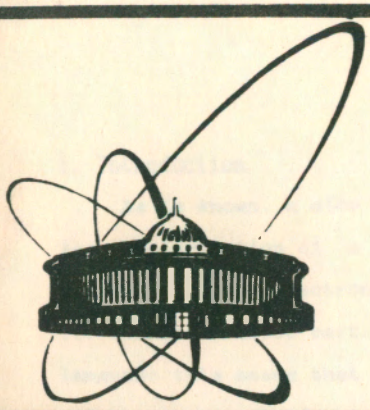

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FROHLICH MULTIPOLARONS

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1. Introduction

As is known, a slow electron in an ionic crystal creates a local polarization of a surrounding medium, which lowers its energy. When the electron moves, the polarization region follows it, forming a quasi particle, a polaron. In a quantum-mechanical language this means that the electron polarizes the phonon vacuum, and the processes of emission and subsequent absorption of virtual phonons result in the renormalization of the electron energy; thus the polaron is a bound state of a charged particle in a quantum scalar field. The most known between the various polaron models is the Frohlich optical polaron, that is the model of a scalar particle in a continious medium interacting with LO-phonons.

Up to now the theory of the Frohlich polaron can be considered as a well developed field of solid state physics. The investigations have been done extensively for various quantities characterizing a one-polaron system: self-energy and effective mass, mobility, optical absorption coefficient and so on. Much less attention has been paid, however, to studying many-polaron systems. For the first time the possibility for two polarons to form a bound state (bipolaron) has been considered in paper [1]. Calculations should be also mentioned of the bipolaron ground state energy and effective mass by the path integral method [2], the critical value of the electron-phonon coupling to form bipolarons and the mean distance between two electrons in a bipolaron [3,4]. From the physical point of view the bipolaron concept can be useful in studying the properties of negative U-centers and D^- complexes in ionic crystals. These systems consist of a defect and two bound electrons and can be considered as intrinsic bipolarons [5-7]. Recent interest in the bipolarons is caused by

their role in attempts of explaining the high-temperature superconductivity. According to the proposed bipolaronic mechanism of superconductivity, the bipolarons of high enough density undergo the Bose-Einstein condensation, which results in a superconductivity state [8].

Naturally, the question arises whether there is a possibility of an N-polaron bound state to be formed for $N \geq 2$. When N electrons propagate in a medium there are feasible processes of phonon exchange between them, which give rise to attraction forces. Therefore a bound state of N polarons can exist. If the constant of electron-phonon interaction is small, $g \ll 1$, the probability of creating a bound state of two polarons is g^2 times as small as the probability of their free propagation. In other words, in the regime of weak coupling polarons hold their individuality and almost independently propagate through a crystal. In this case, it should be expected, their total energy is merely a sum of energies of N isolated polarons.

In the strong coupling regime the processes of phonon exchange are no longer suppressed, and a bound state of N electrons arises which is surrounded by a common cloud of virtual phonons. Polarons lose their individuality completely, and the energy of such a state should strongly depend on the number of electrons N. Really N polarons compose a bound state whose energy is much lower than the total energy of N isolated polarons. In paper [2] we indicated that the formation of macroscopic polaron clusters is more profitable energetically.

It may appear that the Coulomb repulsion forces between electrons will impede the formation of an N-polaron cluster. However, the electron-phonon interaction is itself of a Coulomb

type, and it is clear that at a sufficiently large coupling constant of electron-phonon interaction the electro-static forces will be unable to prevent polarons to merge into a cluster. The same may be concluded from the results on the behaviour of a single polaron in a field of a fixed Coulomb charge [9].

Formation of the polaron clusters with a low energy (owing to large N) may lead to heating a crystal. With increasing temperature the effective constant of electron-phonon interaction diminishes, a polaron "undresses" [10, 11], which in turn may result in a self-destruction of a polaron cluster. So interesting temperature effects can exist in polaron physics.

