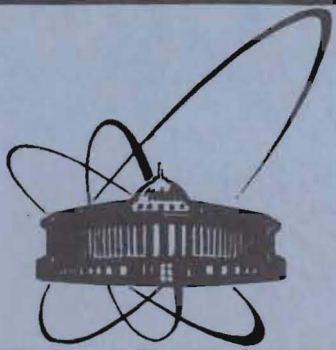

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DIAGRAMS IN THE POLARON MODEL

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1. INTRODUCTION

The polaron model exists for a long time, but as far as we know, no systematic exposition has yet been given for calculations by perturbation theory. As a matter of fact, widely known are only the results of first order in the coupling constant. As to the next, second order, in the literature one can find contradictory assertions, references to incorrect calculations, etc. Higher orders of perturbation theory were not treated at all in view of computational difficulties. Therefore, we consider it reasonable to discuss this question which is of certain theoretical interest at least. Moreover, such an interest is stimulated by some practical reasons. Thus, for values of the coupling constant characteristic of real crystals the first three terms of a perturbation series turn out to provide a better estimate of the ground-state energy than any of the approximate procedures applied earlier. Further, the polaron model traditionally serves as a tool for nonperturbative strong-coupling methods. However, any method of that kind capable to describe the polaron properties throughout the whole range of the coupling constant values should be compared, at small coupling constants, with exact results of the perturbation theory.

Finally some physicists suspicted that at a certain critical value of the coupling constant there occurs a phase transition from the polaron state of weak coupling to the localized state of strong coupling. As one supposes the energy is not analytic in coupling constant at that point, and other characteristics of the polaron (e.g., the average number of phonons) have discontinuities. The perturbation series for polaron being known exactly would help to solve the problem of whether the phase transition really occurs or not.

In this paper we develop the perturbation theory for polaron. In Sec.2 rules are formulated for constructing Feynman diagrams for the energy of the system. In Sec.3 we calculate the polaron energy and mass in the first two perturbation orders. In Sec.4 the energy of the polaron at rest is computed in the third order. In Sec.5 an expansion in coupling constant is constructed for the average number of virtual phonons around the electron. While constructing the diagrammatic technique in the polaron model we shall make use of the quantum-mechanical perturbation theory. So we consider it is worth giving here a sketch of its basic results. For simplicity we shall deal with

corrections to the energy of the ground state which is known to be nondegenerate. So one splits the Hamiltonian H into the perturbation potential V and free part H_0, for which wave functions and eigenvalues are known: $H_0|n\rangle = E_n^{(0)}|n\rangle$. The conventional notation $V_{nm} = \langle n|V|m\rangle$ and $\omega_{nm} = E_n^{(0)} - E_m^{(0)}$ is adopted. Brillouin-Wigner perturbation theory bases on the expansion

$$E = E_0^{(0)} + V_{00} + \sum_{k\geq 2} \sum_{n_1,\ldots,n_{k-1}}{}' \frac{V_{0n_1} V_{n_1 n_2} \cdots V_{n_{k-1}0}}{(E - E_{n_1}^{(0)}) \ldots (E - E_{n_{k-1}}^{(0)})}, \qquad (1.1)$$

where the prime signifies that all $n_i \neq 0$, i.e., the absence of the ground state in the sum over all possible intermediate states.

If we cut the series (1.1) at a certain value $k = k_0$, we obtain the equation for the perturbed energy E, to which the minimal root corresponds. To construct the Rayleigh-Schrödinger perturbation series one needs to expand also the denominators in (1.1). Doing so the first k_0 terms of the series will be reproduced exactly.

It follows from (1.1), that a k-th-order correction to the ground-state energy $E_0^{(0)}$ is written as a sum of connected and disconnected parts. The connected part is as follows:

$$(E_k)_{con} = \sum_{n_1,\ldots,n_{k-1}}{}' \frac{V_{0n_1} V_{n_1 n_2} \cdots V_{n_{k-1}0}}{\omega_{0n_1} \cdots \omega_{0n_{k-1}}}. \qquad (1.2)$$

It contains k matrix elements of the perturbation potential and $k-1$ propagators of the form $1/\omega_{0n}$. The disconnected part is a sum of terms, each being a product of previous energy corrections by a certain factor. The previous energy corrections occur in all possible combinations in orders from 1 to $k-2$: E_1, E_1^2, E_2, $2E_1E_2$, etc. Each of these combinations including the numerical factors can be obtained from expressions of the form

$$(E_1 + E_2 + \ldots + E_{k-2})^m, \qquad m = 1, 2, \ldots, k-2. \qquad (1.3)$$

Let some of these combinations be of order i and contain j propagators. Then it should be multiplied by a factor obtained from $(E_{k-i})_{con}$ by adding into the denominator missing $i-j$ powers of propagators so that the total number of propagators in $(E_k)_{con}$ and in all terms of $(E_k)_{dis}$ be the same. The addition of powers is accomplished in all possible ways to all propagators that enter into $(E_{k-i})_{con}$, each further power giving the factor -1.

It is easy to convince oneself that exactly m propagators should be added when constructing some term of the disconnected part with (1.3) at a certain value of m.

