Physics – Uspekhi **41** (4) 403 – 406 (1998)

METHODOLOGICAL NOTES PACS number: **71.38.+i**

Translation invariance and the problem of the bipolaron

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Contents

Abstract. Differences between translation-invariant and broken-symmetry bipolaron theories are analyzed in detail. It is shown that the Bogolyubov – Tyablikov canonical transformation allows collective coordinates to be introduced in a regular way for two particles in a quantum field and that for the case of the bipolaron the resulting electron-electron interaction in a phonon field depends on the electron coordinate difference alone. Predictions using a revised solution of the nonlinear differential equations for a bipolaron are given. It is shown that solving bipolaron equations numerically reduces the total bipolaron energies compared to known variational results.

1. Introduction

One of the main results of quantum field theory is the statement that the interaction between the particles is caused by the exchange of field quanta. In the case of two particles in a homogeneous isotropic medium this interaction can only depend on the difference in the particle coordinates. The problem of the nature of the interaction between two particles spaced from each other has always attracted the attention of physicists. It will suffice to recall the prolonged debates about the long-range or short-range character of the influence of bodies on each other. In Newtonian mechanics the mutual influence of bodies on each other is characterized by a force. According to Newton's third law, the forces influencing both the particles are equal and opposite, i.e.

$$\frac{\partial U}{\partial \mathbf{r}_1} = -\frac{\partial U}{\partial \mathbf{r}_2}\,, \tag{1}$$

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Received 30 July 1997, revised 27 January 1998
Uspekhi Fizicheskikh Nauk **168** (4) 465 – 469 (1998)
Translated by V D Lakhno; edited by A Radzig

where $\mathbf{r_1}$ and $\mathbf{r_2}$ are the coordinate vectors of both the particles, and $U(\mathbf{r_1}, \mathbf{r_2})$ is the potential energy of the interparticle interaction. Relation (1) can be derived from a fundamental property of the system under consideration, i.e. its translation invariance. Indeed, the interaction energy $U(\mathbf{r_1}, \mathbf{r_2})$ in a homogeneous isotropic medium does not change if we simultaneously displace both the particles by a distance $\mathbf{a}$:

$$U(\mathbf{r}_1, \mathbf{r}_2) = U(\mathbf{r}_1 + \mathbf{a}, \mathbf{r}_2 + \mathbf{a})\,. \tag{2}$$

Since relation (2) is valid for any displacement $\mathbf{a}$, it is fulfilled only if

$$U(\mathbf{r}_1, \mathbf{r}_2) = U(\mathbf{r}_1 - \mathbf{r}_2)\,. \tag{3}$$

Thus, Newton's third law is a consequence of the homogeneity and isotropy of a medium. In classical mechanics, however, such a formulation of Newton's third law is not commonly used, because, when postulating the third law, Newton meant a contact interaction of bodies rather than an interaction via a field.

The statement that the interaction between two particles only depends on the difference in their coordinates is general and central to the contemporary theory of interacting particles. In particular, it was shown in Ref. [1] that the interaction between two electrons in a phonon field is only determined by the difference in the electron coordinates, the result being true for any constant of the electron-phonon coupling. This result is however in contradiction with well-known results of strong coupling bipolaron theory.

Recall that a bipolaron represents a system of two electrons coupled with each other due to a strong interaction with the medium. In polar crystals an electron interacts with a phonon field. Thus, a bipolaron in polar crystals can be considered as two coupled polarons. According to the bipolaron model, which was first suggested by S Pekar, the lattice polarization is assumed to be static. It induces a potential coupling electrons with opposite spins, and the electrons maintain polarization through their electric fields, i.e. the arising state is self-consistent and the symmetry of the

total system appears to be spontaneously broken. Subsequently, the term 'bipolaron' acquired a wider meaning and now refers to electrons interacting with any phonons, magnons and other quasi-particles.

