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Pekar's ansatz and the strong coupling problem in polaron theory

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Abstract. The translationally invariant polaron theory of Tulub, which does not involve Pekar's ansatz (believed to provide an asymptotically exact solution in the strong-coupling limit) and fundamentally produces a lower-energy polaron than when using the ansatz, is discussed in detail. For the bipolaron, the theory yields the best values for bonding energy and for critical stability parameters. A variety of physical implications of the existence of translationally invariant polarons and bipolarons are discussed.

Keywords: Fröhlich Hamiltonian, Lee–Low–Pines transformation, weak coupling, Bose condensate, F-center

1. Introduction. Pekar's ansatz

The polaron theory is known to be one of the first theories describing the particle–quantum-field interaction. Its various aspects are dealt with in many books and review articles [1–10]. Being nonrelativistic, the theory does not contain divergences; for over 60 years, it has provided a platform for testing methods of quantum field theory. Although the exact solution of the polaron problem remains to be found, it is believed that the main properties of the polaron ground state are known fairly well, first and foremost in the limit cases of weak and strong coupling. The solution in the weak-coupling limit was proposed by Fröhlich [11] and in the strong-coupling limit by Pekar [1, 12]. The polaron ground state energy E_0 in the weak-coupling limit was found with a high accuracy in Refs [13, 14]:

$$E_0 = -(\alpha + 0.0159196220\alpha^2 + 0.000806070048\alpha^3 + \ldots)\hbar\omega_0\,, \tag{1.1}$$

where $\hbar\omega_0$ is the optical phonon energy and α is the electron–phonon coupling constant.

The solution in the opposite (strong-coupling) limit was found by Pekar under the assumption that the wave function Ψ of the electron + field system has the form

$$\Psi(r, q_1, \ldots, q_i, \ldots) = \psi(r)\,\Phi(q_1, \ldots, q_i, \ldots)\,, \tag{1.2}$$

where $\psi(r)$ is the electron wave function, depending on the electron coordinates alone, and Φ is the field wave function, depending solely on the field coordinates. Pekar himself regarded ansatz (1.2) as an approximate solution (see his fundamental monograph [1]). The pioneering work of Bogoliubov and Tyablikov [15, 16] demonstrated that the use of ansatz (1.2) (for the split coordinates introduced in [15, 16]) in a consistent translationally invariant theory gives the same results for the polaron ground state energy as in the semiclassical Pekar theory [1, 12]. The ground state energy was determined with a high accuracy using relation (1.2) in Refs [17, 18]:

$$E_0 = (-0.108513\alpha^2 - 2.836)\hbar\omega_0\,. \tag{1.3}$$

The view of Pekar's ansatz (1.2) as an exact solution of the strong-coupling polaron problem became generally accepted after the publication of Ref. [19], in which asymptotic form (1.3) was rigorously proved by integration over trajectories, i.e., without using ansatz (1.2) (see also review [20]).

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Many attempts to improve the strong-coupling theory [21–26] were made before the publication of Ref. [19]. A cause of dissatisfaction with Pekar's ansatz was the translational invariance of the initial polaron Hamiltonian. The use of the ansatz for the wave function $\psi(r)$ in (1.2) leads to a localized solution, which means that the electron is trapped in a localized polarized well created by itself. In other words, this solution lacks the symmetry of the initial Hamiltonian. Electron self-trapping in the localized polaron well leads to spontaneous symmetry breaking of the system. The approach chosen to restore the initial symmetry was based on the use of a degenerate state with broken symmetry. Because the position of the center of the polaron well r_0 in a homogeneous and isotropic medium does not affect anything, an initially localized solution can be extended to all positions of the polaron potential well by choosing the wave function in the form of a linear combination over all well positions.

This approach was most consistently realized in Ref. [24]. The wave function (an eigenfunction of the total momentum) was taken as a superposition of plane waves corresponding to the total momentum times the wave functions derived from (1.2) under the action of the translation operator. In other words, the superposition was taken over all positions of the polaron well r_0.

The main result in Ref. [24] is that the computation of the polaron ground state energy with such a delocalized wave function yields the same value as the calculation with localized function (1.2). The polaron mass value previously obtained by Landau and Pekar [27] was reproduced in [24] based on the assumption of motion of localized state (1.2) in a medium. The results in Ref. [24] greatly contributed to the resolution of the contradiction between the requirements of delocalization of a translationally invariant wave function and localization of the wave function of a self-trapped state.

This approach cannot be regarded as fully satisfactory despite its success, because it retains a number of controversies ensuing from the use of the semiclassical description. Indeed, the superposition reported in Ref. [24], on the one hand, determines the localized polaron position, but on the other hand makes it possible to measure this position without altering the state and discover a localized polaron well with the trapped electron. The cause of this paradox is the classicality of the polaron well in the strong-coupling limit, with the result that the total momentum operator commutes with the polaron well position r_0.[1] This defect was corrected by means of approaches in which the quantity r_0, which is by no means an auxiliary degree of freedom, was considered as such with additional constraints imposed on the function $r_0(r, q_1, \ldots, q_i, \ldots)$. Issues related to the solution of the problem of introducing collective coordinates are discussed in Ref. [30].

Because the results of introducing collective coordinates in the polaron theory by various methods are debatable, it seems appropriate to present rigorous data concerning the translationally invariant theory without recourse to the notion of collective coordinates. The objective of this review is to describe an approach applicable in the strong-coupling limit and not using Pekar's ansatz.

The solution with such properties for a strongly coupled polaron was first found in the work of Tulub [31, 32]. However, the importance of these publications remained unnoticed for almost half a century because the test wave function for evaluation of the ground state was chosen incorrectly in [32]. As a result, the ground state energy $E_0 = -0.105\alpha^2\hbar\omega_0$ obtained in Ref. [32] was higher than that in (1.3). The optimal choice of the wave function was reported quite recently in Ref. [33]. It implies a polaron ground state energy lower than (1.3), $E_0 = -0.125720\alpha^2\hbar\omega_0$, which means the inapplicability of the adiabatic approximation, which forms the basis of solid state physics, in the case of the polaron.

The present review describes the main features of the translationally invariant (TI) polaron theory. In Section 2, Heisenberg's canonical transformation is used to introduce the coordinate-free Pekar–Fröhlich Hamiltonian underlying the translationally invariant description, while the Lee–Low–Pines transformation is used to reproduce the weak-coupling limit.

Section 3 deals with the general translationally invariant Tulub theory that holds for any values of the electron–phonon interaction constant. The paramount importance of Tulub's approach necessitates a more detailed description than in the original work [32] to enable the reader to reproduce and verify the presented results. A general expression for the TI polaron energy at an arbitrary bonding force is reported.

Section 4 considers the limit weak-coupling case. It is shown that the general expression for the polaron energy presented in Section 3 reproduces the weak-coupling limit with high accuracy.

Section 5 concerns the limit case of strong coupling. It demonstrates that the polaron ground state energy is lower in this case than that estimated based on Pekar's ansatz.

The translationally invariant theory is generalized to the case of the bipolaron in Section 6. The bipolaron ground state energy is shown to be much lower than that obtained by the best variational calculations using Pekar's ansatz. The results are used to explain high-temperature superconductivity based on TI bipolarons.

An alternative derivation of the TI polaron and bipolaron energies is proposed in Section 7. It describes an approach allowing an explicit calculation of wave functions for polarons and bipolarons. The results presented in this section indicate that the wave functions thus found describe delocalized states at all values of the electron–phonon coupling constant. This means that Pekar's ansatz is not satisfied in the strong-coupling limit, and no transition to the self-trapped (i.e., localized) state with broken symmetry occurs.

The results obtained radically modify the notion of polarons and bipolarons in general, casting doubt on the concept of autolocalized states in condensed systems. The main results of the recent discussion on the completeness of Tulub's theory are reported in Section 8.

Section 9 deals with certain problems related to the existence of translationally invariant polarons and bipolarons and its practical implications, with special reference to their superconducting properties.

[1] The nature of the arising difficulties was fairly well perceived at the dawn of quantum mechanics by its founders. For example, Bethe noted in [28] that a correct quantum mechanical description of field–particle interactions requires quantization of this field, i.e., quantum field theory: "the fact is quantization of mechanical parameters (coordinates and momenta) implies quantization of their respective fields. Otherwise, as shown by Bohr and Rosenfeld [29], a thought experiment can be suggested that consists of simultaneous measurement of the particle coordinate and momentum from the observation of the field it creates, thereby violating Heisenberg's uncertainty principle."

Section 10 is focused on some fundamental unsolved problems of the strong-coupling theory.

In Appendices 1–3, we collect proofs of certain important assertions underlying our approach.

2. Coordinate-free Hamiltonian. Weak coupling

We proceed from the Pekar–Fröhlich Hamiltonian

$$H = -\frac{\hbar^2}{2m}\Delta_r + \sum_k V_k\left[a_k \exp(\mathrm{i}kr) + a_k^+ \exp(-\mathrm{i}kr)\right] + \sum_k \hbar\omega_k^0 a_k^+ a_k\,, \tag{2.1}$$

where a_k^+ and a_k are creation and annihilation operators of field quanta with the energy $\hbar\omega_k^0 = \hbar\omega_0$, m is the electron effective mass, and V_k is a function of the wave vector k.

Hamiltonian (2.1) is interesting to study because unlike many model Hamiltonians considered in condensed matter theory, Pekar–Fröhlich Hamiltonian (2.1) asymptotically accurately describes the long-wavelength limit of a nonrelativistic electron in a continuous polar medium.

