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исследований
дубна

E17-86-424

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PERTURBATION THEORY FOR THE MULTIDIMENSIONAL POLARON

Submitted to "Physica A"

1986

Intensive theoretical and experimental investigations in condensed matter physics of recent years stimulated the revival of attention to various polaron models described by the well-known Fröhlich Hamiltonian

$$H = \frac{\vec{p}^{\,2}}{2\mu} + \sum_{\vec{k}} \omega_{\vec{k}} a^{+}_{\vec{k}} a_{\vec{k}} + \frac{g}{\sqrt{V}} \sum_{\vec{k}} \left(A_{\vec{k}} e^{i\vec{k}\vec{r}} a_{\vec{k}} + A^{*}_{\vec{k}} e^{-i\vec{k}\vec{r}} a^{+}_{\vec{k}} \right). \tag{1}$$

The utmost physical interest is roused in optical and acoustical polarons, and not only in the bulk, 3-dimensional ones, but also in the surface polarons in two spatial dimensions [1]. In this paper we shall confine ourselves to optical polarons when the phonon frequency does not depend on its momentum: $\omega_{\vec{k}} = \omega$. We shall not fix the number N of spatial dimensions. Such a multidimensional polaron has recently been investigated by Devreese, Peeters and Wu [2]. Here we accept their parametrization

$$A_{\vec{k}} = -\frac{i}{k^{N-1}} \quad , \quad g = \left[\alpha \cdot 2^{N-3/2} \pi^{\frac{N-1}{2}} \Gamma\left(\frac{N-1}{2} \right) \right]^{1/2}. \tag{2}$$

In the representation with the total momentum of the system being a c-number, Hamiltonian (1) can be written as follows

$$H = \left(\vec{W} - \sum_{\vec{k}} \vec{k} a^{+}_{\vec{k}} a_{\vec{k}} \right)^2 + \sum_{\vec{k}} a^{+}_{\vec{k}} a_{\vec{k}} + \frac{g \cdot 2^{1/4}}{\sqrt{V}} \sum_{\vec{k}} \left(A_{\vec{k}} a_{\vec{k}} + A^{*}_{\vec{k}} a^{+}_{\vec{k}} \right), \tag{3}$$

$$\vec{W} = \vec{P} / \sqrt{2\mu\omega} .$$

Note that the energy and mass in Eqs.(2), (3) are expressed in units of ω and μ, respectively.

The goal of this paper is to construct the perturbation theory for such characteristics of the N-dimensional polaron as the ground state energy, effective mass and average number of phonons. Results for the bulk and surface polarons will be obtained as particular cases. Besides, we discuss here the properties of the 1/N-expansion which can provide us with a completely new approach to the polaron problem both in the weak-coupling and in the strong-coupling regimes.

In the paper [3] a special diagrammatic technique has been developed which may easily be generalized to a multidimensional case. The Feynman rules are as follows:

$$
\text{(4)}
$$

 $= \dfrac{1}{K^{N-1}}$;  $= \left[\alpha\Gamma\left(\frac{N-1}{2}\right)/2\pi^{\frac{N+1}{2}}\right]^{1/2}$;

 $= -\left[n - 2\vec{W}\sum_{i=1}^{n}\vec{K}_i + \left(\sum_{i=1}^{n}\vec{K}_i\right)^2\right]^{-1}$;  $= -1$.

Here $\vec{K}_i$ are phonons momenta, and n is the number of phonons in a given virtual state. Let us briefly describe the main distinctions between our diagrams and the conventional ones. In addition to the ordinary strongly connected diagrams we have also the disconnected ones. On the other hand, there are no weakly connected diagrams which can be separated into two parts by cutting an electron propagator. Furthermore, together with the electron-phonon vertices there exists another type of vertices whose role is to change the powers of the corresponding electron propagators. For more details we refer to the paper [3].