This algorithm looks cumbersome being expressed in words, but in fact it is rather simple to deal with. The conviction comes, say, when looking at the well-known formulae for the ground-state energy corrections in the third and fourth orders of the RS perturbation theory. In the next section we use the algorithm to construct Feynman diagrams for the polaron ground-state energy.

2. FEYNMAN DIAGRAMS FOR THE POLARON ENERGY

The Hamiltonian of a nonrelativistic particle (an electron) interacting with a quantized scalar field of lattice vibrations in an ionic crystal (phonons) is of the form

$$H = -\frac{\Delta}{2\mu} + \sum_{\vec{k}} \omega_{\vec{k}} a^{+}_{\vec{k}} a_{\vec{k}} + \frac{g}{\sqrt{V}} \sum_{\vec{k}} (A_{\vec{k}} e^{i\vec{k}\vec{r}} a_{\vec{k}} + A^{*}_{\vec{k}} e^{-i\vec{k}\vec{r}} a^{+}_{\vec{k}}). \qquad (2.1)$$

Here $a^{+}_{\vec{k}}$ and $a_{\vec{k}}$ are operators of creation and annihilation of phonons with the frequency $\omega_{\vec{k}}$ and momentum $\vec{k}$; $A_{\vec{k}}$ are Fourier components of the source density, and V is the volume of the system. The conservation of the total polaron momentum $\vec{P} = -i\vec{\nabla} + \sum_{\vec{k}} \vec{k} a^{+}_{\vec{k}} a_{\vec{k}}$ allows us to make the canonical transformation

$$H \to SHS^{+}, \quad S = \exp(-i\vec{r} \sum_{\vec{k}} \vec{k} a^{+}_{\vec{k}} a_{\vec{k}})$$

and to obtain the following representation for the Hamiltonian:

$$H = \frac{1}{2\mu} (\vec{P} - \sum_{\vec{k}} \vec{k} a^{+}_{\vec{k}} a_{\vec{k}})^2 + \sum_{\vec{k}} \omega_{\vec{k}} a^{+}_{\vec{k}} a_{\vec{k}} + \frac{g}{\sqrt{V}} \sum_{\vec{k}} (A_{\vec{k}} a_{\vec{k}} + A^{*}_{\vec{k}} a^{+}_{\vec{k}}), \qquad (2.2)$$

where the vector $\vec{P}$ is now a c -number.

In the theory of the so-called optical polaron the frequency of phonons is considered being independent of their wave vector. It is usually assumed that

$$\omega_{\vec{k}} = \omega, \quad gA_{\vec{k}} = -i \frac{\omega}{k} \frac{(4\pi\alpha)^{1/2}}{(2\mu\omega)^{1/4}}, \qquad (2.3)$$

where α is the dimensionless coupling constant. It is convenient to rewrite (2.2) in dimensionless units and to split the Hamiltonian into the sum of the free Hamiltonian of noninteracting electron and phonons and the interaction term:

$$H = H_0 + H_{int},$$

$$H_0 = (\vec{W} - \sum_{\vec{k}} \vec{k} a^{+}_{\vec{k}} a_{\vec{k}})^2 + \sum_{\vec{k}} a^{+}_{\vec{k}} a_{\vec{k}}, \qquad (2.4)$$

$$H_{int} = -i \left(\frac{4\pi\alpha}{V}\right)^{1/2} \sum_{\vec{k}} \frac{1}{k} (a_{\vec{k}} - a^{+}_{\vec{k}}).$$

Here the energy is expressed in units of ω and $\vec{W} = \vec{P}/\sqrt{2\mu\omega}$ is the polaron dimensionless momentum.

For small momenta the ground state of the Hamiltonian (2.4) takes the form

$$\mathcal{E}(W) = E/\omega + W^2 \frac{\mu}{m} + O(W^4), \qquad (2.5)$$

where E is the energy of the ground state of the polaron at rest and m is its effective mass. The calculation of these quantities is a basic problem of the polaron equilibrium theory.

Eigenfunctions of the free Hamiltonian (2.4) are $|n_{\vec{k}}>$, where $n_{\vec{k}}$ is the number of phonons with momentum $\vec{k}$; the corresponding energy eigenvalues are

$$\mathcal{E}^{(0)}_{n_{\vec{k}}} = (\vec{W} - \sum_{\vec{k}} \vec{k} n_{\vec{k}})^2 + \sum_{\vec{k}} n_{\vec{k}}. \qquad (2.6)$$

The ground state energy equals

$$\mathcal{E}^{(0)}_{0} = W^2, \qquad (2.7)$$

that is, the kinetic energy of a free electron with mass μ and momentum $\vec{P}$ in units of ω. The propagator which will be called electronic is defined in accordance with the quantum-mechanical perturbation theory as the inverse transition frequency ω^{-1}_{on} :

$$-\frac{1}{n - 2\vec{W} \sum_{i=1}^{n} \vec{k}_i + (\sum_{i=1}^{n} \vec{k}_i)^2}. \qquad (2.8)$$

In diagrams it will be depicted by a solid line. It describes the transition of the system from the vacuum state (free electron) to a state with n phonons which have the momenta $\vec{k}_1, \ldots, \vec{k}_n$ and all frequencies are the same and equal to unity; then the electron has the momentum $\vec{W} - \sum_{i=1}^{n} \vec{k}_i$.