The main goal of this paper is to discuss most thoroughly the physical situation arising in the description of two particles in a quantum field and to consider a mathematical approach to describing a strong particle-field interaction. Since the approach suggested is independent of the details of the interaction between two particles, it can be applied to various cases of interaction of particles with a quantum field.

The problems to be discussed are not new. They first arose in the attempt to develop a translation-invariant theory for one particle strongly interacting with a quantum field. As we show below there is no consensus now even in this simplest case. We hope that this discussion will help to clear up the differences between the translation-invariant theories and the theories with broken symmetry.

2. Physical reasons for the introduction of collective coordinates in the bipolaron problem

In the polaron case the electron interacts with the medium's polarization induced by the electron itself. Thus, the electron resides in a potential field $\varphi(r - r_0)$, where r_0 defines the position of the potential well induced by the polarization. In an isotropic homogeneous medium r_0 can be arbitrary. If the field φ was classical, the value r_0 (in the reference system where the polaron rests), once chosen, would remain fixed. In quantum theory two approaches are possible. Either the well can be considered fixed in space $r_0 = \text{const}$, which corresponds to the case of broken symmetry, or the well is not spatially fixed and executes fluctuative motions so that it can be found at any point in space with equal probability. This latter case corresponds to the conservation of the translation symmetry of the initial problem.

Historically, the polaron theory originally dealt with the former approach based on the Pekar semiclassical theory [2]; the potential well was considered spatially fixed. The subsequent quantum-field description of the polaron, the foundation of which was laid by Fröhlich [3], remained, in fact, within the same paradigm. The most representative is the quotation from Ref. [4]: *'Self-trapping of an electron or a hole presents an interesting example of a situation where the reasoning of symmetry or group theory can lead to erroneous results.'*

The latter approach is based on papers by Bogolyubov and Tyablikov [5, 6] who did not consider the potential well as fixed in space. However, though the initial Hamiltonian was written with a fixed potential well, the degeneration of the Hamiltonian with respect to r_0 was nevertheless taken into account from the outset. This is achieved by the introduction of a collective coordinate (more precisely, a group coordinate). The electron radius-vector $\mathbf{r}$ is presented then as $\mathbf{r} = \mathbf{q} + \lambda$, where $\mathbf{q}$ is the translation-invariant part of the electron coordinates, and λ is the fluctuating part. All the results in Refs [5, 6] are written in the coordinates $\mathbf{q}$ and λ which have mathematical rather than physical meaning. In the case of one particle this situation is quite natural, since in physically meaningful coordinates a potential well possessing translation invariance must not depend on coordinates at all. This would correspond to the existence of solutions only in the form of plane waves.

As the theory with broken symmetry does not introduce physically meaningless variables it has accepted wide recognition, while the translation-invariant approach has been dealt with in only a few works. It is essential that in the case of one polaron both approaches, i.e. that with broken symmetry and the translation-invariant approach, yield the same result in the zero approximation.

The situation changes, however, if we consider two particles in a field. The Hamiltonian of the particle-field interaction H_{int} will be

$$H_{\text{int}} = e\varphi(r_1 - r_0) + e\varphi(r_2 - r_0)\,, \tag{4}$$

where r_1 and r_2 are the coordinates of the first and the second particles, respectively. The fact that the interaction between two particles in an isotropic and homogeneous system depends only on the distance between the particles has never been doubted. In quantum field theory this result follows immediately when the interaction is weak and can be taken into account by the perturbation theory. Suppose, for example, that Hamiltonian (4) describes the interaction of two nonrelativistic particles with a scalar field. Since the interaction is linear in field operators, H_{int} can be written as

$$H_{\text{int}} = \sum_k gC_k \Big\{ b_k^+ \exp\big[-\mathrm{i}(\mathbf{r}_1 - \mathbf{r}_0)\mathbf{k}\big] + b_k \exp\big[-\mathrm{i}(\mathbf{r}_2 - \mathbf{r}_0)\mathbf{k}\big] + \text{H.-c.}\Big\}, \tag{5}$$

where g is the coupling constant of the particle-field interaction, C_k are some constants of the particle-field interaction, and b_k^+, b_k are the operators of creation and annihilation of the field quanta with energy $\omega(k)$. For second order perturbation theory the above interaction takes on the form

$$U(\mathbf{r}_1 - \mathbf{r}_2) = -2\sum_k g^2 \frac{|C_k|^2}{\omega_k} \cos\mathbf{k}(\mathbf{r}_1 - \mathbf{r}_2)\,. \tag{6}$$