The paper is organized as follows. In Sec.2 we introduce the exactly solvable N-particle linear polaron model to illustrate the decreasing N-dependence of the ground state energy. In Sec. 3 a representation is obtained for a partition function of a system of N polarons as path integrals. In Sec. 4, using the variational method, we estimate the ground-state energy and the effective mass of the system. Sec. 5 contains estimations and a discussion of the role of temperature.

2. Linear polaron model

There exists an exactly solvable model of an N-particle system in a phonon field. It is a linear version of the Frohlich Hamiltonian:

$$H = -1/(2\mu)\sum_{j}^{N} \nabla_j^2 + (1/2)\sum_{i,j}^{N} \gamma_{ij}\, r_i r_j + \sum_{k} \omega_k a_k^+ a_k$$

$$+ \sum_{j}^{N}\sum_{k} [i\pi_j(k)/\sqrt{2\omega_k V}\,](kr_j)(a_k^+ - a_k)\,, \qquad (2.1)$$

where

$$\gamma_{ij} = (1/3)\sum_{k} k^2 \,[\pi_j(k)\pi_i(k)]/(\omega_k^2 V) \quad . \qquad (2.2)$$

System (2.1) for $N = 1$ has been proposed by Bogolubov [12] to approximate the Frohlich polaron and now is referred to as the linear or Bogolubov polaron. Relation (2.2) provides the conservation of the set of N momenta :

$$P_j = -i\nabla_j + \sum [k\pi_j(k)(a_k^+ + a_k)]/(\omega_k \sqrt{2\omega_k V}) \quad , \quad j = 1.2....N \; .$$

The energy of the system at fixed total momentum $P = \sum P_j$ takes the form

$$\mathcal{E}(P) = E + P^2/2m \; .$$

where E is the energy of the multipolaron at rest and m - its effective mass. The functions $\pi_j(k)$ are introduced to characterize the interaction between an j-th particle and a phonon with a wave vector k . They are assumed to be in the form

$$\pi_j(k) = \alpha_j \pi(k). \quad j = 1, 2, \ldots, N. \qquad (2.3)$$

System (2.1) under constraints (2.3) turns out to be exactly solvable. Due to (2.3) the particles interacting with a field distinguish from one another only by different "charges" α_j .

Let us now introduce a new set of coordinates $\{y_j\}$ instead of $\{r_j\}$ through the linear orthogonal transformation

$$y_j = \sum_{j=1}^{N} W_{ji} r_i \; . \qquad (2.4)$$

matrix W being taken to diagonalize the quadratic form $\sum \gamma_{ij} r_i r_j = \gamma^2 \sum \alpha_i \alpha_j r_i r_j$:

$$\hat{W} : \sum_{i,j} \alpha_i \alpha_j r_i r_j \Rightarrow S(N) y_N^2 . \qquad (2.5)$$

Here, the use has been made of the relations

$$\gamma^2 = (1/3)\sum_k \frac{\pi^2(k)k^2}{\omega_k^2 V} \qquad \text{and} \qquad S(n) = \sum_{i=1}^{n} \alpha_i^2 .$$

There should be kept in mind that (2.5) is due to the fact that the matrix $\| \alpha_i \alpha_j \|$, $i,j = 1,\ldots, N$ possesses the principal values 0 of an $(N-1)$-fold degeneracy and $S(N)$. The matrix W is readily obtained : $W = \| W_{nj} \|$, where

$W_{nj} = 0$, $1 \le n \le N-2$, $n+2 \le j \le N$;

$W_{nj} = (\alpha_{n+1}\alpha_j)/\sqrt{S(n)S(n+1)}$, $1 \le n \le N-1$, $1 \le j \le n$;

$W_{n,n+1} = -\sqrt{S(n)/S(n+1)}$; $W_{Nj} = \alpha_j/\sqrt{S(N)}$, $1 \le j \le N$.