The matrix element of the interaction Hamiltonian (2.4) differs from zero only between states in which the number of phonons differs by unity for some value of the momentum:

$$\langle \vec{k}_1,\ldots,\vec{k}_n | H_{int} | \vec{k},\vec{k}_1,\ldots,\vec{k}_n \rangle = -i\left(\frac{4\pi a}{V}\right)^{1/2}\frac{1}{k}. \qquad (2.9)$$

As in the initial and final states real phonons are absent, all the expressions will contain squares of the modulus of the matrix element (2.9). The transition from summation to integration over momenta is performed in a standard way:

$$\frac{1}{V}\sum_{\vec{k}} \to \frac{1}{(2\pi)^3}\int d\vec{k},$$

which gives additional factor $1/(2\pi)^3$ so that the square of each matrix element of H_{int} yields the factor

$$\frac{a}{2\pi^2}\,\frac{1}{k^2}. \qquad (2.10)$$

The emission and absorption of a virtual phonon will be represented by a wavy line between two vertices on a solid line. We shall represent each wavy line by the propagator $1/k^2$ and each vertex by the factor $\sqrt{a/2\pi^2}$, thus reproducing the factor (2.10). We call the wavy line the "phonon line" in a rather symbolic sense: we can merely assign to it a unit factor and attach the square root of the whole factor (2.10) to the vertex. However, the notation we have adopted shows a more close analogy with the diagrams of quantum field theory where propagators of the form $1/k^2$ describe the propagation of massless particles. Naturally, all virtual momenta in diagrams are integrated over and the momentum conservation takes place in each vertex. The polaron diagrams look like the diagrams of quantum field theory of the ϕ^3 type without external lines.

Note that in the polaron theory the electron is considered as a quantum-mechanical particles. As there is no electronic quantum field, there are no diagrams with electronic loops: electrons cannot be created and annihilated.

We also stress that in the quantum-mechanical perturbation theory the summation over virtual states does not include the state to which corrections are searched for, i.e., in our case the ground state. This means that we have no diagrams containing a free electron line without phonon lines, i.e., weakly connected diagrams which can be divided into two disconnected parts by cutting the electron line.

At the same time the theory should include disconnected diagrams corresponding to disconnected terms of the quantum-mechanical perturbation theory discussed in the preceding section. The procedure of increasing the power of the propagator can be described by introducing a new type of the vertex on the

solid line: a point to which the factor -1 corresponds. As the momentum should be conserved at the point vertex, the latter will increase the power of the corresponding propagator by unity. For constructing any of the factors we speak about in the first section we place on connected diagrams of the proper order a necessary number of points in all possible ways. The obtained factor miltiplied by the corresponding diagram without points is a term of the sum of all disconnected diagrams. The number of points is chosen by the above-mentioned algorithm so that the total number of electron propagators be the same in connected and disconnected diagrams of the same order.

Like in quantum mechanics, the above rules for constructing diagrams are more easily to use in practice than to formulate.

3. LOWEST PERTURBATION ORDERS

Prior to proceed to particular calculations we note that all the corrections of odd orders to the energy in the polaron theory vanishes so that the expansion is made in powers of $g^2 \approx a$. So, what we call the first perturbation order corresponds to the second order of the quantum-mechanical perturbation theory.

In the first perturbation order we have one diagram which, by the formulated rules, corresponds to the contribution

$$\mathcal{E}_1 = \quad = -\frac{a}{2\pi^2}\int \frac{d\vec{k}}{k^2}\,\frac{1}{1-2\vec{W}\vec{k}+k^2}. \qquad (3.1)$$

This integral can be easily calculated: for $W \le 1$ we have

$$\mathcal{E}_1 = -\frac{a}{W}\arcsin W = -a\left(1+\frac{W^2}{6}+O(W^4)\right). \qquad (3.2)$$

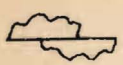
Summing $\mathcal{E}_1$ and the free-electron energy (2.7) and comparing with (2.5) we get for the first perturbation order of the energy and mass of a polaron:

$$E = -a\omega, \qquad m = \mu(1+a/6). \qquad (3.3)$$

This result was known almost from the very creation of the polaron model. To the second perturbation order two strongly connected diagrams contribute:

$$= -\frac{a^2}{4\pi^4}\int \frac{d\vec{q}\,d\vec{k}}{q^2k^2}\,\frac{1}{(1-2\vec{W}\vec{q}+q^2)^2\left[2-2\vec{W}(\vec{q}+\vec{k})+(\vec{q}+\vec{k})^2\right]} =$$

$$= -a^2\left[\ln(\sqrt{2}+1)-\frac{1}{2}\ln 2-\frac{\sqrt{2}}{2}+\frac{1}{2}\right]-a^2W^2\left[\frac{4}{3}\ln(\sqrt{2}+1)-\frac{2}{3}\ln 2-\frac{17\sqrt{2}}{24}+\frac{1}{2}\right]+\ldots$$



$$= -\frac{\alpha^2}{4\pi^4}\int \frac{d\vec{q}\,d\vec{k}}{q^2k^2}\,\frac{1}{(1-2\vec{W}\vec{q}+q^2)[2-2\vec{W}(\vec{q}+\vec{k})+(\vec{q}+\vec{k})^2](1-2\vec{W}\vec{k}+k^2)} =$$

$$= -\alpha^2[\ln(\sqrt{2}+1)-\ln 2] - \alpha^2 W^2\frac{\sqrt{2}}{12}+\ldots \qquad (3.4)$$

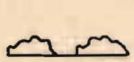
We stress that by the formulated rules the form of the propagator shown by the solid line depends on the number of phonons in a given virtual state. In the above diagrams of second order the end electron propagators depend only on the momentum of one phonon; and a vertical cut crossing such a propagator will intersect only one phonon line. Therefore free terms in these propagators equal unity. For the middle propagator the vertical cut intersects two phonon lines, or, which is the same, the electron propagator depends on the momenta of two phonons. Therefore, the free term equals two. This general rule valid also for higher-order diagrams follows directly from formula (2.8).