The sum of all diagrams defines the energy of a moving polaron

$$\mathcal{E}(W) = \mathcal{E}_0(W) + \alpha\,\mathcal{E}_1(W) + \alpha^2\mathcal{E}_2(W) + \dots$$

at small momentum taking the form

$$\mathcal{E}(W) \simeq E + W^2/m \; .$$

In the zeroth order in coupling constant $\mathcal{E}_0(W) = W^2$ so that the required expansions for the ground state energy E and the polaron effective mass m are as follows

$$E = \alpha E_1 + \alpha^2 E_2 + \dots \; ,$$

$$m = 1 + \alpha m_1 + \alpha^2 m_2 + \dots \qquad (5)$$

In the first order in α, in accordance with tules (4), we obtain

$\alpha\,\mathcal{E}_1(W) =$  $= -\alpha\,\dfrac{\Gamma\left(\frac{N-1}{2}\right)}{2\pi^{\frac{N+1}{2}}}\displaystyle\int\frac{d^N K}{K^{N-1}}\,\frac{1}{K^2 - 2\vec{W}\vec{K} + 1} \simeq$

$$\simeq -\alpha\,\frac{\sqrt{\pi}}{2}\,\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma(N/2)}\left(1 + \frac{W^2}{2N}\right),$$

from which there follow the first coefficients of expansions (5)

$$E_1 = -\frac{\sqrt{\pi}}{2}\,\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma(N/2)}\;, \qquad m_1 = \frac{\sqrt{\pi}}{4N}\,\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma(N/2)}\;. \qquad (6)$$

In the second order in α the polaron energy is defined by a sum of three diagrams. The disconnected diagram contribution can be obtained in the analytical form

  $= -\alpha^2\,\mathcal{E}_1(W)\,\dfrac{\Gamma\left(\frac{N-1}{2}\right)}{2\pi^{\frac{N+1}{2}}}\displaystyle\int\frac{d^N K}{K^{N-1}}\,\frac{1}{(K^2 - 2\vec{W}\vec{K} + 1)^2} \simeq$ (7)

$$\simeq \frac{\alpha^2}{2}\left[\frac{\sqrt{\pi}}{2}\,\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma(N/2)}\right]^2\left(1 + W^2\,\frac{2}{N}\right).$$

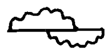
Unfortunately, this cannot be performed for the remaining two diagrams. However, we succeeded in representing their contributions by one-dimensional integrals of elementary functions for which numerical calculations can be carried out by means of a simplest programmable calculator such as HP-34C:

 $= -\alpha^2\left[\dfrac{\Gamma\left(\frac{N-1}{2}\right)}{2\pi^{\frac{N+1}{2}}}\right]^2\displaystyle\int\frac{d^N K\, d^N q}{K^{N-1}q^{N-1}}\,\frac{1}{(q^2 - 2\vec{W}\vec{q} + 1)^2\,[(\vec{q}+\vec{K})^2 - 2\vec{W}(\vec{q}+\vec{K}) + 2]} \simeq$

$$\simeq G_1 + B_1 W^2 \; , \qquad (8)$$

$$G_1 = -\alpha^2\,\frac{\Gamma\left(\frac{N-1}{2}\right)}{2\sqrt{\pi}\,\Gamma(N/2)}\int_0^1\frac{dx}{\sqrt{1-x^2}}\,\frac{x^{N-2}}{2-x^2}\left(x + 2\,\frac{1-x^2}{\sqrt{2-x^2}}\arccos\frac{x}{\sqrt{2}}\right),$$

$$B_1 = -\alpha^2\,\frac{\Gamma\left(\frac{N-1}{2}\right)}{2N\sqrt{\pi}\,\Gamma(N/2)}\int_0^1\frac{dx}{\sqrt{1-x^2}}\,\frac{x^{N-2}}{(2-x^2)^3}\Big[x(7 - 14x^2 + 9x^4) + \frac{2}{\sqrt{2-x^2}}(7 - 11x^2 + 8x^4 - 4x^6)\arccos\frac{x}{\sqrt{2}}\Big] ;$$