Electron coordinates can be eliminated from (2.1) by means of a Heisenberg transformation [34]:

$$S_1 = \exp\left[\frac{\mathrm{i}}{\hbar}\left(\mathbf{P} - \sum_k \hbar\mathbf{k}a_k^+ a_k\right)\mathbf{r}\right], \tag{2.2}$$

where $\mathbf{P}$ is the total momentum of the system. Acting with S_1 on the field operators yields

$$S_1^{-1} a_k S_1 = a_k \exp(-\mathrm{i}kr)\,, \qquad S_1^{-1} a_k^+ S_1 = a_k^+ \exp(\mathrm{i}kr)\,.$$

Accordingly, the transformed Hamiltonian $\tilde{H} = S_1^{-1} H S_1$ takes the form

$$\tilde{H} = \frac{1}{2m}\left(\mathbf{P} - \sum_k \hbar\mathbf{k}a_k^+ a_k\right)^2 + \sum_k V_k(a_k + a_k^+) + \sum_k \hbar\omega_k^0 a_k^+ a_k\,. \tag{2.3}$$

Hamiltonian (2.3) does not contain electron coordinates; therefore, the solution of the polaron problem based on (2.3) is translationally invariant. To study the ground state of (2.3), Lee, Low, and Pines [35] used the test wave function

$$|\Psi\rangle_{\mathrm{LLP}} = S_2|0\rangle\,, \tag{2.4}$$

where

$$S_2 = \exp\left[\sum_k f_k(a_k^+ - a_k)\right], \tag{2.5}$$

f_k are variational parameters having the meaning of the displacement of field operators from their equilibrium positions, and $|0\rangle$ is the vacuum wave function. To find f_k, we minimize the energy $E = \langle 0|S_2^{-1}\tilde{H}S_2|0\rangle$, which at $P = 0$ gives

$$E = 2\sum_k f_k V_k + \frac{\hbar^2}{2m}\left[\sum_k \mathbf{k} f_k^2\right]^2 + \sum_k \frac{\hbar^2 k^2}{2m} f_k^2 + \sum_k \hbar\omega_k^0 f_k^2\,, \tag{2.6}$$

$$f_k = -\frac{V_k}{\hbar\omega_k^0 + \hbar^2 k^2/(2m)}\,. \tag{2.7}$$

For an ionic crystal,

$$V_k = \frac{e}{k}\sqrt{\frac{2\pi\hbar\omega_0}{\tilde{\varepsilon}V}} = \frac{\hbar\omega_0}{k u^{1/2}}\left(\frac{4\pi\alpha}{V}\right)^{1/2}, \qquad u = \left(\frac{2m\omega_0}{\hbar}\right)^{1/2}, \quad \alpha = \frac{1}{2}\frac{e^2 u}{\hbar\omega_0\tilde{\varepsilon}}\,, \quad \tilde{\varepsilon}^{-1} = \varepsilon_\infty^{-1} - \varepsilon_0^{-1}\,, \tag{2.8}$$

where e is the electron charge, ε_∞ and ε_0 are high-frequency and static dielectric permittivities, and α is the electron–phonon coupling constant. Substituting (2.8) in (2.6) and (2.7) yields the ground state energy $E = -\alpha\hbar\omega_0$, i.e., the energy of the weak-coupling polaron in the first order in α.

The problem of transition to the case of strong coupling in coordinate-free Hamiltonian (2.3) was solved based on the general translationally invariant theory proposed by Tulub in Ref. [32]. The main features of this theory are described in Section 3.

3. Coordinate-free Hamiltonian. The general case.

The general translationally invariant theory was constructed in Refs [31, 32] using the canonical transformation of Hamiltonian (2.3) by the operator S_2 in (2.5), leading to a shift of field operators:

$$S_2^{-1} a_k S_2 = a_k + f_k\,, \qquad S_2^{-1} a_k^+ S_2 = a_k^+ + f_k\,. \tag{3.1}$$

The result of the transformation of the Hamiltonian $\tilde{H} = S_2^{-1}\tilde{H}S_2$ is

$$\tilde{\tilde{H}} = H_0 + H_1\,, \tag{3.2}$$

where

$$H_0 = \frac{\mathbf{P}^2}{2m} + 2\sum_k V_k f_k + \sum_k\left(\hbar\omega_k^0 - \frac{\hbar\mathbf{k}\mathbf{P}}{m}\right) f_k^2 + \frac{1}{2m}\left(\sum_k \mathbf{k} f_k^2\right)^2 + \mathcal{H}_0\,, \tag{3.3}$$

$$\mathcal{H}_0 = \sum_k \hbar\omega_k a_k^+ a_k + \frac{1}{2m}\sum_{k,k'} \mathbf{k}\mathbf{k}' f_k f_{k'}(a_k a_{k'} + a_k^+ a_{k'}^+ + a_k^+ a_{k'} + a_{k'}^+ a_k)\,, \tag{3.4}$$

$$\hbar\omega_k = \hbar\omega_k^0 - \frac{\hbar\mathbf{k}\mathbf{P}}{m} + \frac{\hbar^2 k^2}{2m} + \frac{\hbar\mathbf{k}}{m}\sum_{k'} \hbar\mathbf{k}' f_{k'}^2\,. \tag{3.5}$$

The Hamiltonian H_1 contains linear, cubic, and quartic terms in creation/annihilation operators. With the properly chosen wave function diagonalizing the quadratic form in (3.4), the expectation value of H_1 vanishes (see Appendix 1). In what follows, we set $\hbar = 1$, $\omega_0 = 1$, $m = 1$, and $P = 0$.

To reduce $\mathcal{H}_0$ to the diagonal form, we set

$$q_k = \frac{1}{\sqrt{2\omega_k}}(a_k + a_k^+)\,, \qquad p_k = -\mathrm{i}\sqrt{\frac{\omega_k}{2}}(a_k - a_k^+)\,, \qquad \mathbf{z}_k = \mathbf{k} f_k\sqrt{2\omega_k}\,. \tag{3.6}$$

With (3.6) taken into account, expression (3.4) takes the form

$$\mathcal{H}_0 = \frac{1}{2}\sum_k (p_k^+ p_k + \omega_k^2 q_k^+ q_k) + \frac{1}{2}\left(\sum_k \mathbf{z}_k q_k\right)^2 - \frac{1}{2}\sum_k \omega_k \,. \tag{3.7}$$

The equation of motion for the operator q_k follows from (3.7):

$$\ddot{q}_k + \omega_k^2 q_k = -\mathbf{z}_k \sum_{k'} \mathbf{z}_{k'} q_{k'} \,. \tag{3.8}$$

We seek a solution of system (3.8) in the form

$$q_k(t) = \sum_{k'} \Omega_{kk'} \xi_{k'}(t) \,, \qquad \xi_k(t) = \xi_k^0 \exp(\mathrm{i}\nu_k t) \,. \tag{3.9}$$

This gives the following set of equations for the matrix $\Omega_{kk'}$:

$$(\nu_{k'}^2 - \omega_k^2)\Omega_{kk'} = \mathbf{z}_k \sum_{k''} \mathbf{z}_{k''} \Omega_{k''k'} \,. \tag{3.10}$$

We consider the determinant of this system obtained by replacing the eigenvalues ν_k^2 in (3.10) by a quantity s that may differ from ν_k^2. The determinant of such a system has the form

$$\det\left|(s-\omega_k^2)\delta_{kk'} - \mathbf{z}_k \mathbf{z}_{k'}\right| = \prod_k (s - \nu_k^2) \,. \tag{3.11}$$

On the other hand, in accordance with Wentzel's work [36],[2]

$$\det\left|(s-\omega_k^2)\delta_{kk'} - \mathbf{z}_k \mathbf{z}_{k'}\right| = \prod_k (s-\omega_k^2)\left(1 - \frac{1}{3}\sum_{k'} \frac{\mathbf{z}_{k'}^2}{s-\omega_{k'}^2}\right)^3 . \tag{3.12}$$

It is convenient to introduce

$$\Delta(s) = \frac{\prod_k (s-\nu_k^2)}{\prod_k (s-\omega_k^2)} \,. \tag{3.13}$$

It follows from (3.11) and (3.12) that

$$\Delta(s) = \left(1 - \frac{1}{3}\sum_k \frac{\mathbf{z}_k^2}{s-\omega_k^2}\right)^3 . \tag{3.14}$$

It also follows from (3.11) and (3.12) that the field frequencies ν_k renormalized by interaction are determined by the equation

$$\Delta(\nu_k^2) = 0 \,. \tag{3.15}$$

The change in the system energy ΔE due to the electron–field interaction is expressed as

$$\Delta E = \frac{1}{2}\sum_k (\nu_k - \omega_k) \,. \tag{3.16}$$

[2] In [36], z_k is a scalar but not a vector function; therefore, there is no 'cube' in (3.12). A generalization to the vector case can be found in [31].

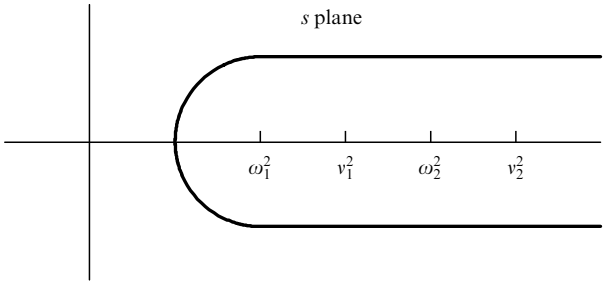

Figure 1. Contour C.

To express ΔE in terms of $\Delta(s)$, we use the Wentzel approach [36]. Following [36], we write the identity

$$\begin{aligned}\sum_k \left(f(\nu_k^2) - f(\omega_k^2)\right) &= \frac{1}{2\pi\mathrm{i}}\oint_C \mathrm{d}s\, f(s) \sum_k \left(\frac{1}{s-\nu_k^2} - \frac{1}{s-\omega_k^2}\right) \\ &= \frac{1}{2\pi\mathrm{i}}\oint_C \mathrm{d}s\, f(s)\, \frac{\mathrm{d}}{\mathrm{d}s}\ln\Delta(s) = -\frac{1}{2\pi\mathrm{i}}\oint_C \mathrm{d}s\, f'(s)\ln\Delta(s) \,,\end{aligned} \tag{3.17}$$

where integration is performed along the contour shown in Fig. 1.