The W - transformation being applied to Hamiltonian (2.1) yields

$$\hat{W} : H[\mathbf{r}_1 \ldots \mathbf{r}_N] \Rightarrow H[\mathbf{y}_1 \ldots \mathbf{y}_N] = -(1/2\mu)\sum_j^{N-1} \frac{\partial^2}{\partial \mathbf{y}_j^2} + H_R[\mathbf{y}_N] ,$$

$$H_R = -(1/2\mu)\frac{\partial^2}{\partial \mathbf{y}_N^2} + (\gamma_R^2/2)\mathbf{y}_N^2 + \sum_k \omega_k a_k^+ a_k + \qquad (2.6)$$

$$+ \sum_k \frac{i\pi_R(k)}{\sqrt{2\omega_k V}} (\mathbf{k}\mathbf{y}_N)(a_k^+ - a_k) .$$

Hamiltonian H_R describes a linear polaron with the renormalised interaction:

$$\pi_R(k) = \sqrt{S(N)}\,\pi(k) , \qquad \gamma_R^2 = S(N)\gamma^2 .$$

A one-polaron linear model is known to be exactly solvable [12,13] and for the ground-state energy and the effective mass of the N - polaron linear model the following expressions are readily obtained:

$$E = (3/2)\omega\,[\sqrt{1 + g_R^2(N)} - 1] , \quad m = \mu N[1 + g_R^2(N)/N] . \qquad (2.7)$$

where

$$g_R^2(N) = \sum_k (\pi_R^2 k^2)/3\mu\omega_k^4 V$$

is the dimensionless renormalised coupling constant. In the regime of weak coupling ($g_R^2 \ll 1$) N linear polarons are independent up to the order g_R^4. As we shall see, this is very likely to the system of N Frohlich polarons at small coupling constant. In the strong coupling limit ($g_R^2 \gg 1$) there is formed an N-particle bound complex with a self-energy $E \sim \sqrt{N}$.

If the "charges" α_i are the same for all the polarons, the renormalized coupling constant is expressed as

$$g_R^2(N) = N g^2 ,$$

where g is the one-polaron coupling constant. Then Eqs. (2.7) take the more simple form

$$E = (3/2)\omega \left[\sqrt{1 + g^2 N} - 1\right], \quad m = \mu N[1 + g^2]. \qquad (2.8)$$

It is clear that at any coupling constant $E < N E_1$ for $N > 1$, that is the energy of the multipolaron bound state is lower than the sum of the energies E_1 of N independent polarons. Besides, it is worth noting that for all the values of g_R^2 the effective mass of system (2.1) is a sum of the masses of individual polarons, which is a result of the momentum conservation for each of them. This is the main distinction as compared with the Frohlich polaron.

It is obvious that the specific behaviour of the multipolaron energy and effective mass on N strongly depend on the concrete model under consideration. For example, the Coulomb interaction leads to the energy proportional to N^3. To convince let us consider a simple quantum-mechanical model, a system of N identical particles with mass μ and charges q interacting with each other by the Coulomb attraction law:

$$H = \sum_{i=1}^{N} p_i^2/2\mu - \sum_{i<j} q^2/|r_i - r_j| .$$

Let R be a characteristic size of the system. Then the potential energy of interaction of a pair of particles has an order of $-q^2/R$, and the total potential energy of the system equals $-q^2/R$ times the number of pairs, $N(N-1)/2$. The kinetic energy of every particle equals $1/2\mu R^2$ in order of magnitude, whereas the total kinetic energy is N times as large. As a result, the ground-state energy of the system is given by the expression

$$E = \frac{N}{2\mu R^2} - \frac{q^2 N(N-1)}{2R} \quad ,$$

that gets its minimum at $R = 2/\mu q^2 (N-1)$. Therefore we obtain

$$E = -\frac{\mu q^4}{8} N(N-1)^2$$

When N=2, i.e. the problem has a clear physical meaning, we arrive at the known result for a particle with a reduced mass placed in the Coulomb potential. For arbitrary N the problem simulates an N-polaron cluster and shows a characteristic N^3-dependence of the ground-state energy of the Frohlich multipolaron.