 $= -\alpha^2\left[\dfrac{\Gamma\left(\frac{N-1}{2}\right)}{2\pi^{\frac{N+1}{2}}}\right]^2\displaystyle\int\frac{d^N K\, d^N q}{K^{N-1}q^{N-1}}\,\frac{1}{(q^2 - 2\vec{W}\vec{q} + 1)(K^2 - 2\vec{W}\vec{K} + 1)}\cdot$

$$\cdot\frac{1}{(\vec{q}+\vec{K})^2 - 2\vec{W}(\vec{q}+\vec{K}) + 2} \simeq G_2 + B_2 W^2 ,$$

$$G_2 = -\alpha^2 \frac{\Gamma\left(\frac{N-1}{2}\right)}{\sqrt{\pi}\,\Gamma(N/2)} \int_0^1 \frac{dx}{\sqrt{1-x^2}}\, x^{N-2} \left(\frac{1}{\sqrt{2-x^2}} \arccos\frac{x}{\sqrt{2}} - \frac{1}{2\sqrt{1-x^2}} \arccos x \right),$$

$$B_2 = -\alpha^2 \frac{\pi}{8N} \left[\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma(N/2)} \right]^2 + \alpha^2 \frac{\Gamma\left(\frac{N-1}{2}\right)}{N\sqrt{\pi}\,\Gamma(N/2)} \int_0^1 \frac{dx}{\sqrt{1-x^2}}\, \frac{x^{N-2}}{(2-x^2)^2} \cdot \tag{9}$$

$$\cdot \left[\frac{x}{2}(1+x^2) + \frac{1-2x^2}{\sqrt{2-x^2}} \arccos\frac{x}{\sqrt{2}} \right].$$

By means of Eqs. (7)-(9) we can calculate the coefficients E_2 and m_2 for arbitrary N. As to the E_2, we obtained the same values as Devreese et al. did[2]. They used the path-integral technique and expressed their final result in the form of double integral. Thus, we confirm their numerical calculations in the scope of a completely different method. For this reason, here we shall only present our calculations for the multidimensional polaron mass for the same values of N, for which the energy has been calculated in the paper[2].

Table
Expansion Coefficients of the Exact Perturbation Series for the N-Dimensional Polaron Effective Mass

N	m_1	m_2
2	0.392 699 08	0.127 234 83
3	0.166 666 67	0.023 627 63
4	0.098 174 77	0.008 332 33
5	0.066 666 67	0.003 880 44
6	0.049 087 39	0.002 117 73
7	0.038 095 24	0.001 281 48
8	0.030 679 62	0.000 834 05
9	0.025 396 83	0.000 573 05
10	0.021 475 73	0.000 410 67
20	0.007 283 41	0.000 047 68
30	0.003 912 49	0.000 013 80

As expected, for the bulk, 3-dimensional polaron we have obtained the well-known results which can be expressed in an analytical form[4]. For another interesting case of a surface polaron (N=2) integrals in Eqs.(8),(9) can be simplified. We'll take the pleasure to cite our results for the N=2 case:

$$E_2 = \frac{\pi^2-\pi}{8} - \frac{3}{32}\sqrt{\frac{\pi}{2}}\,\Gamma^2(1/4) + \frac{\pi^2}{4}\sqrt{\frac{\pi}{2}}\frac{1}{\Gamma^2(1/4)} + G -$$

$$- \frac{1}{4}\int_0^{\pi/2} d\theta \frac{\theta}{\sqrt{\sin\theta}} \frac{1+2\sin\theta}{1+\sin\theta} = -0{,}063\,973\,966,$$

$$m_2 = -\frac{3\pi^2}{64} + \frac{25\pi}{128} - \frac{5}{8} + \frac{5}{128}\sqrt{\frac{\pi}{2}}\,\Gamma^2(1/4) - \frac{3\pi^2}{16}\sqrt{\frac{\pi}{2}}\frac{1}{\Gamma^2(1/4)} +$$

$$+ \frac{1}{8}\int_0^{\pi/2} d\theta \frac{\theta}{\sqrt{\sin\theta}} \frac{1+6\sin\theta-6\sin^2\theta+4\sin^3\theta}{(1+\sin\theta)^3} = 0{,}127\,234\,835.$$