Setting $f(s) = \sqrt{s}$, we obtain

$$\Delta E = \frac{1}{2}\sum_k (\nu_k - \omega_k) = -\frac{1}{8\pi\mathrm{i}}\oint_C \frac{\mathrm{d}s}{\sqrt{s}} \ln\Delta(s) \,. \tag{3.18}$$

Passing from summation to integration in (3.14) using the relation

$$\sum_k = \frac{1}{(2\pi)^3}\int \mathrm{d}^3 k \,,$$

with expression (3.14) for $\mathbf{z}_k$, we obtain

$$\Delta(s) = D^3(s) \,, \qquad D(s) = 1 - \frac{2}{3(2\pi)^3}\int \frac{k^2 f_k^2 \omega_k^2}{s-\omega_k^2}\, \mathrm{d}^3 k \tag{3.19}$$

in the continuum case. For the total electron energy, we then have

$$E = \Delta E + 2\sum_k V_k f_k + \sum_k f_k^2 \omega_k^0 \,. \tag{3.20}$$

These results are universal and hold for various polaron models, i.e., for any functions V_k and ω_k^0. In Sections 4 and 5, we discuss the limit cases of weak and strong coupling that follow from general expression (3.20). We note that in accordance with [31], expression (3.20) at $\mathbf{P} \neq 0$ takes the form

$$E = \frac{P^2}{2m} + \Delta E(\mathbf{P}) + 2\sum_k V_k f_k + \sum_k f_k^2 \omega_k^0 \,,$$

$$\Delta E(\mathbf{P}) = -\frac{1}{8\pi\mathrm{i}}\oint_C \frac{\mathrm{d}s}{\sqrt{s}} \ln\prod_{i=1}^3 D^i(s) \,,$$

$$D^i(s) = 1 - \sum_k \frac{(z_k^i)^2}{s-\omega_k^2} \,,$$

where z_k^i is the ith component of the vector $\mathbf{z}_k$. In this case, the functions f_k, ω_k, and z_k should be regarded as depending on both $|\mathbf{k}|$ and $\mathbf{kP}$.

4. Weak-coupling limit in the Tulub theory

The quantities f_k in the expression for the total energy E in (3.20) must be found from the minimum condition $\delta E/\delta f_k = 0$, which leads to an integral equation for f_k:

$$f_k = -\frac{V_k}{1+k^2/2\mu_k}\,, \quad \mu_k^{-1} = \frac{\omega_k}{2\pi\mathrm{i}}\oint_C \frac{\mathrm{d}s}{\sqrt{s}}\,\frac{1}{(s-\omega_k^2)D(s)}\,. \quad (4.1)$$

In the case of weak coupling, $\alpha \to 0$ and Eqns (4.1) can be solved in the framework of the perturbation theory. In the first approximation as $\alpha \to 0$, $D(s) = 1$, and the following expression for μ_k^{-1} is obtained:

$$\mu_k^{-1} = \frac{\omega_k}{2\pi\mathrm{i}}\oint_C \frac{\mathrm{d}s}{\sqrt{s}}\,\frac{1}{s-\omega_k^2} = 1\,. \quad (4.2)$$

Accordingly, for f_k from (4.1), we have

$$f_k = -\frac{V_k}{1+k^2/2}\,. \quad (4.3)$$

For the quantity ΔE entering the total energy, we then obtain

$$\Delta E = -\frac{3}{8\pi\mathrm{i}}\oint_C \frac{\mathrm{d}s}{\sqrt{s}}\ln D(s)\,,$$
$$\ln D(s) = -\frac{2}{3(2\pi)^3}\int \frac{k^2 f_k^2 \omega_k}{s-\omega_k^2}\,\mathrm{d}^3k\,. \quad (4.4)$$

Calculating the integrals in (4.4) with (4.3) taken into account gives $\Delta E = (\alpha/2)\hbar\omega_0$. Calculating the remaining terms in (3.20), we obtain the first term of the polaron total energy expansion in the coupling constant α, $E = -\alpha\hbar\omega_0$.

The authors of Refs [31, 37, 38] developed a general scheme for calculating the next terms of the expansion with respect to α. Specifically, they obtained the following expressions for the self-energy and the effective mass of the polaron [38]:

$$E = -(\alpha + 0.01592\alpha^2)\hbar\omega_0\,,$$
$$m^* = \left(1 + \frac{\alpha}{6} + 0.02362\alpha^2\right)m\,. \quad (4.5)$$

Thus, up to $O(\alpha^3)$ terms, the expression for the polaron energy calculated based on the Tulub approach using the perturbation theory coincides with the results of exact calculation (1.1) (see Section 7).

5. Strong coupling

The case of strong coupling is much more complicated. To elucidate the character of the solution in the strong-coupling region, we first consider analytic properties of the function $D(s)$. For this, we represent $D(s)$ in the form

$$D(s) = D(1) + \frac{s-1}{3\pi^2}\int_0^\infty \frac{k^4 f_k^2 \omega_k\,\mathrm{d}k}{(\omega_k^2-1)(\omega_k^2-s)}\,, \quad (5.1)$$

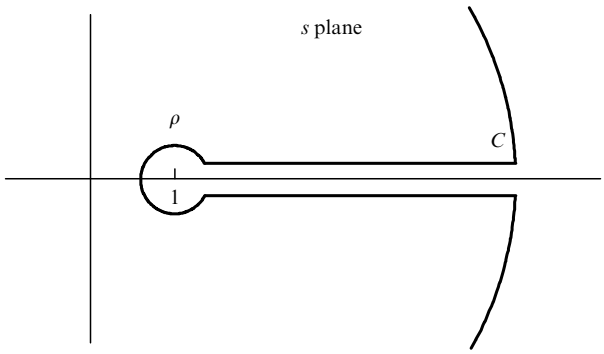

Figure 2. Contour $C + \rho$.

where

$$D(1) = 1 + Q \equiv 1 + \frac{1}{3\pi^2}\int_0^\infty \frac{k^4 f_k^2 \omega_k}{\omega_k^2 - 1}\,\mathrm{d}k \quad (5.2)$$

is the value of $D(s)$ at $s = 1$. It also follows from (3.19) that

$$D(s) = 1 - \frac{1}{3\pi^2}\int_0^\infty \frac{\omega_k k^4 f_k^2}{s-\omega_k^2}\,\mathrm{d}k\,. \quad (5.3)$$

The function $D(s)$, as a function of the complex variable s, has the following properties: (1) $D(s)$ has a cut along the real axis from $s = 1$ to $s = \infty$ and has no other singularities, (2) $D^*(s) = D(s^*)$, (3) $sD(s)$ increases not slower than s as $s \to \infty$. These properties allow representing the function $[(s-1)D(s)]^{-1}$ in the form (see Appendix 2)

$$\frac{1}{(s-1)D(s)} = \frac{1}{2\pi\mathrm{i}}\oint_{C+\rho}\frac{\mathrm{d}s'}{(s'-s)(s'-1)D(s')}\,. \quad (5.4)$$

The integration contour $C + \rho$ is shown in Fig. 2.

The integrand in (5.4) has a pole at $s' = 1$ and a cut from $s' = 1$ to $s' = \infty$. Integrating (5.4) along the upper and lower sides of the cut gives integral equation (3.18) for $D^{-1}(s)$:

$$\frac{1}{D(s)} = \frac{1}{1+Q} + \frac{s-1}{3\pi^2}\int_0^\infty \frac{k^4 f_k^2 \omega_k\,\mathrm{d}k}{(s-\omega_k^2)(\omega_k^2-1)\left|D(\omega_k^2)\right|^2}\,. \quad (5.5)$$

By integration by parts, expression (3.18) for ΔE can be represented in the form

$$\Delta E = \frac{1}{2\pi^2}\int_0^\infty \mathrm{d}k\,k^4 f_k^2 \omega_k\,\frac{1}{2\pi\mathrm{i}}\oint_C \frac{\sqrt{s}}{(s-\omega_k^2)^2}\,\frac{1}{D(s)}\,\mathrm{d}s\,. \quad (5.6)$$

It follows from (5.5) and (5.6) that

$$\Delta E = \frac{1}{2\pi^2}\int_0^\infty \frac{k^4 f_k^2\,\mathrm{d}k}{2(1+Q)} + \frac{1}{12\pi^4}\int_0^\infty\int_0^\infty \frac{k^4 f_k^2 p^4 f_p^2 \omega_p\left[\omega_k\omega_p + \omega_k(\omega_k+\omega_p)+1\right]}{(\omega_k+\omega_p)^2(\omega_p^2-1)\left|D(\omega_p^2)\right|^2}\,\mathrm{d}p\,\mathrm{d}k\,. \quad (5.7)$$

Equation (4.1) for μ_k^{-1} can be represented in accordance with (5.5) as

$$\mu_k^{-1} = \frac{1}{1+Q} + \frac{1}{3\pi^2}\int_0^\infty \frac{p^4 f_p^2(\omega_k\omega_p+1)\,\mathrm{d}p}{(\omega_p^2-1)(\omega_k+\omega_p)\left|D(\omega_p^2)\right|^2}\,. \quad (5.8)$$

Equations (4.1) and (5.8) for f_k and the polaron energy in (3.20) and (5.7) are very complicated, and solving them exactly is hardly possible. The direct variational principle was used in Ref. [32] to approximately calculate the energy E in (3.20) and (5.7). The Gaussian function

$$f_k = -V_k \exp\left(-\frac{k^2}{2a^2}\right), \tag{5.9}$$

where a is a variable parameter, was taken as a test function in the case of strong coupling $a \gg 1$. Substituting (5.9) in (3.19) yields the real and imaginary parts of $D(s)$ (see Appendix 3)

$$\begin{aligned}
&\operatorname{Re} D(\omega_k^2) = 1 + \lambda v(y), \qquad \operatorname{Im} D(\omega_k^2) = \frac{k^3 f_k^2}{6\pi}, \\
&v(y) = 1 - y\exp(-y^2)\int_0^y \exp(t^2)\,\mathrm{d}t \\
&\qquad\qquad - y\exp(y^2)\int_y^\infty \exp(-t^2)\,\mathrm{d}t, \\
&\lambda = \frac{4\alpha a}{3\sqrt{2\pi}}, \qquad y = \frac{k}{a}.
\end{aligned} \tag{5.10}$$

In the strong-coupling limit ($\alpha \gg 1$), the expression for the energy E defined by (3.20) with (5.7) taken into account assumes the form

$$E = \frac{3}{16}\,a^2\left[1 + q\left(\frac{1}{\lambda}\right)\right] - \frac{\alpha a}{\sqrt{\pi}}\left(2 - \frac{1}{\sqrt{2}}\right), \tag{5.11}$$

$$q\left(\frac{1}{\lambda}\right) = \frac{2}{\sqrt{\pi}}\int_0^\infty \frac{\exp(-y^2)\bigl(1 - \Omega(y)\bigr)\,\mathrm{d}y}{\bigl(1/\lambda + v(y)\bigr)^2 + \pi y^2 \exp(-2y^2)/4}, \tag{5.12}$$

$$\Omega(y) = 2y^2\left[(1 + 2y^2)y\exp(y^2)\int_y^\infty \exp(-t^2)\,\mathrm{d}t - y^2\right].$$

As $\lambda \to \infty$, the integral in (5.12) has a maximum at $y^4 = 3\lambda/4$ if the function f_k is chosen in form (5.9); however, this feature is absent when the actual boundedness of the region of integration over y is taken into account (see Section 8).