It follows that the interaction caused by the exchange of the field quanta depends only on the difference in the particle coordinates. It should be emphasized that the inference about the dependence of the interparticle interaction only on the coordinate difference is valid in any order of the perturbation theory. The second order of perturbation theory is considered here only for interaction (6) to be written in an explicit form. An interaction of the form (6), obtained with the use of perturbation theory, provides the basis for many theories, particularly, for the theory of nucleon-nucleon interaction caused by the exchange of the meson-field quanta [7].

The most troublesome is the other limiting case, when $g \gg 1$, i.e. the case of a strong particle-field interaction. In the theories with broken symmetry (semiclassical theories) the field φ in (4) in the zero approximation is considered as classical, which is consistent with the intuitive idea of the motion of a particle in a fixed potential well. Thus, in this case the interaction depends on each individual coordinates of the particles and is not translation-invariant. The particles move in a potential well whose position is fixed in space. The situation is quite similar to a quantum field if r_0 is fixed. In this event the bipolaron theory leads to an interaction which only depends on the individual vectors r_1 and r_2, and thereby is not translation-invariant in physical variables.

In the translation-invariant theories this intuitive idea appears wrong. Actually, even in the limit $g \to \infty$ the idea of the existence of a classical component in the solution to a translation-invariant quantum problem is untrue. Thus, for example, in the case of a strong coupling polaron, which is the simplest example of a particle interacting with a quantum field, the Bogolyubov transformation converts the classical static solution to an operator where only the group variable q, which is the functional of the field operators, responds to the translation transformations.

The bipolaron theory where the potential well is not spatially fixed, i.e. r_0 is considered as a collective variable, was developed in Ref. [1]. The fundamental difference of the case of two particles from that of one particle is in the fact that the translation-invariant theory for two particles can be built in physical coordinates. The reason is that in this event there is a translation-invariant and nonconstant expression, given by the interaction of two particles with the field, which only depends on the difference in the particle coordinates.

3. Introduction of collective coordinates in the bipolaron theory

To introduce collective coordinates, following Ref. [1], we pass from the coordinates of particles $\mathbf{r}_1$ and $\mathbf{r}_2$ in Hamiltonian (5) to the coordinates of their centre of mass $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ and the relative coordinates $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$. In what follows the quantity r_0 in (5) will be considered as a collective coordinate rather than a fixed position of the potential well. It should be reiterated that the Hamiltonian of a system in which collective coordinates are not introduced and the Hamiltonian which immediately includes collective coordinates describe one and the same physical system. The collective coordinates are introduced in order to develop a translation-invariant theory. Using the complex coordinates of the field q_k related to operators of the creation and annihilation of the field quanta b_k^+, b_k as

$$q_k = \frac{\epsilon(b_k + b_{-k}^+)}{\sqrt{2}}, \qquad -\mathrm{i}\,\frac{\partial}{\partial q_k} = \frac{\mathrm{i}(b_k^+ - b_{-k})}{\epsilon\sqrt{2}}, \tag{7}$$

where ϵ is a dimensionless small parameter introduced with the aim of showing explicitly that the oscillator frequencies $\omega_k = \epsilon^2 v_k$ are small, we express Hamiltonian (2) in the form

$$H_{\mathrm{int}} = \sum_k 2A_k \cos\frac{\mathbf{kr}}{2} \exp\left[\mathrm{i}\mathbf{k}(\mathbf{R} - \mathbf{r}_0)\right] q_k\,,$$