3. Path integrals

The Frohlich Hamiltonian for a system of N identical spinless charged particles is of the form

$$H = \sum_{i=1}^{N} \mathbf{p}_i^2/2\mu + \sum_{\mathbf{k}} \omega_{\mathbf{k}} a_{\mathbf{k}}^+ a_{\mathbf{k}} + g \sum_{i=1}^{N} \sum_{\mathbf{k}} (A_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_i} + A_{\mathbf{k}}^* a_{\mathbf{k}}^+ e^{-i\mathbf{k}\mathbf{r}_i}) +$$

$$+ \sum_{i<j} V(|\mathbf{r}_i - \mathbf{r}_j|), \qquad (3.1)$$

where $\mathbf{r}_i$ and $\mathbf{p}_i$ are, respectively, the coordinate and momentum of an i-th electron. $a_{\mathbf{k}}$ is the amplitude of a $\mathbf{k}$-th mode of a phonon field with energy $\omega_{\mathbf{k}}$, and $V(|\mathbf{r}_i - \mathbf{r}_j|) = e^2/|\mathbf{r}_i - \mathbf{r}_j|$ is the Coulomb potential of repulsion between i-th and j-th particles. In Ref.[2] we used Hamiltonian (3.1) at N=2 for studying the bound state of two

polarons, whereas J.T.Devreese et al.[14] employed it for analyzing optical properties of a two-dimensional electron gas.

For a Frohlich optical polaron it is usually assumed that

$$\omega_k = \omega \,,\quad gA_k = -\frac{i}{k}\left[\frac{2\sqrt{2}\alpha\pi\omega^{3/2}}{V\sqrt{\mu}}\right]^{1/2},\quad g^2\sum_k |A_k|^2 \Rightarrow \frac{\alpha\omega^{3/2}}{2\sqrt{2\mu}\pi^2}\int\frac{dk}{k^2}\,,$$

where α is a dimensionless coupling constant, and V is the volume of the system.

Let us consider the operator

$$\hat{Z}(u) = \exp\left[-\beta\,(H - u\hat{P})\right]\,|\,\Phi\,><\,\Phi\,|\quad,$$

where $\hat{P}$ is the operator of the total conserved momentum

$$\hat{P} = -i\sum_{j=1}^{N}\nabla_j + \sum_k k\,a_k^+ a_k\quad,$$

and $|\Phi>$ is an arbitrary state. The vector u has a meaning of average velocity. The operator $\hat{Z}$ defines a distribution of the grand canonical type and to it there corresponds the partition function $Z(u) = Sp\,\hat{Z}(u)$, from which the ground state energy at a fixed value of P can be defined:

$$\varepsilon(P) = uP - \lim_{\beta\to\infty}\frac{1}{\beta}\ln Z(u),\qquad \lim_{\beta\to\infty}\frac{1}{\beta}\frac{\partial\ln Z}{\partial u} = P. \tag{3.2}$$

If we take different states $|\Phi>$, we arrive at different boundary conditions in the functional integral for Z which does not influence the definition of energy $\varepsilon(P)$. For simplicity, we take $|\Phi>$ in the form

$$|\Phi\,> = |0>|r_1>|r_2>\ldots|r_N>|r_1 = r_2 = \ldots = r_N$$

which results in zeroth boundary conditions in the N-fold integral along paths over each of the integration variables. For Z it is possible to get the following representation as N-fold path integral

$$Z(u) = \int_{x_i(0)=x_j(0)=0}\mathcal{D}x_1\,\mathcal{D}x_2\ldots\mathcal{D}x_N\,\exp S[x_1,x_2,\ldots,x_N;u]\quad. \tag{3.3}$$

$$S[x_1, x_2, \ldots, x_N; u] = \beta\mu u^2 N/2 - (\mu/2)\sum_{j=1}^{N} \int_0^\beta \dot{x}_j^2\, ds +$$

$$+ (1/2) \sum_{i,j=1}^{N} \sum_k |A_k|^2 \int_0^\beta ds_1 ds_2 \exp\{-\omega|s_1 - s_2| + ku(s_1 - s_2) -$$

$$- ik[x_i(s_1) - x_j(s_2)]\} -$$

$$- \sum_{i<j} \int_0^\beta V(|x_i(\sigma) - x_j(\sigma)|)\, d\sigma \quad . \tag{3.4}$$

Derivation of formulae (3.3-4) for two polarons is given in [2] and can be extended without difficulty to the case of arbitrary N.