The calculation of (5.12) in Ref. [32] was based on the assumption that $1/\lambda = 0$ in the strong-coupling limit. Numerical integration yielded $q(0) = 5.75$, whence

$$E = -0.105\alpha^2\hbar\omega_0 \tag{5.13}$$

was found by varying the energy E in (5.11) with respect to a. A comparison of (5.13) and (1.3) shows that the E in (5.13) at $\alpha \to \infty$ is higher than its exact value (1.3) in the Pekar theory. For this reason, it has been believed until recently that the Tulub theory gives no new results for the polaron.

This opinion changed drastically after the publication of Ref. [33], where it was shown that for minimizing energy (3.20), the choice of the test function in form (5.9) was far from optimal, because it failed to satisfy virial relations. It was shown in [33] that the optimal choice of f_k must contain the factor $\sqrt{2}$ in front of the exponential in (5.9). Minimizing energy (3.20) with the optimal test function leads to

$$E = -0.125720\alpha^2\hbar\omega_0\,. \tag{5.14}$$

This is a fundamental result indicating first and foremost that Pekar's ansatz does not give an exact solution. Although (5.14) refers to a concrete case of the Pekar–Fröhlich Hamiltonian with V_k given by (2.8), the conceptual conclusion must hold for all types of autolocalized states. Of special interest is the case of bipolarons due to their potentially important role in superconductivity.

6. Translationally invariant bipolarons

Much attention has been given recently to bipolarons in connection with attempts to explain the phenomenon of superconductivity based on the Bose condensation mechanism in a bipolaron gas. In this context, it is important to study conditions for stability of bipolaron states. The theory of large-radius bipolarons, considered to be the leading candidate for the role of charged bosons forming the Bose–Einstein condensate with pairing in real space, is expounded in reviews [7, 8, 39].

The study of the formation of a stable two-electron state in a crystal, or a bipolaron, typically implies finding the pairwise interaction of two polarons as a function of the distance between them [8]. The range of the existence of a large-radius bipolaron is bounded in terms of the coupling constant α by a rather large value α_c; the bound bipolar state is nonexistent at $\alpha < \alpha_c$. Because the requirement for large α_c may not be satisfied in high-temperature superconductors, a number of papers have been devoted to studying the contribution of other types of interaction and pairing symmetries [40, 41].

In what follows, we confine ourselves to considering the Pekar–Fröhlich electron–phonon interaction, because this approach can be generalized to interactions of other types. It is of special importance in view of the recently obtained strong indications that the electron–phonon interaction in high-temperature superconductors is strong [42–44]. Other arguments suggest that the weak screening of high-frequency optical phonons makes the description of strong electron–phonon interactions in high-temperature superconductors via the long-range Fröhlich interaction [45] more reasonable than their description in the framework of contact interaction in the Holstein polaron model [46].

Before the publication of Refs [47–49], the lowest energies of bipolaron states determined by the electron–phonon interaction were obtained for $\alpha < 8$ in [50–52] and for $\alpha > 8$ in [52–55]. Attempts to find a translationally invariant solution of the bipolaron problem using variational methods, e.g., by means of direct variation of the wave function of a two-electron system [39, 56, 57], led to higher values of the ground-state bipolaron energy than those calculated with the use of the wave function lacking translational invariance [51, 52, 55, 58]. Results obtained for bipolarons in Refs [47–49] using the translationally invariant approach are presented below.

We proceed from the Pekar–Fröhlich Hamiltonian for the bipolaron [8],

$$\begin{aligned}
H = &-\frac{\hbar^2}{2m}\,\Delta_{r_1} - \frac{\hbar^2}{2m}\,\Delta_{r_2} + \sum_k \hbar\omega_k^0 a_k^+ a_k + U\bigl(|\mathbf{r}_1 - \mathbf{r}_2|\bigr) \\
&+ \sum_k \bigl[V_k \exp(\mathrm{i}k r_1)a_k + V_k \exp(\mathrm{i}k r_2)a_k + \text{h.c.}\bigr], \\
U\bigl(|\mathbf{r}_1 - \mathbf{r}_2|\bigr) = &\frac{e^2}{\varepsilon_\infty |\mathbf{r}_1 - \mathbf{r}_2|},
\end{aligned} \tag{6.1}$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the coordinates of the first and second electrons, U describes Coulomb repulsion between electrons, and h.c. are Hermitian conjugate terms.

In the center-of-mass system, Hamiltonian (6.1) takes the form

$$H = -\frac{\hbar^2}{2M_e}\Delta_R - \frac{\hbar^2}{2\mu_e}\Delta_r + U(r) + \sum_k \hbar\omega_k^0 a_k^+ a_k + \sum_k 2V_k \cos\frac{\mathbf{kr}}{2}\left[a_k \exp(\mathrm{i}\mathbf{kR}) + \text{h.c.}\right], \quad (6.2)$$

$$\mathbf{R} = \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}, \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \quad M_e = 2m, \quad \mu_e = \frac{m}{2}.$$

In what follows, we set $\hbar = 1$, $\omega_k^0 = 1$, and $M_e = 1$ (accordingly, $\mu_e = 1/4$).

The center-of-mass coordinates can be eliminated from Hamiltonian (6.2) by the Heisenberg canonical transformation

$$S_1 = \exp\left(-\mathrm{i}\sum_k \mathbf{k} a_k^+ a_k\right)\mathbf{R},$$

$$\tilde{H} = S_1^{-1} H S_1 = -2\Delta_r + U(r) + \sum_k a_k^+ a_k + \sum_k 2V_k \cos\frac{\mathbf{kr}}{2}(a_k + a_k^+) + \frac{1}{2}\left(\sum_k \mathbf{k} a_k^+ a_k\right)^2. \quad (6.3)$$

It follows from formula (6.3) that the exact solution of the bipolaron problem depends on the translationally invariant wave function $\psi(r)$ containing only relative coordinates r.

Averaging $\tilde{H}$ over $\psi(r)$ yields the Hamiltonian

$$\bar{H} = \frac{1}{2}\left(\sum_k \mathbf{k} a_k^+ a_k\right)^2 + \sum_k a_k^+ a_k + \sum_k \bar{V}_k (a_k + a_k^+) + \bar{T} + \bar{U}, \quad (6.4)$$

$$\bar{V}_k = 2V_k \left\langle \psi \middle| \cos\frac{\mathbf{kr}}{2} \middle| \psi \right\rangle,$$

$$\bar{U} = \langle \psi | U(r) | \psi \rangle, \quad \bar{T} = -2\langle \psi | \Delta_r | \psi \rangle.$$

This Hamiltonian differs from Hamiltonian (2.3) in that V_k in the latter is substituted by $\bar{V}_k$ and constants $\bar{T}$ and $\bar{U}$ are added. Repeating the derivation described in Section 3, we obtain the bipolaron energy in the form

$$E_{bp} = \Delta E + 2\sum_k \bar{V}_k f_k + \sum_k f_k^2 + \bar{T} + \bar{U}, \quad (6.5)$$

where ΔE is defined in (5.7). Relation (6.5) can be used to derive an equation for the bipolaron energy by varying E_{bp} with respect to f_k and ψ. Because solving the equations thus obtained is quite difficult, the real bipolaron energy is determined by the direct variational method with [49]

$$f_k = -N\bar{V}_k \exp\left(-\frac{k^2}{2\mu}\right), \quad \psi(r) = \left(\frac{2}{\pi\ell^2}\right)^{3/4} \exp\left(-\frac{r^2}{\ell^2}\right), \quad (6.6)$$

where N, μ, and ℓ are the variational parameters. At $N = 1$, expression (6.6) reproduces the results in Ref. [47] and at $N = 1$ and $\mu \to \infty$, the results in [48].

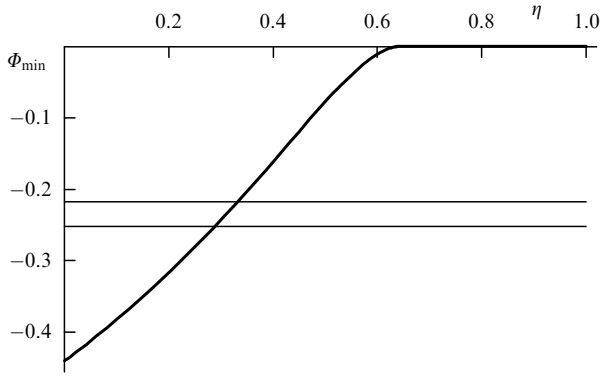

Figure 3. Function $\Phi_{\min}(\eta)$.