Besides connected diagrams (3.4) we should take account of the disconnected diagram, that is, the energy in first order times a factor constructed out of the same first-order diagram but having one more electron propagator. As we discussed diagrammatically this is depicted by a point on the electron line:

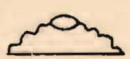
(3.5)

$$= \frac{\alpha^2}{4\pi^4}\int \frac{d\vec{q}\,d\vec{k}}{q^2k^2}\,\frac{1}{(1-2\vec{W}\vec{q}+q^2)(1-2\vec{W}\vec{k}+k^2)^2} = \frac{\alpha^2}{2}+W^2\frac{\alpha^2}{3}+\ldots$$

Diagrams (3.4) and (3.5) cover all second-order diagrams as the polaron theory does not include weakly connected diagrams and diagrams with electron loops of the form



and



Summing the contributions (3.4) and (3.5) we get for the polaron energy in the second perturbation order

$$\mathcal{E}_2 = -\alpha^2[2\ln(\sqrt{2}+1)-\frac{3}{2}\ln 2-\frac{\sqrt{2}}{2}]+ \qquad (3.6)$$

$$+W^2\alpha^2[-\frac{4}{3}\ln(\sqrt{2}+1)+\frac{2}{3}\ln 2+\frac{5\sqrt{2}}{8}-\frac{1}{6}]+\ldots$$

This expression, together with formulae (2.5), (2.7) and (3.2), leads to the following expansion for the polaron energy and mass up to second order in α:

$$E/\omega = -\alpha-\alpha^2[2\ln(\sqrt{2}+1)-\frac{3}{2}\ln 2-\frac{\sqrt{2}}{2}] = -\alpha-1{,}591\,962\,(\frac{\alpha}{10})^2 \qquad (3.7)$$

$$m/\mu = 1+\frac{\alpha}{6}+\alpha^2[\frac{4}{3}\ln(\sqrt{2}+1)-\frac{2}{3}\ln 2-\frac{5\sqrt{2}}{8}+\frac{7}{36}] = 1+\frac{\alpha}{6}+2{,}362\,763\,(\frac{\alpha}{10})^2.$$

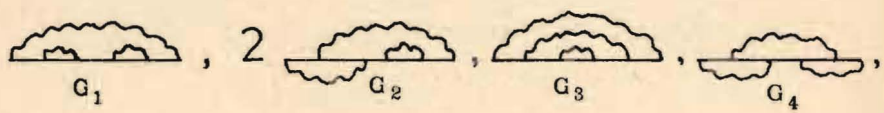
To complete this section, we make some historical remarks. The diagrammatic technique for the polaron has been developed by Pines[1]. He started with a general quantum-field approach and constructed diagrams for the Green functions which included integration not only over momenta of virtual phonons but also over their frequencies. In diagrams we have made use of, the frequency of virtual phonons coincides with that of real phonons. As a result, the vertices do not contain the δ-function providing the energy conservation. Instead, there appeared a rule according to which the free terms in the electron propagator depends on just where this propagator is situated in the diagram and equals the number of phonons in a corresponding virtual state. We kept a different way, but it appears that both the variants of diagrammatic technique should give the same results.

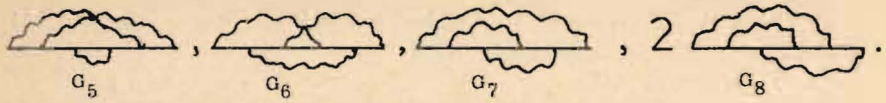
Numerically formulae (3.6) in the form $\mathcal{E}_2 = -\alpha^2\cdot 0{,}016 + W^2\alpha^2\cdot 0{,}0042$ have been obtained by Höhler and Müllensiefen[2]. Analytic expressions (3.7) have been found by Röseler[3] by a variational method. As an exact result these expressions have been derived in our work in collaboration with Kochetov[4] (see also reviews[5]) from the expression for the polaron free energy at finite temperature.

4. THE POLARON ENERGY IN THE THIRD PERTURBATION ORDER

We set here $\vec{W}=0$, i.e., for the time being we do not consider the mass but only the energy of the polaron at rest. This removes terms, linear in momenta, from the propagators. As a result, calculations will get simplified.