$$A_k = \frac{\sqrt{2} g C_k}{\epsilon}\,. \tag{8}$$

In the translation-invariant bipolaron theory Hamiltonian (8) is invariant with respect to the translational group $R \to R + a$, $q_k \to q_k \exp(-\mathrm{i}ka)$. These transformations determine the choice of the collective coordinates in the bipolaron Hamiltonian in the form

$$\mathbf{R} = \mathbf{r}_0 + \mathbf{q}\,, \tag{9}$$

where r_0 represents the fluctuating part of the coordinates, and all the translations are applied to the coordinate q. According to (9), the electron centre of mass fluctuates together with the position of the potential well. In this case rectilinear and steady motion of the electrons is described by the collective coordinate q. Let us replace the coordinates q_k by the complex field coordinates Q_k:

$$q_k = (U_k + \epsilon Q_k) \exp\left[-\mathrm{i}(kq)\right]. \tag{10}$$

Since the total number of dynamic variables for the system of two electrons plus the field must be conserved, the new coordinates (10) must meet several additional conditions

$$\sum_k \mathbf{k} v_k^* Q_k = 0\,, \tag{11}$$

where v_k are the complex numbers, satisfying the condition of reality $v_{-k} = v_k^*$ and the condition of orthogonality

$$\sum_k k^\alpha k^\beta v_k^* U_k = \delta_{\alpha\beta}\,. \tag{12}$$

Relations (9)–(12) represent a canonical transformation which was first used by Bogolyubov and Tyablikov in the polaron theory.

Substituting in (8) the new variables $\mathbf{r}_0, \mathbf{q}, Q_k$ instead of $\mathbf{R}$, q_k and taking into account the confinement (11), (12) we obtain for the total Hamiltonian in [1] the expansion $H = H_0 + \epsilon H_1 + \epsilon^2 H_2 + \ldots$ In doing so the zero order Hamiltonian contains an interaction which depends only on the relative coordinates of two particles $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$:

$$U(\mathbf{r}_1 - \mathbf{r}_2) = 4\sum_k \frac{|A_k|^2}{v_k} \int \cos\frac{\mathbf{kr}}{2} \left|\psi(r)\right|^2 \mathrm{d}^3 r \cos\frac{\mathbf{k}}{2}(\mathbf{r}_1 - \mathbf{r}_2)\,, \tag{13}$$

where $\psi(r)$ is the wave function.

It should be reiterated that the interaction between two particles is only determined by the difference in the particle coordinates, and this conclusion is independent of the value of the coupling constant. The parameter ϵ (strong coupling) was taken small only to express interaction (13) explicitly.

The results of Ref. [1] whose main concepts are presented above, can be applied to the case of one particle. The energy of the particle-field interaction will be written as

$$U = \sum_k 2g^2 \frac{|C_k|^2}{\omega_k}\,. \tag{14}$$

This expression diverges if C_k is the interaction of the electron with longitudinal polarization phonons. It should be pointed out regarding this conclusion that, as was shown above in the case of one particle, the translation-invariant approach based on the description of the particle in physically meaningful coordinates leads to the interaction energy (14), which is independent of the particle coordinates. Therefore, expression (14) does not lead to any contradictions. Moreover, it exactly corresponds to the expression for the small-radius polaron energy: $U = e^2/\tilde{\epsilon} r_{\mathrm{p}}$, where r_{p}^{-1} stands for the upper limit at which the sum (14) is cut out. The physical reason for this correspondence is quite clear. According to Ref. [1], the electron in this situation fluctuates together with the polarization potential well, which instantly follows its motions.

4. Numerical calculations

The potential energy (13) involved in the Schrödinger equation for two particles in a field in the limiting case of a strong coupling can be considered as an exact result of the translation-invariant theory. The phrase 'exact solution of a

Table 1.