We shall estimate the integral (3.3) by the Feynman method [15]:

$$\int_{x_i(0)=x_i(\beta)=0} \mathcal{D}x_1 \ldots \mathcal{D}x_N \exp S[x_1, \ldots, x_n; u] = \int_{x_i(0)=x_i(\beta)=0} \mathcal{D}x_1 \ldots \mathcal{D}x_N\, e^{S'} \exp(S - S')$$

$$\geq \int_{x_i(0)=x_i(\beta)=0} \mathcal{D}x_1 \ldots \mathcal{D}x_N\, e^{S'} \exp\langle S - S' \rangle , \tag{3.5}$$

where the symbol $\langle \ldots \rangle$ stands for averaging of the functional over the measure $\exp S'$. As an approximating action S', we take a sufficiently plain action for which the path integral may be computed exactly. It is natural to take S' as a quadratic form over variables $x_i(s)$, the coefficients of which being considered as variational parameters. One should take into account that the action S is invariant under exchange of the positions of any two particles. An approximating action S' should possess the same symmetry. Then a trial wave function of the ground state we are interested in will be symmetric *a priori* under permutations of any two particles. This takes into account the effects of the Bose-statistics of the system. The fermion case should be considered separately.

So we choose S' as follows:

$$S'[x_1,\ldots,x_n] = -\frac{\mu}{2}\sum_{i=1}^{N}\int_0^\beta x_i^2\,ds \;-\; \frac{\mu}{2}\sum_{i=1}^{N} C_{ij}\int_0^\beta x_i x_j\,ds\ . \qquad (3.6)$$

where the matrix C takes the form

$$C_{ij} = B + (A - B)\,\delta_{ij}\ ,\ i,j = 1,\ldots,N\ . \qquad (3.7)$$

The relation (3.7) follows from the symmetry properties. coefficients A and B are variational parameters. It is easy to convince oneself that the matrix C has two different eigenvalues

$$\Omega^2 = A - B\ , \qquad \Omega_N^2 = A + B\,(N-1)\ , \qquad (3.8)$$

where Ω^2 is $(N-1)$-fold degenerated. The quadratic form in (3.6) should be positive definite so the variational parameters vary in the range, where eigenvalues Ω^2 and Ω_N^2 are positive.

It is not difficult to calculate the orthogonal $N*N$ matrix U which diagonalizes C. One variant has the form:

$$U_{ij} = b + (a - b)\,\delta_{ij}\ ,\ i,j = 1,\ldots,N-1,$$

$$U_{iN} = U_{Ni} = 1/\sqrt{N}\ ,\ i = 1,\ldots,N\ ,$$

$$a = b + 1\ ,\qquad b = -(\sqrt{N}+1)/(N-1)\sqrt{N}\ . \qquad (3.9)$$

Note that any other realization of the matrix U does not influence the results obtained in what follows.

4. Variational estimates

Eqs. (3.2), (3.5) provide an upper bound on the ground-state energy of the system in the vicinity of the point $P = 0$:

$$\mathcal{E}(P) \le E + P^2/2m\ ,$$

where E is an upper bound on the ground-state energy at $P = 0$, and m is a lower bound on the effective mass of the system. To perform the calculations, we change the variables in (3.3) with the help of liner transformation U:

$$x_i(s) = \sum_{j=1}^{N} U_{ij}\, y_j(s). \qquad (4.1)$$

In new variables $y_i(s)$ the approximating action (3.6) is diagonal:

$$S'[y_1,\ldots,y_n] = -\frac{\mu}{2}\sum_{i=1}^{N}\int_0^\beta y_i^2\, ds \;-\; \frac{\mu}{2}\sum_{i=1}^{N}\Omega_i^2\int_0^\beta y_i^2\, ds\,. \qquad (4.2)$$

where in accordance with (3.8) the frequencies Ω_i are equal for all $i = 1,\ldots,N-1$: $\Omega_i = \Omega$.