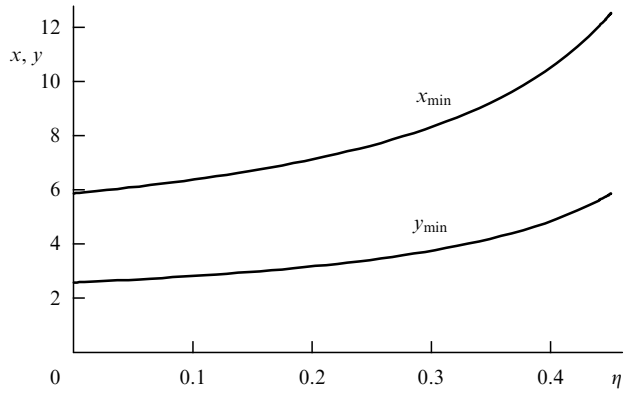

Figure 4. Functions $x_{\min}(\eta)$ and $y_{\min}(\eta)$.

Substituting (6.6) in the expression for the total energy after minimization with respect to N yields the equation

$$E(x, y; \eta) = \Phi(x, y; \eta)\alpha^2, \quad (6.7)$$

$$\Phi(x, y; \eta) = \frac{6}{x^2} + \frac{20.25}{x^2 + 16y} - \frac{16\sqrt{x^2 + 16y}}{\sqrt{\pi}(x^2 + 8y)} + \frac{4\sqrt{2/\pi}}{x(1 - \eta)}.$$

Here, x and y are the variable parameters, $x = \ell\alpha$, $y = \alpha^2/\mu$; $\eta = \varepsilon_\infty/\varepsilon_0$. We let $\Phi_{\min}$ denote the minimal value of the function Φ of x and y. Figure 3 shows the dependence of $\Phi_{\min}$ on η and Fig. 4 illustrates the dependences of $x_{\min}$ and $y_{\min}$ on η.

It follows from Fig. 3 that $E_{\min}(\eta = 0) = -0.440636\alpha^2$ is the lowest bipolaron ground state energy of all values previously obtained by the variational method. The horizontal lines in Fig. 3 correspond to energies $E_1 = -0.217\alpha^2$ and $E_2 = -0.2515\alpha^2$, where $E_1 = 2E_{p_1}$, E_{p_1} is Pekar's polaron ground state energy (1.3), $E_2 = 2E_{p_2}$, and E_{p_2} is the ground state energy of translationally invariant polaron (5.14). The intersections of these lines with the $E_{\min}(\eta)$ curve give critical values of the parameters $\eta = \eta_{c_1} = 0.3325$ and $\eta = \eta_{c_2} = 0.289$. A bipolaron decays into two translationally invariant polarons at $\eta > \eta_{c_2}$ and into Pekar's polarons at $\eta > \eta_{c_1}$. The values of minimizing parameters $x_{\min}$ and $y_{\min}$ for the above η values are $x_{\min}(0) = 5.87561$, $y_{\min}(0) = 2.58537$, $x_{\min}(0.289) = 8.16266$, $y_{\min}(0.289) = 3.68098$, and $x_{\min}(0.3325) = 8.88739$, $y_{\min}(0.3325) = 4.03682$.

The critical value of the electron–phonon coupling constant α for the formation of a TI bipolaron found from a

comparison of expressions for the energies in the weak-coupling limit (twice the weak-coupling polaron energy $E=-2\alpha\hbar\omega_0$) and in the strong-coupling limit ($E=-0.440636\alpha^2\hbar\omega_0$) is $\alpha_c\approx 4.54$ (the lowest of the estimates obtained by the variational method). The last value is conventional. Hamiltonian (6.4) coincides with single-electron Hamiltonian (2.3) in terms of structure. Therefore, according to [20], the bipolaron energy is an analytic function of α as in the case of the polaron. Hence, the polaron energy has no singularities at the point $\alpha=\alpha_c$, and the bipolaron state exists over the entire range of the parameters α and η, $0<\alpha<\infty$ and $0<\eta<1-1/2\sqrt{2}$, at which $E<0$.

To elucidate the existence of the value α_c at which the bipolaron state can be split into individual polarons, calculations at an intermediate coupling strength are needed. According to one of the possible scenarios, the bipolaron energy for certain η values is lower than that of each of the two individual polarons at any α values, which means that the bipolaron state always exists. We note that the virial theorem is fulfilled with a high degree of accuracy for the obtained ground state.

The origin of high-temperature superconductivity (HTSC) and its relation to the formation of bipolaron states have been considered in numerous articles and reviews [7, 8, 59, 60], where the existence of HTSC was explained by Bose condensation of the bipolaron gas. The Bose condensation temperature $T_0=3.31\hbar^2 n_0^{2/3}/(k_B m_{bp})$, supposed to equal the critical temperature T_c of the superconducting transition at $m_{bp}\approx 10m$, varies over a wide range from $T_0=3$ K at $n=10^{18}$ cm^{-3} to $T_0\approx 300$ K at $n\approx 10^{21}$ cm^{-3}, depending on the bipolaron concentration n_0. In the latter case, the bipolaron concentration is so high that the bipolaron composite character has to manifest itself, as in the case of Cooper pairs; specifically, bipolarons cease to behave as separate particles and decay into polarons as their concentration increases further. In accordance with (6.6), the characteristic size of the bipolaron state ℓ in dimensional units is $\ell_{corr}=\hbar^2\tilde{\varepsilon}x(\eta)/(me^2)$, where ℓ_{corr} has the meaning of the correlation length, and the dependence $x(\eta)$ is shown in Fig. 4. It follows from Fig. 4 that x changes only insignificantly, from $x(\eta=0)\approx 6$ to $x(\eta=0.289)\approx 8$, over the entire range of η in which the bipolaron state remains stable.

This means that the critical concentration at which the composite character of bipolarons becomes noticeable is of the order of $n_c\approx 10^{21}$ cm^{-3}, even at $\eta=\eta_c$. This result suggests the possibility of the existence of a bipolaron HTSC mechanism in copper oxides.

7. Ground state functional. The Tulub ansatz

The quadratic form in (3.4) can be diagonalized using the Bogoliubov–Tyablikov transformation [61]. We let α_k denote operators of physical particles in terms of which $\mathcal{H}_0$ is a diagonal operator.

The quadratic form is diagonalized by means of the transformation

$$a_k=\sum_{k'}M_{1kk'}\alpha_{k'}+\sum_{k'}M^*_{2kk'}\alpha^+_{k'}\,,$$
$$a^+_k=\sum_{k'}M^*_{1kk'}\alpha^+_{k'}+\sum_{k'}M_{2kk'}\alpha_{k'}\,, \tag{7.1}$$

with the following relations satisfied:

$$[a_k,\,a^+_{k'}]=[\alpha_k,\alpha^+_{k'}]=\delta_{kk'}\,,\qquad [H_0,\alpha^+_k]=\omega_k\alpha^+_k\,. \tag{7.2}$$

It follows from the properties of unitary transformation (7.1) that

$$M_2M_1^+=M_1^*M_2^{\mathrm{T}}\,,$$
$$(M_1^+)^{-1}=M_1-M_2^*(M_1^*)^{-1}M_2\,. \tag{7.3}$$

The transformation of operators inverse to (7.1), with the use of (7.3), has the form

$$\alpha_k=\sum_{k'}M^*_{1kk'}a_{k'}-\sum_{k'}M^*_{2kk'}a^+_{k'}\,,$$
$$\alpha^+_k=\sum_{k'}M_{1kk'}a^+_{k'}-\sum_{k'}M_{2kk'}a_{k'}\,. \tag{7.4}$$

According to [31, 32], the matrices M_1 and M_2 are

$$(M_{1,2})_{kk'}=\frac{1}{2}(\omega_k\omega_{k'})^{-1/2}(\omega_k\pm\omega_{k'})$$
$$\times\left[\delta(k-k')+(\mathbf{kk}')\,f_kf_{k'}\frac{2(\omega_k\omega_{k'})^{1/2}}{(\omega^2_{k'}-\omega^2_k\pm\mathrm{i}\varepsilon)D_\pm(\omega^2_k)}\right], \tag{7.5}$$
$$D_\pm(\omega_p^2)=1+\frac{1}{3\pi^2}\int_0^\infty\frac{f_k^2k^4\omega_k}{\omega_k^2-\omega_p^2\mp\mathrm{i}\varepsilon}\,\mathrm{d}k\,.$$

The upper sign in the right-hand side of (7.5) is for M_1, and the lower sign is for M_2. Diagnolization of the quadratic form in (3.4) leads to

$$\mathcal{H}_0=\Delta E+\sum_k v_k\alpha^+_k\alpha_k\,. \tag{7.6}$$

The ground state functional $\Lambda_0|0\rangle$ is chosen from the condition

$$\alpha_k\Lambda_0|0\rangle=0\,. \tag{7.7}$$

To find the explicit form of the functional Λ_0, it is convenient to use the Fock representation [62, 63] establishing a correspondence between the operator a^+_k and a certain c-number $\bar{a}_k$ and between operators a_k and $\mathrm{d}/\mathrm{d}\bar{a}_k$. Then condition (7.7) becomes [taking (7.4) into account]

$$\left(\sum_{k'}M^*_{1kk'}\frac{\mathrm{d}}{\mathrm{d}\bar{a}_{k'}}-\sum_{k'}M^*_{2kk'}\bar{a}_{k'}\right)\Lambda|0\rangle=0\,. \tag{7.8}$$

Direct substitution in (7.8) gives the solution of this equation

$$\Lambda_0=C\exp\left(\frac{1}{2}\sum_{k,k'}a^+_kA_{kk'}a^+_{k'}\right), \tag{7.9}$$

where C is a constant. Here, it is enough to return from a^+_k to $\bar{a}_k$ in (7.9). The matrix A satisfies the relations

$$A=M_2^*(M_1^*)^{-1}\,,\qquad A=A^{\mathrm{T}}\,. \tag{7.10}$$

Thus, the ground state energy corresponding to the functional Λ_0 is

$$\langle 0|\Lambda_0^+\mathcal{H}_0\Lambda_0|0\rangle=\Delta E\,. \tag{7.11}$$

As shown in Appendix 1, $\langle 0|\Lambda_0^+H_1\Lambda_0|0\rangle\equiv 0$.