η	0	0.053	0.094	0.132	0.166	0.199	0.228	0.256	0.282	0.305	0.317
E_{L1}	−1.36	−1.28	−1.22	−1.15	−1.09	−1.03	−0.97	−0.92	−0.86	−0.81	−0.78
E_{L2}	−1.41	−1.33	−1.25	−1.19	−1.12	−1.05	−0.99	−0.93	−0.87	−0.82	−0.79
E_L	−1.44	−1.35	−1.28	−1.21	−1.15	−1.08	−1.02	−0.96	−0.90	−0.85	−0.82

two-particle problem in a quantum field' was used in paper [1] in just this sense. In truth, the nonlinear differential equations obtained for the bipolaron in Ref. [1] have no analytical solution and were integrated approximately.

The authors of Refs [8, 9] applied probe wave functions to these equations and obtained a total bipolaron energy less than in Ref. [1]. So, the numerical solutions in Ref. [1] were not of very high accuracy. The discrepancy is $7-14\%$. Table 1 compares the results of calculations for the total energy of the bipolaron E_{L1} obtained by probe functions (9) in paper [8], E_{L2} obtained by probe functions (11) in the same paper [8], and E_L found from improved numerical integration [10] of the system (43) from Ref. [1]. It is seen that E_L is less than the values obtained by the variational computations of E_{L1} and E_{L2}. The deviation of the results listed in Tables 1–3 of Ref. [1] from those obtained with the use of improved solutions is approximately 5% [10]. The results of improved calculations of other physical quantities significant in the bipolaron theory are given in Refs [10, 11].

5. Various versions of translation-invariant theories

Historically, the Bogolyubov–Tyablikov theory was one of the first translation-invariant theories considering the problem of retaining the symmetry properties of the Hamiltonian, which were lost as a result of separation of the classical part of the boson field. The methodological significance of this theory lies in the fact that a system with a constraint was quantized for the first time. As distinct from classical mechanics, where the study of systems with constraints is reduced to solving a conditional extremum problem, in the quantum theory there is no universal approach to the solution of such problems. The consideration of systems with constraints within quantum field theory became an actual problem as late as a quarter of century after the publication of the Bogolyubov–Tyablikov papers. They attracted interest in the context of the problem of quantization in the curved space and the problem of quantizing nonperturbative solutions of the field theory, such as kinks, instantons, solitons, etc. Nowadays various approaches have been developed in quantum field theory in which collective coordinates are introduced immediately in the initial Hamiltonian just as r_0 in expressions (4), (5). There are various ways of imposing additional conditions which are used to keep the total number of variables in the system constant. For example, expanding a field into a Fourier series, the authors of Refs [12, 13] do not use the Bogolyubov–Tyablikov condition, and from the outset reduce the number of Fourier components by a number equal to the number of collective variables introduced.

In the bipolaron theory, the Bogolyubov–Tyablikov method was used in papers [14, 15]. In these works the Bogolyubov–Tyablikov transformation was applied to Hamiltonian (5) but collective coordinates were not introduced. In this approach the zero approximation yields the same results as in the theories with broken symmetry. As in the case of the polaron these theories manipulate only split, physically meaningless coordinates. Thus, a physical theory which would use only physical variables, such as relative coordinates $r = r_1 - r_2$ and the potential energy $U(r_1 - r_2)$, was not developed in these works.

In the previous discussion we considered in detail the behaviour of particles in nonrelativistic quantum field theory. In the relativistic theory, the analysis of the problem should include the retardation of the interaction caused by the finiteness of the signal propagation. Since the corresponding field equations in the relativistic theory are formulated in terms of variables unaffected by symmetry transformations, in particular, by space-time transformations, the conclusion about the dependence of the interaction on the difference in the particle coordinates only is valid in this case as well.

In summary it should be noted that the method of introducing collective coordinates and the Bogolyubov–Tyablikov transformation in a two-particle problem considered in this work was applied to the deuteron problem [16]. This approach yields a physically correct result for nuclear forces which only depend on the difference in the nucleon coordinates.

In conclusion the author expresses his gratitude to V K Fedyanin, N M Plakida, I V Puzynin, G N Chuev, V A Osipov and E A Kochetov for numerous discussions and valuable comments.

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