The averages entering into the estimate (3.5) are as follows:

$$\langle \exp -ik\,[x_i(s_1)-x_j(s_2)]\rangle = \langle \exp -ik\sum_{\ell=1}^{N}[U_{i\ell}y_\ell(s_1)-U_{j\ell}y_\ell(s_2)]\rangle =$$

$$\exp\left\{-\frac{k^2}{2\mu}\sum_{\ell=1}^{N}[2U_{i\ell}U_{j\ell}G^{(\ell)}(s_1,s_2)-U_{i\ell}^2G^{(\ell)}(s_1,s_1)-U_{j\ell}^2G^{(\ell)}(s_2,s_2)]\right\}, \qquad (4.3)$$

where $G^{(\ell)}(s_1,s_2)$ is the Green function of a linear oscillator with frequency Ω_ℓ obeying the corresponding boundary conditions:

$$(d^2/ds^2 - \Omega_\ell^2)G^{(\ell)}(s,\sigma) = \delta(s-\sigma),\quad G^{(\ell)}(0,\sigma) = G^{(\ell)}(\beta,\sigma) = 0,$$

$$G^{(\ell)}(s,\sigma) = [\operatorname{ch}\Omega_\ell(\beta-s-\sigma) - \operatorname{ch}\Omega_\ell(\beta-|s-\sigma|)]/2\Omega_\ell \operatorname{sh}\Omega_\ell\beta\,. \qquad (4.4)$$

It can easily be found that

$$\int_{y_i(0)=y_i(\beta)=0} \mathcal{D}y_1\ldots\mathcal{D}y_N\, e^{S'} = (\mu/2\pi\beta)^{3N/2}\prod_{\ell=1}^{N}(\Omega_\ell\beta/\operatorname{sh}\Omega_\ell\beta)^{3/2}. \qquad (4.5)$$

$$(\mu\Omega_\ell^2/2)\int_0^\beta ds\,\langle y_\ell^2(s)\rangle = \frac{3}{4}\left[\Omega_\ell\beta\coth\Omega_\ell\beta - 1\right]. \qquad (4.6)$$

Using (4.3-6) we can obtain an estimate for the energy as a function of the parameters Ω and Ω_N. For the ground-state energy of the multipolaron at rest and its effective mass we get the estimates

$$E = \frac{3}{4}\left[(N-1)\Omega + \Omega_N\right] - \frac{N\alpha\omega^{3/2}}{\sqrt{\pi}} \int_0^\infty d\sigma\, e^{-\omega\sigma}\left[\Phi_N^{-1/2}(\sigma) + (N-1)\Psi_N^{-1/2}(\sigma)\right]$$

$$+ \frac{N(N-1)}{2}\frac{e^2\sqrt{2\mu}}{\sqrt{\pi}}\sqrt{\Omega}\ . \qquad (4.7)$$

$$m = \mu N\left(1+\frac{\alpha\omega^{3/2}}{3\sqrt{\pi}}\int_0^\infty d\sigma\,\sigma^2\, e^{-\omega\sigma}\left[\Phi_N^{-3/2}(\sigma) + (N-1)\Psi_N^{-3/2}(\sigma)\right]\right), \qquad (4.8)$$

where

$$\Phi_N(\sigma) = \frac{N-1}{\Omega N}\left(1-e^{-\Omega\sigma}\right) + \frac{1}{N\Omega_N}\left(1-e^{-\Omega_N\sigma}\right)\ ,$$

$$\Psi_N(\sigma) = \frac{1}{\Omega N}\left(N-1+e^{-\Omega\sigma}\right) + \frac{1}{N\Omega_N}\left(1-e^{-\Omega_N\sigma}\right)\ . \qquad (4.9)$$