It follows from (7.9), (2.2), and (2.5) that the wave function of the polaron ground state $|\psi\rangle_{\rm p}$ has the form

$$|\psi\rangle_{\rm p} = C\exp\left(-\frac{\rm i}{\hbar}\sum_k \hbar\mathbf{k}a_k^+ a_k\mathbf{r}\right)\exp\left[\sum_k f_k(a_k^+ - a_k)\right]\Lambda_0|0\rangle\,. \tag{7.12}$$

Accordingly, the bipolaron wave function $|\psi\rangle_{\rm bp}$ is expressed, taking (5.3), (5.4) into account, as

$$|\psi\rangle_{\rm bp} = C\psi(r)\exp\left(-\frac{\rm i}{\hbar}\sum_k \hbar\mathbf{k}a_k^+ a_k\mathbf{R}\right) \times\exp\left[\sum_k f_k(a_k^+ - a_k)\right]\Lambda_0|0\rangle\,. \tag{7.13}$$

It follows from (7.12) and (7.13) that the polaron and bipolaron wave functions are delocalized across the entire space and cannot be represented in the form of ansatz (1.2).

It also follows from (7.12) and (7.13) that the attempts of Lee, Low, and Pines [35] to evaluate the polaron ground state energy over the entire range of α variations failed because of an unsuccessful choice of test function (2.4), which lacked a factor corresponding to functional Λ_0.

However, it should be emphasized that even a radical improvement of the test function by the introduction of a factor Λ_0 allowing us to consider both strong and weak coupling cases in the Lee–Low–Pines functions does not produce an exact result. The fact that Tulub's function is an ansatz comes from its properties:

$$\langle 0|\Lambda_0^+ H_1\Lambda_0|0\rangle = 0\,,\ E = \langle 0|\Lambda_0^+ H_0\Lambda_0|0\rangle\,,\ H_0\Lambda_0|0\rangle = E\Lambda_0|0\rangle\,. \tag{7.14}$$

Being an ansatz, the Tulub solution solves the polaron problem in a certain class of functions with the structure $\Lambda_0|0\rangle$. That Tulub's ansatz is not an exact solution of the problem follows from the fact that the use of expression (3.20) alone to calculate energy, e.g., in the weak-coupling case, gives the result [31]

$$E = -\alpha - \frac{1}{6}\left(\frac{1}{2} - \frac{4}{3\pi}\right)\alpha^2\,.$$

To obtain the exact value of the coefficient at α^2 in the expansion of the energy as a power series in α, Eqn (1.1), it is necessary to take the contribution of the Hamiltonian H_1 into account in accordance with the perturbation theory [38].

Delocalization of wave functions (7.12) and (7.13) has many important implications, which are discussed in Section 9.

8. Discussion of the completeness of the Tulub theory

The authors of Refs [64, 65] raised the question of the completeness of the Tulub theory [31, 32]. Their objections were based on the work of Porsch and Röseler [37] reproducing the results of the Tulub theory. In the last section of their article, Porsch and Röseler considered possible consequences of replacing the infinite integration limit with a finite one in the Tulub theory, followed by a transition back to the infinite limit. Surprisingly, it turned out that simultaneously with the cut-off in the integration over phonon wave vectors in the functional of total polaron energy, that functional needs to be supplemented by a term $\delta E^{\rm PR}$ that makes a nonzero contribution as the upper limit tends to infinity [37, 65]. Based on this result, the authors of Refs [64, 65] concluded that Tulub disregarded this addition, which makes his theory incomplete.

To resolve this paradox, we consider the function $\Delta(s)$ defined by formula (3.14) [or (3.19) in the continuum case]. According to (3.14) and (3.19), the zeros of these functions make a contribution to the 'polaron recoil' energy ΔE defined by (3.16); in accordance with (3.15), they are found from the equation

$$1 = \frac{2}{3}\sum_k \frac{k^2 f_k^2\omega_k}{s - \omega_k^2}\,. \tag{8.1}$$

If there is no cutoff in the sum in the right-hand side of (8.1), the solution gives a spectrum of s values determined by frequencies ν_{k_i} lying between the neighboring values of ω_{k_i} and $\omega_{k_{i+1}}$ for all wave vectors k_i. These frequencies determine the recoil energy

$$\Delta E = \frac{1}{2}\sum_{k_i}(\nu_{k_i} - \omega_{k_i})\,. \tag{8.2}$$

We next discuss what happens to the contribution of the frequencies ν_{k_i} to ΔE in the region of wave vectors k where f_k tends to zero but never exactly vanishes. It follows from (8.1) that solutions of Eqn (8.1) tend to ω_{k_i} as $f_k \to 0$: $\nu_{k_i} \to \omega_{k_i}$. Accordingly, the contribution to ΔE in the region of wave vectors where $f_k \to 0$ must also tend to zero.

Specifically, introducing a certain k^0 such that f_k values in the region $k > k^0$ are small leads to the expression

$$\Delta E = \frac{1}{2}\sum_{k_i \leqslant k^0}(\nu_{k_i} - \omega_{k_i})\,, \tag{8.3}$$

containing no additional terms. This corresponds to fixing an upper limit k^0 in the Tulub functional, with no additional terms appearing.

For example, to study the minimum of Tulub's functional (3.20), (5.7), we choose the test function f_k without a cutoff, in the form [49]

$$f_k = -V_k\exp\left(-\frac{k^2}{2a^2(k)}\right), \qquad a(k) = \frac{a}{2}\left[1 + \tanh\left(\frac{k_{\rm b} - k}{a}\right)\right], \tag{8.4}$$

where a is a parameter of Tulub's test function (5.9), $k_{\rm b}$ satisfies the condition $a \ll k_{\rm b} \ll k_{\rm oc}$, and $k_{\rm oc} = a\sqrt[4]{3\lambda/4}$ is the value of the wave vector at which Tulub's integral (5.12) has a maximum [32, 66]; in this case, the use of (8.4) in the $a \to \infty$ limit gives the following expression for the integral $q(1/\lambda)$:

$$q\left(\frac{1}{\lambda}\right) \approx 5.75 + 6\left(\frac{a}{k_{\rm b}}\right)^3\exp\left(-\frac{k_{\rm b}^2}{a^2}\right). \tag{8.5}$$

The second term in the right-hand side of (8.5) vanishes as $k_{\rm b}/a \to \infty$, which leads, as expected, to Tulub's result $q(1/\lambda) \approx 5.75$.

However, Eqn (8.1) has a singularity. It has an isolated solution ν_{k^0} differing from the frequency ω_{k^0} by a finite value, even for the continuum spectrum at $f_k = 0$ if $k > k^0$. This

isolated solution leads to an additional contribution to ΔE,

$$\Delta E = \frac{1}{2}\sum_{k_i<k^0}(v_{k_i}-\omega_{k_i}) + \delta E^{\mathrm{PR}}\,,$$
$$\delta E^{\mathrm{PR}} = \frac{3}{2}(v_{k^0}-\omega_{k^0})\,, \tag{8.6}$$

where v_{k^0} has the meaning of 'plasma frequency' [37]. In other words, there is no continuous transition here from the case where $f_k \to 0$ at $k > k^0$ to the case where $f_k = 0$ at $k > k^0$. Direct calculation [67] of the contribution made by the term with the 'plasma frequency' δE^{PR} to (8.6) shows that the Porsch–Röseler theory does not turn into the Tulub theory, even as $k^0 \to \infty$.

In the Tulub theory, we choose those f_k that lead to a minimum of the total polaron energy functional. Specifically, the choice of the test function in form (8.4) guarantees the absence of a contribution of the 'plasma frequency' to the total energy; for practical purposes, it is possible to choose the cut-off f_k without introducing any additional terms into Tulub's functional [66, 67].

To summarize, the critical remarks in [64, 65] were shown to be invalid both in Refs [66, 67] and in Ref. [49] cited above. At present, the Tulub theory and the data obtained using it [33, 47–49] are regarded as certain.

9. Implications of the existence of translationally invariant polarons and bipolarons

The available data indicate that the ground state of a TI polaron is a delocalized state of the electron–phonon system: the probability of finding an electron is the same at any spatial point. The explicit form of the ground state wave function is presented in Section 7. Both the electron density and amplitudes of phonon modes corresponding to the frequencies v_{q_i} renormalized by interaction are delocalized.

Importantly, according to (3.15), the renormalized phonon frequencies v_{q_i} in the case of TI polarons have the energy higher than nonrenormalized frequencies of optical phonons, i.e., they are higher than renormalized frequencies of polarons with spontaneously broken symmetry [68]. This gives hope to discover such phonon modes in Raman scattering and optical absorption experiments. If a polaron (bipolaron) is bound at a Coulomb center, i.e., forms an F-center (F′-center), all renormalized local phonon frequencies ω_n are lower in energy than the optical phonon frequency ω_0 [68]. This fact facilitates experimental verification of the presence of delocalized TI phonon modes $v_{q_i} > \omega_0$.

The translationally invariant theory does not contain the concept of a 'polaron potential well' (a well formed by local phonons [68]) in which an electron is localized, i.e., a self-trapped state. Therefore, the induced polaron charge for a TI polaron is zero. The absence of a localized 'phonon coat' for a TI polaron suggests that its effective mass is not significantly different from the effective electron mass. The energy of the TI polaron ground state is lower than that of Pekar's polaron; it is defined by formula (5.14), while Pekar's polaron energy is given by (1.3).

This means that the polaron zero total momentum is associated with an energy gap between the TI polaron state and the Pekar state, i.e., a state with broken translational invariance. The TI polaron is a structureless particle (see Ref. [68] for the results of a structural survey of Pekar's polaron).