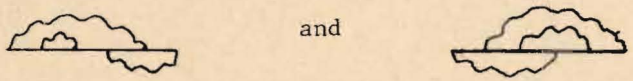
In the third order there are eight strongly connected diagrams whose contributions will be denoted by $G_1, \ldots, G_8$:





G_5 G_6 G_7 G_8

Note is to be made that the diagrams G_2 and G_8 enter with symmetry factors 2 allowing for contributions of the diagrams



and

which follow from the initial ones if the latter are considered in the opposite direction: from the right to left. The remaining diagrams possess the left-right symmetry and thus have no symmetry factors. Calculations yield:

$$G_1 = -\frac{\alpha^3}{8\pi^6}\int \frac{d\vec{q}\,d\vec{k}\,d\vec{\ell}}{q^2k^2\ell^2}\,\frac{1}{(1+q^2)^3[\,2+(\vec{q}+\vec{k})^2\,][\,2+(\vec{q}+\vec{\ell})^2\,]} =$$

$$= -\alpha^3\frac{2}{\pi}\int_0^\infty \frac{dq}{q^2(1+q^2)^3}\left(\operatorname{arc\,tg}\frac{q}{\sqrt{2}}\right)^2 = -0{,}173\,361\,050\,\alpha^3\,,$$

$$G_2 = -\frac{\alpha^3}{4\pi^6}\int \frac{d\vec{q}\,d\vec{k}\,d\vec{\ell}}{q^2k^2\ell^2}\,\frac{1}{(1+k^2)[\,2+(\vec{q}+\vec{k})^2\,](1+q^2)^2[\,2+(\vec{q}+\vec{\ell})^2\,]} =$$

$$= -\alpha^3\frac{4}{\pi}\int_0^\infty \frac{dq}{q^2(1+q^2)^2}\operatorname{arc\,tg}\frac{q}{\sqrt{2}}\left[\operatorname{arc\,tg}\frac{q}{\sqrt{2}} - \operatorname{arc\,tg}\frac{q}{\sqrt{2}+1}\right] = -0{,}170\,935\,051\alpha^3,$$

$$G_3 = -\frac{\alpha^3}{8\pi^6}\int \frac{d\vec{q}\,d\vec{k}\,d\vec{\ell}}{q^2k^2\ell^2}\,\frac{1}{(1+q^2)^2[\,2+(\vec{q}+\vec{k})^2\,]^2[\,3+(\vec{q}+\vec{k}+\vec{\ell})^2\,]} =$$

$$= -\alpha^3\frac{1}{\pi}\int_0^\infty \frac{dk}{(2+k^2)^2}\operatorname{arc\,tg}\frac{k}{\sqrt{3}}\left[\,2\operatorname{arc\,ctg}k - \frac{k}{k^2+1}\,\right] = -0{,}037\,613\,108\alpha^3\,,$$

$$G_4 = -\frac{\alpha^3}{8\pi^6}\int \frac{d\vec{q}\,d\vec{k}\,d\vec{\ell}}{q^2k^2\ell^2}\,\frac{1}{(1+k^2)[\,2+(\vec{q}+\vec{k})^2\,](1+q^2)[\,2+(\vec{q}+\vec{\ell})^2\,](1+\ell^2)} =$$

$$= -\alpha^3\frac{2}{\pi}\int_0^\infty \frac{dq}{q^2(1+q^2)}\left[\operatorname{arc\,tg}\frac{q}{\sqrt{2}} - \operatorname{arc\,tg}\frac{q}{\sqrt{2}+1}\right]^2 = -0{,}045\,165\,941\,\alpha^3\,,$$

$$G_5 = -\frac{\alpha^3}{8\pi^6}\int \frac{d\vec{q}\,d\vec{k}\,d\vec{\ell}}{q^2k^2\ell^2}\,\frac{1}{(1+q^2)[\,2+(\vec{q}+\vec{k})^2\,]^2[\,3+(\vec{q}+\vec{k}+\vec{\ell})^2\,](1+k^2)} =$$

$$= -\alpha^3\frac{2}{\pi}\int_0^\infty \frac{dq}{(2+q^2)^2}\operatorname{arc\,tg}\frac{q}{\sqrt{3}}\left[\,2\operatorname{arc\,ctg}q - \operatorname{arc\,ctg}\frac{q}{2}\,\right] = -0{,}032\,259\,338\,\alpha^3.$$

The contributions of diagrams $G_1 - G_5$ given by simple integrals may be expressed in an analytic form in terms of a special function, the Euler dilogarithm. As the analytic expressions are bulky, we present here only the numerical values.

As to the remaining three diagrams, we failed to simplify them to such an extent and expressed them through triple integrals calculated at computer. As a result we get:

$$G_6 = -\frac{\alpha^3}{8\pi^6}\int \frac{d\vec{q}\,d\vec{k}\,d\vec{\ell}}{q^2k^2\ell^2}\,\frac{1}{(1+k^2)[\,2+(\vec{q}+\vec{k})^2\,][\,3+(\vec{q}+\vec{k}+\vec{\ell})^2\,][\,2+(\vec{q}+\vec{\ell})^2\,](1+\ell^2)} =$$

$$= -0{,}015\,020\,0(2)\,\alpha^3\,,$$

$$G_7 = -\frac{\alpha^3}{8\pi^6}\int \frac{d\vec{q}\,d\vec{k}\,d\vec{\ell}}{q^2k^2\ell^2}\,\frac{1}{(1+q^2)^2[\,2+(\vec{q}+\vec{k})^2\,][\,3+(\vec{q}+\vec{k}+\vec{\ell})^2\,][\,2+(\vec{q}+\vec{\ell})^2\,]} =$$