Note that the part of the action (4.2) with the parameter Ω approximates the inner motion within the polaron cluster. It follows from (3.9) and (4.1) that

$$y_N(s) = \frac{1}{\sqrt{N}}\sum_{i=1}^{N} x_i(s)\ .$$

So, motion of the centre of inertia of the system is approximated by an oscillator action with frequency Ω_N. The action (3.4) is invariant under simultaneous translations of all the coordinates $x_i(s)$. The centre of inertia of the system (3.1) moves along a straight line when there is no electron-phonon interaction. In this case $\Omega_N=0$, which one can see easily from (4.7) taking $\alpha = 0$ and changing the sign of e^2 (the system of gravitating masses). The approximating action S' occurs to be invariant under translations. Minimization over Ω results in an expression analogous to (2.9).

When $\alpha \neq 0$, the centre of inertia of the system moves along a rather intricate trajectory, the more different from a straight line, the larger is α. Bogolubov was the first who had paid attention to this fact[16]. Correspondingly, the variational

parameter Ω_N will not be equal to zero as we shall see later. In any case the values of the parameters Ω and Ω_N are defined by minimizing the multipolaron energy (4.7).

Let us now examine various limiting cases. In the weak coupling regime ($\alpha \ll 1$) $\Omega = \Omega_N = 0$ and

$$E = -\frac{N\alpha\omega^{3/2}}{\sqrt{\pi}} \int_0^\infty \frac{d\sigma}{\sqrt{\sigma}} e^{-\omega\sigma} = -N\alpha\omega \,, \qquad (4.10)$$

$$m = \mu N \left(1 + \frac{\alpha\omega^{3/2}}{3\sqrt{\pi}} \int_0^\infty d\sigma \sqrt{\sigma}\, e^{-\omega\sigma}\right) = \mu N(1+\alpha/6), \qquad (4.11)$$

i.e. to the first approximation in coupling constant α the cluster falls into N independent polarons. Corrections to the additive formula (4.10-11) for the system energy and effective mass arise only in the two-phonon approximation and are of an order of α^2. For two polarons these corrections have been found in [2]. Formula (4.10) has been derived without taking into account the Coulomb repulsion which at small α does not allow a bound state of polarons to be formed at all.

In the strong coupling regime ($\alpha \gg 1$) Ω and Ω_N are large, and (4.7) acquires the form

$$E = \frac{3}{4}\left[(N-1)\Omega + \Omega_N\right] - \frac{N^2\alpha\omega^{3/2}}{\sqrt{\pi}}\left[\frac{N-1}{\Omega N} + \frac{1}{N\Omega_N}\right]^{-1/2} + \frac{N(N-1)}{2}\frac{e^2\sqrt{2\mu}}{\sqrt{\pi}}\sqrt{\Omega} \,. \qquad (4.12)$$

If the Coulomb repulsion is neglected, (4.12) reaches its minimum at $\Omega=\Omega_N$, so that

$$E = \frac{3}{4}N\Omega - \frac{N^2\alpha\omega^{3/2}}{\sqrt{\pi}}\sqrt{\Omega} \,, \qquad \Omega_{min} = \omega\,\frac{4}{9\pi}\,(\alpha N)^2 \qquad (4.13)$$

whereas for the ground-state energy of the system we get the estimate

$$E = -\omega\,(\alpha^2/3\pi)\,N^3 \,. \qquad (4.14)$$

Here $-\omega\ (\alpha^2/3\pi)$ is the energy of one polaron in the strong coupling regime. Qualitative dependence of the energy of a polaron cluster was discussed in Sec.2. The result of Ref. [2] is reproduced when one puts $N=2$.

The expression for the multipolaron effective mass is as follows:

$$m = (16\alpha^4/81\pi^2)N^6 . \qquad (4.15)$$

For $N = 2$ relation (4.15) coincides with the result of Ref.[2]. Thus the N-polaron system goes from a weakly correlated, loosely formed state at small α to a compact, strongly correlated configuration at large α with an enormous mass. So, in the strong coupling limit, an N-polaron cluster is proved to be practically localized.