According to the TI polaron theory, the terms 'large-radius polaron' (LRP) and 'small-radius polaron' (SRP) are arbitrary, because the electron state is delocalized with respect to the crystal. The difference between the LRP and SRP in the TI theory lies in the fact that the inequality $k_{\mathrm{char}}a < \pi$ is satisfied for the LRP and the inequality $k_{\mathrm{char}}a > \pi$ holds for the SRP (where a is the lattice constant and k_{char} is the characteristic value of phonon wave vectors making the leading contribution to the polaron energy). This inference holds not only for the Pekar–Fröhlich polaron but also for the whole class of polarons in which the coupling constant is unrelated to the electron wave vector, as in the case of the Holstein polaron. These criteria may not be satisfied for the class of polarons with the coupling constant depending on the electron wave vector (as in the Su–Schrieffer–Heeger model [69]).

The above features of TI polarons account for their physical properties being qualitatively different from those of Pekar's polarons. In the presence of minor local defects in a crystal, TI polarons remain in a delocalized state. For example, delocalized polaron states give rise to F-centers in an ionic crystal, with vacancies only at a certain critical value $\varepsilon_{0\mathrm{c}}$ of the static dielectric constant. For $\varepsilon_0 > \varepsilon_{0\mathrm{c}}$, the crystal contains delocalized TI polarons and free vacancies. At $\varepsilon_0 = \varepsilon_{0\mathrm{c}}$, a transition occurs from the delocalized state to the vacancy-associated localized state (wave function collapse). Such a behavior of TI polarons is qualitatively different from that of Pekar's polarons, which localize at vacancies at any ε_0 values. This explains, in particular, the absence of absorption (i.e., structure) by a free Pekar polaron, because a TI polaron is then realized. Absorption occurs only after the formation of a bound Pekar polaron, i.e., an F-center. These observations are confirmed by recent publications concerning Holstein polarons [70–72]. We generalized the above approach to the case of the Holstein polaron in Ref. [73].

We note that only a physical interpretation of free strong-coupling polarons needs modification. The overwhelming majority of the data on strong-coupling polaron physics refer to Pekar-type polaron states bound at lattice vacancies or defects and do not need any correction.

Taking translational invariance into account in the case of polarons slightly affects the assessment of the ground state which, however, does throw new light on its properties. As Tulub showed in the part of his work devoted to TI polaron scattering, increasing the electron–phonon coupling constant to a certain critical value results in the disappearance of polaron scattering on optical phonons [32].

This means that polarons become superconducting at coupling constants above a critical value. Although scattering on optical phonons is the principal mechanism of electron scattering in ionic crystals [74], it may seem that the contribution of acoustic phonons should also be taken into consideration. However, it follows in general from the energy and momentum conservation laws that the scattering of TI polarons on acoustic phonons is possible only if their velocity is higher than the speed of sound [75].

The energy of TI bipolarons is much higher than that of polarons, which has important physical implications. Specifically, TI bipolarons remain in a delocalized state if a crystal has small local defects. For example, the formation of F′-centers by delocalized bipolaron states in an ionic crystal with vacancies occurs only at a certain critical value $\varepsilon_{0\mathrm{c}_1}$ of the static dielectric constant. For $\varepsilon_0 > \varepsilon_{0\mathrm{c}_1}$, the crystal contains delocalized TI bipolarons and free vacancies. At $\varepsilon_0 = \varepsilon_{0\mathrm{c}_1}$,

transition occurs from the delocalized state to the vacancy-associated localized state, i.e., to the F′-center. Such a behavior of TI bipolarons is qualitatively different from that of Pekar-type bipolarons with spontaneously broken symmetry [8] localized at vacancies at any ε_0 values.

The fundamental difference of TI bipolarons from bipolarons with spontaneously broken symmetry is that the former are inseparable, while the latter are separable; the interaction between electrons and polarization in the case of bipolarons with spontaneously broken symmetry has the form $\Phi(\mathbf{r}_1, \mathbf{r}_2) = F(\mathbf{r}_1) + F(\mathbf{r}_2)$. At $|\mathbf{r}_1 - \mathbf{r}_2| \gg R$, where R is the bipolaron radius, the equation for a bipolaron splits into two decoupled polaron equations. This fact allows the bipolaron state with spontaneously broken symmetry to be interpreted as the bound state of two polarons [8]. In the case of TI bipolarons, $\Phi(\mathbf{r}_1, \mathbf{r}_2) = \Phi(\mathbf{r}_1 - \mathbf{r}_2)$. Splitting the interaction functional for a bipolaron into interaction functionals of individual polarons is impossible, regardless of $|\mathbf{r}_1 - \mathbf{r}_2|$ values, and the notion of TI bipolarons as composite states becomes invalid. This inference is consistent with the modern concept of the impossibility of dividing a quantum mechanical system into independent subsystems [76].

TI bipolarons delocalized at $P = 0$, where P is the total bipolaron momentum, are separated by an energy gap from bipolaron states with broken translational invariance described by a localized wave function. Similar to polarons, TI bipolarons become superconducting when the coupling constant exceeds a certain critical value. Explaining high-temperature superconductivity in terms of the bipolaron mechanism of Bose condensation is known to encounter difficulties arising from the large mass of bipolarons and, consequently, the low temperature of Bose condensation. The possibility of the smallness of TI bipolaron mass resolves the problem.

We emphasize that the aforementioned properties of TI bipolarons impart superconducting features to them even in the absence of Bose condensation, while the high bonding energy of bipolarons makes such a superconductivity scenario realistic, even in strongly defective crystals.

10. Conclusion

Presently, there are no doubts about the Tulub theory or quantitative data obtained using it. This quantum field theory is nonperturbative and can be used to reproduce not only strong and weak coupling limits but also an intermediate coupling regime.

Integration over trajectories [77] is considered to be one of the most effective methods to calculate polarons and bipolarons within this bonding force range. This approach is not translationally invariant without proper modification, because the main contribution to energy levels in this framework comes from classical solutions (i.e., extrema of the exponential of the classical action entering the integral over trajectories). Due to translational invariance, such solutions are not isolated stationary points but belong to a continuum family of classical solutions resulting from the action of the translation operator on the initial classical solution. This makes the stationary phase approximation inapplicable to translationally invariant systems.

Approaches to the restoration of translational invariance in quantum field theory based on the introduction of collective coordinates into functional integral [78] have not been used so far in the polaron theory. Not surprisingly, integration over trajectories yields a result coinciding with the results of the semiclassical theory of the strong-coupling polaron [79].

It has recently been proposed to use the quantum Monte Carlo method as a powerful calculation tool for the polaron theory [80, 81]. However, this tool itself cannot reproduce the results of Tulub's ansatz without the modification mentioned in preceding paragraphs. At the same time, verification of Tulub's ansatz in the strong-coupling limit by the diagrammatic Monte Carlo method is precluded by the necessity to calculate very high-order diagrams.

To summarize, Pekar's ansatz (1.2) is a baseline assumption regarding the form of the solution, confirmed by numerous calculations and evidence. It has been universally accepted during the more than 80-year history of polaron theory (starting from Landau's note [82]) that ansatz (1.2) is an asymptotically exact solution of the polaron problem in the strong-coupling limit.

Tulub's ansatz (see Section 7) is another assumption on the form of the solution, whose structure is determined by the form of the function $\Lambda_0|0\rangle$. The Tulub solution in the framework of this assumption is also asymptotically exact. Tulub's ansatz should be preferred from the variational standpoint, because the Tulub solution gives a lower energy value for polarons.

It follows from the above that the polaron theory is far from complete. Great effort is needed in the framework of Tulub's ansatz to revise many concepts (e.g., superconductivity) and claims of condensed matter physics. Extension of the scope of application of Tulub's ansatz to other aspects of quantum field theory may lead to a radical reconsideration of many previously obtained results currently believed to be unquestionable, and vice versa. For example, the inseparability of the bipolaron state in the polaron model of quarks [83] (with the role of phonons played by the gluon field in [83]) fairly well explains their confinement. It was shown in Ref. [73] that the TI theory does not need to resort to the Higgs mechanism of spontaneous symmetry breaking to estimate the mass of elementary particles.

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11. Appendices

Appendix 1

The Hamiltonian H_1 in (3.2) has the form

$$H_1 = \sum_k (V_k + f_k \hbar\omega_k)(a_k + a_k^+) + \sum_{k,k'} \frac{\mathbf{k}\mathbf{k}'}{m} f_{k'} (a_k^+ a_k a_{k'} + a_k^+ a_{k'}^+ a_k) + \frac{1}{2m} \sum_{k,k'} \mathbf{k}\mathbf{k}' a_k^+ a_{k'}^+ a_k a_{k'}, \quad \text{(A1.1)}$$

where $\hbar\omega_k$ is given by expression (3.5). Let the operator H_1 act on the functional Λ_0 in (7.9). Then $\langle 0|\Lambda_0^+ H_1 \Lambda_0|0\rangle = 0$.

Indeed, the action of Λ_0 on the terms of the Hamiltonian H_1 that include an odd number of operators (the first and the second terms of H_1) always contains their odd number, and the expectation values of these terms vanish.

We consider the expectation value of the last term in H_1:

$$\left\langle 0\left|\Lambda_0^+ \sum_{k,k'} \mathbf{k}\mathbf{k}'\, a_k^+ a_{k'}^+ a_k a_{k'} \Lambda_0\right|0\right\rangle . \tag{A1.2}$$

The function $\langle 0|\Lambda_0^+ a_k^+ a_{k'}^+ a_k a_{k'} \Lambda_0|0\rangle$ is the norm of the vector $a_k a_{k'} \Lambda_0|0\rangle$, positive definite at all k and k'. The substitution $\mathbf{k} \to -\mathbf{k}$ in (A1.2) changes the sign of the entire expression, and (A1.2) vanishes. Hence, $\langle 0|\Lambda_0^+ H_1 \Lambda_0|0\rangle = 0$.

