia.

[13] M. A. Smondyrev and J. T. Devreese, subm. to Phys. Rev. B (1995).

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