$$= -0{,}022\,882\,3(1)\,\alpha^3\,,$$

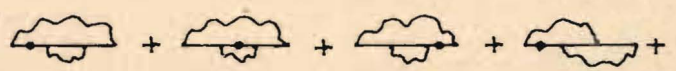
$$G_8 = -\frac{\alpha^3}{4\pi^6}\int \frac{d\vec{q}\,d\vec{k}\,d\vec{\ell}}{q^2k^2\ell^2}\,\frac{1}{(1+q^2)[\,2+(\vec{q}-\vec{k})^2\,][\,3+(\vec{q}+\vec{k}+\vec{\ell})^2\,][\,2+(\vec{q}+\vec{\ell})^2\,](1+\ell^2)} =$$

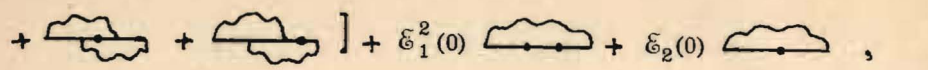
$$= -0{,}034\,581\,4(3)\,\alpha^3\,.$$

Thus, the sum of all connected diagrams contributes to the energy

$$\sum_{i=1}^{8} G_i = -0{,}531\,818\,2(4)\,\alpha^3\,. \qquad (4.1)$$

Now let us turn to the contributions of disconnected diagrams; these may be written:

$$\Delta = \mathcal{E}_1(0)\,[$$  $+$

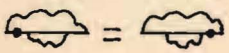


(4.2)

where $\mathcal{E}_1(0)$ and $\mathcal{E}_2(0)$ are, respectively, corrections of the first and second order to the polaron energy defined by formulae (3.2) and (3.6) at $\vec{W}=0$. Calculations yield:

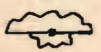
$$= -\frac{\alpha}{2\pi^2}\int\frac{d\vec{q}}{q^2(1+q^2)^2} = -\frac{\alpha}{2},$$

$$= -\frac{\alpha}{2\pi^2}\int\frac{d\vec{q}}{q^2(1+q^2)^3} = -\alpha\frac{3}{8},$$

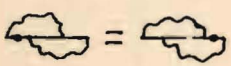


$$= -\frac{\alpha^2}{4\pi^4}\int\frac{d\vec{q}\,d\vec{k}}{q^2k^2}\frac{1}{(1+q^2)^2[2+(\vec{q}+\vec{k})^2]} =$$

$$= -\alpha^2[\ln(\sqrt{2}+1) - \frac{1}{2}\ln 2 - \frac{3}{8}\sqrt{2} + \frac{1}{4}], \qquad (4.3)$$



$$= -\frac{\alpha^2}{4\pi^4}\int\frac{d\vec{q}\,d\vec{k}}{q^2k^2}\frac{1}{(1+q^2)^2[2+(\vec{q}+\vec{k})^2]^2} = -\alpha^2\left(\frac{1}{4} - \frac{\sqrt{2}}{8}\right),$$



$$= -\frac{\alpha^2}{4\pi^4}\int\frac{d\vec{q}\,d\vec{k}}{q^2k^2}\frac{1}{(1+q^2)^2[2+(\vec{q}+\vec{k})^2](1+k^2)} =$$

$$= -\alpha^2[\ln(\sqrt{2}+1) - \ln 2 - \frac{3\sqrt{2}}{4} + 1],$$

$$= -\frac{\alpha^2}{4\pi^4}\int\frac{d\vec{q}\,d\vec{k}}{q^2k^2}\frac{1}{(1+q^2)[2+(\vec{q}+\vec{k})^2]^2(1+k^2)} = -\alpha^2\left(\frac{3\sqrt{2}}{4} - 1\right).$$

Inserting (4.3), (3.2) and (3.6) into (4.2) we obtain the contribution of disconnected diagrams:

$$\Delta = \alpha^3\left[5\ln(\sqrt{2}+1) - \frac{15}{4}\ln 2 - \frac{15\sqrt{2}}{8} + \frac{11}{8}\right] = 0{,}530\ 915\ 579\,\alpha^3. \qquad (4.4)$$

Summing up (4.1) and (4.4) we get the energy of a polaron at rest in the third perturbation order:

$$\mathcal{E}_3(0) = -\alpha^3 \cdot 0{,}000\ 902\ 6(4). \qquad (4.5)$$

Formulae (4.5) and (3.7) give the following expansion for the polaron energy:

$$E/\omega = -\alpha - 1{,}591\ 962\left(\frac{\alpha}{10}\right)^2 - 0{,}903\left(\frac{\alpha}{10}\right)^3 + \ldots \qquad (4.6)$$

In our work with Seljugin [6] we have found the same result proceeding from the representation of the polaron partition function at finite temperature in terms of path integrals. Therefore, we can draw the conclusion on adequacy of these two approaches. Expression (4.6) may be used for an approximate calculation of the polaron energy at not very large values of the coupling constant. In the Table we collect the results of the best variational calculations and those of ref. [7] obtained numerically by the Monte-Carlo method. Numbers in parentheses stand for uncertainty in the last digits of the result (for instance, -1.020(10) means -1.020±0.010). Calculations in the scope of the known Feynman variational method [8] can be found in refs. [9,10]. In the latter column we write the results following from the expansion (4.6).