The correction δE for the Coulomb two-body repulsion can be found by substituting Ω_{min} defined by (4.13) into the last term in (4.12) and is given by

$$\delta E = \frac{N^2(N-1)}{3\pi}\,\alpha\, e^2 \sqrt{2\mu\omega} \quad .$$

It is, naturally, valid when

$$\delta E/E = \frac{N-1}{N}\,(2\mu e^4/\omega\alpha^2)^{1/2} \ll 1 . \qquad (4.16)$$

The physical meaning of the condition (4.16) is obvious.

5. Conclusion

Thus, when the electron-phonon interaction is strong, the Coulomb repulsion does not really preclude formation of a cluster, a bound state of N polarons. It may, however, happen that for concrete substances the strong coupling regime is not reached. Indeed, a characteristic scale of the Coulomb repulsion energy E_c is given by the potential of ionization of a hydrogen atom, i.e. $E_c \approx 10$ eV; a characteristic value of the frequency, $\omega \approx (10^{13}-$

10^{14}) $c^{-1} \approx (10^{-1} - 10^{-2})$ eV. Hence it follows that a bound state becomes feasible when $\alpha \approx (E_c/\omega)^{1/2} \approx 10\text{-}20$. In this case the polaron radius [17] defined by $R \approx 4\pi^2/\alpha\sqrt{2\mu\omega}$ turns out to be equal to several dozen angstroms, which is much larger than the lattice constant. This means that even at such, almost unreal large values of α, we are all the same dealing with a collective effect so that the Frohlich polaron concept remains valid.

The energy of one polaron in the strong coupling regime when $\alpha \approx 10$ equals about several tenths of eV. However, as a result of a strong dependence on the number of particles in a polaron cluster, the cluster energy may on the whole be significantly lower. If that energy in the process of formation of a cluster is transferred to the lattice, it may be sufficient for heating the crystal and even for melting it (i.e. at electron concentration of the order of $10^7 - 10^8$ mol^{-1} which is not very large as compared to the Avogadro number).

However, the polaron cluster will be destroyed before the crystal. If in the process of its formation heat is really released, then heating of the medium should diminish the effective constant of electron-phonon interaction. In our paper [10], we have studied a high-temperature expansion of the ground-state energy of one polaron. The obtained result is as follows:

$$E/\omega = -0{,}5\sqrt{\pi/\beta}\,[\alpha + 0{,}029\,\alpha^2\sqrt{\beta} + O(\beta)]\,, \quad \beta = \omega/k\theta \ll 1\,,$$

from which it is seen that when the second term in brackets is smaller than the first one, the system effectively goes into the regime of weak coupling and its energy is described by the first order in α. In an N-particle problem this regime means, as we have seen, that a polaron cluster has fallen into N independent polarons. This occurs when $1/\beta \gg (0.03\alpha)^2$, i.e. when $k\theta \gg k\theta_c = 10^{-3}\alpha^2\omega \approx$

$0.01\ E_{pol}$, where E_{pol} represents the polaron energy in the strong coupling regime at zero temperature. Qualitatively, θ_c is estimated to be of an order of 50 K.

Recall that we have considered the behaviour of charged bosons. It may happen that for fermions a similar effect will be weakened owing to the Pauli principle. It can occur that Fermi particles in a crystal prefer to form bipolarons so the collapse into the multipolaron state becomes impossible. Still, may be, some temperature effects do exists in fermion systems too. This needs the investigation.

Note the great significance of the mass value of a "bare" particle polarizing a medium. Heavy charged particles (deuterons, e.g.) form polarons of a very small radius. The coupling constant α is proportional to the square root of the particle mass [17], and the polaron radius will be inversely proportional to its mass. For a proton in the strong coupling regime the polaron radius will be significantly smaller than the lattice constant, and the Frohlich model is no longer applicable. This problem also requires further studies in the framework of a more realistic theory in which the structure of a lattice is taken into account.

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