Appendix 2

We show that Eqns (5.4) and (5.5) follow from (5.1) and (5.2). We first note that the analytic properties of $D(s)$ reported in Ref. [32] follow directly from (3.19). Indeed, a pole of $D(s)$ can lie only on the real axis, because the equation

$$1 + \frac{1}{3\pi^2} \int_0^\infty \frac{\omega_k k^4 f_k^2 (\omega_k^2 - s_0 + \mathrm{i}\varepsilon)}{(\omega_k^2 - s_0)^2 + \varepsilon^2}\, \mathrm{d}k = 0 \tag{A2.1}$$

can be satisfied only at $\varepsilon = 0$ due to the positive definiteness of $\omega_k k^4 f_k^2$ in (3.19). Moreover, $D(s)$ is a monotonically increasing function of s because $D'(s) > 0$ at $s < 1$ and $D(s)$ becomes unity as $s_0 \to \infty$. Therefore, $D(s)$ cannot have zeros for $-\infty < s_0 < 1$ and the function $(s-1)D(s)$ can be represented in the form

$$\frac{1}{(s-1)D(s)} = \frac{1}{2\pi\mathrm{i}} \oint_{C+\rho} \frac{\mathrm{d}s'}{(s'-s)(s'-1)D(s')} . \tag{A2.2}$$

The contour of integration in Cauchy's integral (A2.2) is shown in Fig. 2. The integrand in (A.2.2) has the plus sign at $s' = 1$ and contains a cut from $s' = 1$ to $s' \to \infty$. Integration in (A2.2) along the upper and lower sides of the cut yields integral equation (5.5).

Appendix 3

We calculate ΔE in (5.7) with the use of test function (5.9).

The real part of $D(\omega_p^2)$ in (5.7) can be found using Sokhotsky's formula,

$$\frac{1}{\omega_k^2 - \omega_p^2 - \mathrm{i}\varepsilon} = \mathcal{P}\, \frac{1}{\omega_k^2 - \omega_p^2} + \mathrm{i}\pi\delta(\omega_k^2 - \omega_p^2) ,$$

$$\mathrm{Re}\, D(\omega_p^2) = 1 + \frac{1}{3\pi^2} \int_0^\infty f_k^2 k^4 \mathcal{P}\, \frac{\omega_k}{\omega_k^2 - \omega_p^2}\, \mathrm{d}k .$$

It is convenient to represent $\mathrm{Re}\, D$ in the form

$$\mathrm{Re}\, D = 1 + I_1 + I_2 ,$$

$$I_1 = \frac{1}{3\pi^2} \int_0^\infty f_k^2 k^4\, \frac{\mathrm{d}k}{\omega_k + \omega_p} ,$$

$$I_2 = \mathcal{P}\, \frac{\omega_p^2}{3\pi^2} \int_0^\infty \frac{f_k^2 k^4\, \mathrm{d}k}{(\omega_k - \omega_p)(\omega_k + \omega_p)} .$$

Substituting f_k in form (5.9) in these expressions yields

$$I_1 = \frac{8\alpha}{3\sqrt{2}\pi} \int_0^\infty \exp\left(-\frac{k^2}{a^2}\right) \mathrm{d}k - \frac{8\alpha(p^2+4)}{3\sqrt{2}\pi} \int_0^\infty \frac{\exp(-k^2/a^2)}{k^2 + p^2 + 4}\, \mathrm{d}k .$$

Setting $k/a = \tilde{k}$, in the strong-coupling limit ($a \to \infty$) we find

$$I_1 = \frac{8\alpha a}{3\sqrt{2}\pi} \left\{ \frac{\sqrt{\pi}}{2} - \frac{\pi}{2}\, \tilde{p} \exp(\tilde{p}^2) \left[1 - \frac{2}{\sqrt{\pi}} \int_0^{\tilde{p}} \exp(-t^2)\, \mathrm{d}t \right] \right\} .$$

Accordingly,

$$I_2 = \mathcal{P}\, \frac{4\alpha\omega_p}{3\pi\sqrt{2}} \int_0^\infty \frac{\exp(-k^2/a^2) k^2\, \mathrm{d}k}{(\omega_k - \omega_p)(\omega_k + \omega_p)} .$$

The last integral can be represented as the sum

$$I_2 = I_{20} + I_{21} ,$$

where

$$I_{20} = \frac{16\alpha\omega_p}{3\pi\sqrt{2}} \left(1 - \frac{\omega_p - 1}{p^2 + 2} \right) \int_0^\infty \frac{\exp(-k^2/a^2)}{k^2 + p^2 + 4}\, \mathrm{d}k ,$$

$$I_{21} = \frac{16\alpha\omega_p(\omega_p - 1)}{3\pi\sqrt{2}(p^2+2)}\, \mathcal{P} \int_0^\infty \frac{\exp(-k^2/a^2)}{k^2 - p^2}\, \mathrm{d}k .$$

For the integrals entering I_{20} and I_{21}, we have

$$\int_0^\infty \frac{\exp(-k^2/a^2)}{k^2 + p^2 + 4}\, \mathrm{d}k = \frac{1}{a} \left[1 - \frac{2}{\sqrt{\pi}} \int_0^{\tilde{p}} \exp(-t^2)\, \mathrm{d}t \right] \frac{\pi}{2}\, \frac{\exp(\tilde{p}^2)}{\tilde{p}} ,$$

$$\mathcal{P} \int_0^\infty \frac{\exp(-k^2/a^2)}{k^2 - p^2}\, \mathrm{d}k = -\frac{\sqrt{\pi}}{a}\, \frac{\exp(-\tilde{p}^2)}{\tilde{p}} \int_0^{\tilde{p}} \exp(t^2)\, \mathrm{d}t .$$

As a result,

$$I_2 = \frac{2}{3}\, \frac{\alpha a \tilde{p}}{\sqrt{2}} \exp(\tilde{p}^2) \left[1 - \frac{2}{\sqrt{\pi}} \int_0^{\tilde{p}} \exp(-t^2)\, \mathrm{d}t \right] - \frac{4\alpha a \tilde{p}}{3\sqrt{2}\pi} \exp(-\tilde{p}^2) \int_0^{\tilde{p}} \exp(t^2)\, \mathrm{d}t .$$

Finally,

$$\mathrm{Re}\, D = 1 + \frac{4\alpha a}{3\sqrt{2}\pi} \left[1 - \tilde{p} \exp(\tilde{p}^2) \int_{\tilde{p}}^\infty \exp(-t^2)\, \mathrm{d}t - \tilde{p} \exp(-\tilde{p}^2) \int_0^{\tilde{p}} \exp(t^2)\, \mathrm{d}t \right] .$$

This result reproduces the quantity given by formula (5.10). The imaginary part $\mathrm{Im}\, D$ found with the help of Sokhotsky's formula is

$$\mathrm{Im}\, D = \frac{1}{3\pi} \int_0^\infty f_k^2 k^4 \omega_k \delta(\omega_k^2 - \omega_p^2)\, \mathrm{d}k = \frac{1}{6\pi} f_p^2 p^3 .$$

As a result, we express $|D(\omega_k^2)|$ as

$$|D|^2 = (\mathrm{Re}\, D)^2 + (\mathrm{Im}\, D)^2 = \frac{2}{9}\, \alpha^2 a^2 \left\{ \exp(-2\tilde{p}^2)\, \tilde{p}^2 + \frac{8}{2\pi} \left[1 - \tilde{p} \int_{\tilde{p}}^\infty \exp(-t^2)\, \mathrm{d}t - \tilde{p} \exp(-\tilde{p}^2) \int_0^{\tilde{p}} \exp(t^2)\, \mathrm{d}t \right]^2 \right\} .$$

The first term in formula (5.7) is easy to calculate as

$$\frac{1}{4\pi^2}\int_0^\infty \frac{k^4 f_k^2}{1+Q}\,\mathrm{d}k = \frac{3}{16}\,a^2\,.$$

In calculating the second term in (5.7), we segregate the integral

$$I_p = \int_0^\infty \exp\left(-\frac{k^2}{a^2}\right)\frac{k^2\left(\omega_k\omega_p + \omega_k(\omega_k+\omega_p)+1\right)}{(\omega_k+\omega_p)^2}\,\mathrm{d}k\,.$$

As $a\to\infty$, we have

$$I_p = a^3\,\frac{\sqrt{\pi}}{4}\left[1-\tilde{p}^3\exp(\tilde{p}^2)\right.$$
$$\left.\times\int_{\tilde{p}}^\infty \exp(-t^2)\,\mathrm{d}t\,(2+4\tilde{p}^2)+2\tilde{p}^4\right] = \frac{a^3\sqrt{\pi}}{4}\left(1-\Omega(\tilde{p})\right),$$

where

$$\Omega(\tilde{p}) = 2\tilde{p}\left[(1+2\tilde{p}^2)\,\tilde{p}\exp(\tilde{p}^2)\int_{\tilde{p}}^\infty \exp(-t^2)\,\mathrm{d}t - \tilde{p}^2\right],$$

which corresponds to the expression for $\Omega(y)$ in (5.12).

As a result, the following expression for the second term in the right-hand side of (5.7) is obtained:

$$\frac{1}{12\pi^4}\,\frac{4\pi\alpha}{\sqrt{2}}\int_0^\infty I_p\,p^4 f_p^2\,\frac{\omega_p}{(\omega_p^2-1)\left|D(\omega_p^2)\right|^2}\,\mathrm{d}p\,.$$

As $a\to\infty$, the last expression takes the form

$$\frac{\alpha^2 a^4}{3\pi\sqrt{\pi}}\int_0^\infty \left(1-\Omega(\tilde{p})\right)\frac{\exp(-\tilde{p}^2)}{\left|D(\omega_{\tilde{p}}^2)\right|^2}\,\mathrm{d}\tilde{p} = \frac{3}{16}\,a^2 q\,,$$

where $q=q(0)$ is given by (5.12). Finally, for ΔE in (5.7), we have

$$\Delta E = \frac{3}{16}\,a^2(1+q)\,,$$

which corresponds to the first term in the right-hand side of (5.11).

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