Table

α	Feynman	Larsen [10]	AGL [11]	BGS [7]	Our result
0.5	-0.5032	-0.5040	-0.5032	-0.505(5)	-0.5041
1	-1.0130	-1.0160	-1.0139	-1.020(10)	-1.0168
1,5	-1.5302	-1.5361	-1.5317	-1.545(15)	-1,5389
2	-2,0554	-2.0640	-2.0577	-2.080(21)	-2.0709
2.5	-2.5894	-2.5995	-2.5928	-2.627(26)	-2.6136
3	-3.1333	-3.1421	-3.1379	-3.184(32)	-3.1676
3.5	-3.6885	-3.6915	-3.6946	-3.747(37)	-3.7337
4	-4.2565	-4.2471	-4.2644	-4.314(43)	-4.3125
5	-5.4401				-5.5108
7	-8.1127				-8.0896
9	-11.486				-10.9475
11	-15.710				-14.1278

From the Table it is seen that the developed approximate methods do provide the results very close to the exact calculations and that the first three perturbation orders give values below the energy values obtained by any other approximate approach, up to $\alpha \approx 5$-6. It is to be kept in mind that the following, not considered fourth term of the perturbation expansion, is, to all appearances, of an order of $(\alpha/10)^4$ so to use the perturbation theory at large values of the coupling constant we should know a larger number of the expansion terms. In the α-range of the applicability of perturbation theory the latter differs from the above indicated approximate methods not more than by 1.5%, which, naturally, is of no practical relevance. However, as has been said, the investigation of the perturbation expansion may turn out to be necessary for studying more fundamental problems of the polaron theory.

5. AVERAGE NUMBER OF VIRTUAL PHONONS

The rule formulated for constructing diagrams allows us to calculate not only the energy but also other equilibrium characteristics of the polaron. Thus, it would be of further interest to compute the polaron mass in the third perturbation order. If at a certain value of the coupling constant there occurs a phase transition, what is doubtful, the polaron mass at that point changes abruptly. One more important characteristic of the polaron with similar properties is represented by the average number of phonons in the cloud around the electron defined by

$$N = \langle \Psi | \sum_{\vec{k}} a^{+}_{\vec{k}} a_{\vec{k}} | \Psi \rangle , \tag{5.1}$$

where $|\Psi\rangle$ is the wave function of the polaron ground-state. For an optical polaron the operator of the phonon number can be determined as a derivative of the Hamiltonian (2.2) with respect to the frequency ω on condition that $\alpha\omega^{3/2} = \text{const}$, that is denoted by the prime of the derivative:

$$\sum_{\vec{k}} a^{+}_{\vec{k}} a_{\vec{k}} = \frac{\partial' H}{\partial \omega} . \tag{5.2}$$

(A straightforward differentiation with respect to ω is not suited as ω enters also into expression (2.2) for the coupling constant). Taking account of (5.2) and Feynman-Hellman theorem we obtain, instead of (5.1), the following representation:

$$N = \frac{\partial'}{\partial \omega} (\omega \mathcal{E}) = (1 - \frac{3}{2} \alpha \frac{\partial}{\partial \alpha} - \frac{W}{2} \frac{\partial}{\partial W}) \mathcal{E} . \tag{5.3}$$

whence there follows the perturbative series:

$$N = \sum_{n=1}^{\infty} \alpha^n N_n(W),$$
$$N_n(W) = (1 - \frac{3n}{2}) \mathcal{E}_n(W) - \frac{W}{2} \frac{\partial \mathcal{E}_n(W)}{\partial W} , \tag{5.4}$$

where $\mathcal{E}_n(W)$ are expansion coefficients of the polaron energy we have calculated in the preceding sections. With due regard to (3.2) we find in the first perturbation order

$$N_1(W) = \frac{\alpha}{2\sqrt{1 - W^2}} . \tag{5.5}$$

The first terms of expansion (5.5) in powers of the polaron momentum squared coincide with those derived by Lee, Low and Pines[12]. With the electron energy approaching the threshold of production of real phonons ($P^2/2\mu \to \omega$, i.e., $W \to 1$) the average number of virtual phonons, according to (5.5), increases to infinity. This is another manifestation of the effect similar to the Cherenkov effect: for $W>1$ owing to the production of real phonons, the polaron energy acquires an imaginary part, i.e., the polaron acquires a finite lifetime.

The relation (5.3) makes it easy to find a perturbation series for the average number of phonons if we know such series for the polaron energy. For example, for a polaron at rest we have from (4.6) and (5.3) the following expansion for the average number of phonons:

$$N = \frac{\alpha}{2} + 3{,}183\,924 (\frac{\alpha}{10})^2 + 3{,}159(1) \cdot (\frac{\alpha}{10})^3 + \dots \tag{5.6}$$

The relation (5.3) is useful not only for deriving a perturbation series. For example it is well known that in the strong coupling limit the energy of a polaron at rest is of the form

$$E/\omega = -A\alpha^2 - B - \frac{C}{\alpha^2} + O(1/\alpha^4) , \tag{5.7}$$

whence it follows that the average number of virtual phonons at large α equals

$$N = 2A\alpha^2 - B - \frac{4C}{\alpha^2} + O(1/\alpha^4) . \tag{5.8}$$

A numerical calculation by Miyake[13] gives for the coefficient A:

$$A = 0{,}108\,513. \tag{5.9}$$

We recall that for the coefficient A Feynman found the value $A = 1/3\pi = 0{,}1061$ which is very close to the exact result by Miyake.

As for the coefficient B, Allcock made a conclusion[14] that

$$3\ln 2 + \frac{3}{4} = 2{,}829 \leq B \leq 4{,}159 = 6\ln 2. \tag{5.10}$$

The lower bound for B coincides with the value obtained in the scope of the Feynman variational method. Numerical calculations by Miyake[15] give

$$B = 2{,}836. \tag{5.11}$$

For the coefficient C no direct estimations as far as I know, were obtained. However, the Feynman variational expression for the polaron energy gives the value

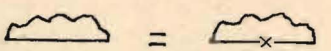
$$C = \frac{27\pi}{4}\left(\frac{7}{16} + 2\ln^2 2 - \frac{1}{2}\ln 2 - \frac{\pi^2}{12}\right) = 4{,}864. \tag{5.12}$$

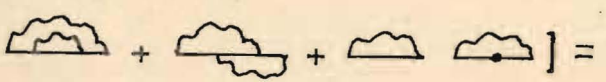
In the absence of other estimations the value (5.12) may serve as a guide since the Feynman method provides a really good approximations for all values of the coupling constant. Then eq. (5.8) takes the form

$$N = 0{,}217\,026\,a^2 - 2{,}836 - \left(\frac{20}{a^2}\right)_{?} + \ldots. \tag{5.13}$$

If we know the larger number of terms in the strong coupling expansion and in the perturbation series, we could trace how solutions (5.6) and (5.13) approach each other and whether the average number of phonons has a discontinuity at some critical value of the coupling constant.

The quantity $N_n(W)$ may be also represented by diagrams. For doing so note that the differentiation with prime (5.2) means the differentiation with respect to frequencies of phonons entering into the electron propagators. Therefore, we may introduce the operation of "crossing" P(×) acting on diagrams for the polaron energy, which supplies each of the propagators with a new vertex marked by a cross:

$N_1 = P(\times)$  ,

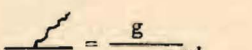
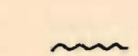
$N_2 = P(\times)[$  $]$ =

= 

+ 

+  .

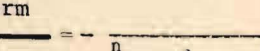
and so on. It may be easily understood that to a vertex of that kind there corresponds a factor n, equal to the number of phonons in a given virtual state. So, vertices marked by a dot and a cross differ by a numerical factor, therefore, results of preceding calculations can be used here as well. However, the diagrammatic representation for $N_n(W)$ is useful when direct differentiation of the Hamiltonian is impossible, for instance, when phonons possess dispersion, i.e., the frequency ω depends on the momentum $\vec{k}$. Obviously, the particular choice (2.3) of $A_{\vec{k}}$ and $\omega_{\vec{k}}$ is not crucial for the diagrammatic technique. The very form of diagrams for $\mathcal{E}_n$ and N_n as well the contribution of vertices marked by a dot and a cross remain unchanged. Clear are also changes to be introduced into the correspondence rules for vertices, electron and phonon lines:

 $= \dfrac{g}{(2\pi)^{3/2}}$,  $= |A_{\vec{k}}|^2$,

 $= -\dfrac{1}{\sum\limits_{i=1}^{n}\omega(\vec{k}_i) - \dfrac{\vec{P}}{\mu}\sum\limits_{i=1}^{n}\vec{k}_i + \dfrac{1}{2\mu}\left(\sum\limits_{i=1}^{n}\vec{k}_i\right)^2}$.

Diagrams construted with these more general rules describe an arbitrary Hamiltonian of the form (2.2) and permit us to go beyond the optical-polaron theory and to study other models of physical interest.

For the BW expansion one can also derive the diagrammatic technique which will be even more simple than that of RS perturbation theory. The main difference is in the absence of disconnected diagrams. In addition electron propagators take the form

 $= -\dfrac{1}{\sum\limits_{i=1}^{n}\omega(\vec{k}_i) + \dfrac{1}{2\mu}\left(\vec{P} - \sum\limits_{i=1}^{n}\vec{k}_i\right)^2 - E}$,

as it follows from (1.1). On diagrams this will be depicted as a thick solid line. BW perturbation theory can be used to improve the results of RS series by partially summing the diagrams.

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Диаграммы в модели полярона

Работа посвящена систематическому изложению теории возмущений для энергии движущегося полярона на основе диаграммной техники. Сформулированные правила построения фейнмановских диаграмм позволили рассчитать энергию полярона с точностью до членов третьего порядка по константе связи. Аналогичные расчеты проведены для среднего числа виртуальных фононов. Полученные разложения имеют, соответственно, вид:

$$E/\omega = -\alpha - 1{,}591\,962\left(\frac{\alpha}{10}\right)^2 - 0{,}903\left(\frac{\alpha}{10}\right)^3 + \ldots,$$

$$N = \frac{\alpha}{2} + 3{,}183\,924\left(\frac{\alpha}{10}\right)^2 + 3{,}16\left(\frac{\alpha}{10}\right)^3 + \ldots .$$

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