Here G = 0.915 965 594 is Catalan's constant. Note that in the recent paper[5] by Das Sarma and Mason, devoted to the optical polaron in two dimensions, the coefficients E_2 and m_2 are expressed through triple integrals and their numerical values are calculated with a much lesser accuracy: $E_2 = -0.062$ and $m_2 = 0.13$. More precisely the value for E_2 has been calculated by Devreese et al. in the paper[6].

In the paper[3] the relation between the average number of phonons $\mathcal{N}$ and the polaron energy $\mathcal{E}(w)$ has been derived:

$$\mathcal{N} = \left(1 - \frac{3}{2}\alpha\frac{\partial}{\partial\alpha} - \frac{w}{2}\frac{\partial}{\partial w}\right)\mathcal{E}(w). \tag{10}$$

With the help of Eq.(10) we can construct the perturbation series for $\mathcal{N}$. In particular, for the surface polaron with small momentum we have

$$\mathcal{N} \simeq \alpha\frac{\pi}{4} + \alpha^2 \cdot 0{,}127\,947\,93 + O(\alpha^3) +$$

$$+ w^2\left(\alpha\frac{3\pi}{16} - \alpha^2 \cdot 0{,}080\,933\,20 + O(\alpha^3)\right).$$

Note, that in the paper[3] the energy of a bulk polaron in the third order in powers of α have been obtained: $E_3 = -0.806 \cdot 10^{-3}$. In the same paper one can also find the first three terms of perturbation series for $\mathcal{N}$.

Let us now revert to the case of multidimensional polaron. Calculations of the polaron energy and effective mass demonstrate that the polaron effects weaken with the increase of the number of dimensions. Equations (6)-(9) give us an opportunity to obtain the asymptotic behaviour of the expansion coefficients at large N:

$$E_1 \simeq -\sqrt{\frac{\pi}{2N}}, \qquad E_2 \simeq -\frac{1}{N^2}\left(\frac{\pi}{8} - \frac{1}{3}\right), \tag{11}$$

$$m_1 \simeq \frac{1}{2N}\sqrt{\frac{\pi}{2N}}, \qquad m_2 \simeq \frac{1}{N^3}\left(\frac{3\pi}{4} - 2\right).$$

It follows from Eq.(11) that a nontrivial limit at large N can be obtained through redefinition of the coupling constant, e.g., through scaling of the type $\alpha \to \alpha N^{3/2}$. Such a redefinition of the coupling constant is not an innovation. For example, we used an analogous scaling while constructing the 1/N-expansions for the anharmonic oscillator[7], which allowed us to reproduce the results of perturbation theory as well as the strong coupling limit. The 1/N-expansion could provide us with a new method of description of the polaron properties at all possible values of coupling constant α. We still have no regular procedure of 1/N-expansion, but the results just obtained can help us to guess its leading term.

Indeed, it has been noticed by Devreese et al.[2] that in the Feynman variational approximation there exist scaling laws

$$E_F^{(N)}(\alpha) = \frac{N}{3} E_F^{(3)}\left(\alpha \frac{3\sqrt{\pi}}{2N} \frac{\Gamma(\frac{N-1}{2})}{\Gamma(N/2)}\right), \tag{12}$$

$$m_F^{(N)}(\alpha) = m_F^{(3)}\left(\alpha \frac{3\sqrt{\pi}}{2N} \frac{\Gamma(\frac{N-1}{2})}{\Gamma(N/2)}\right),$$

where the index in parentheses indicates the space dimensionality. For exact solutions these scaling laws (12) are valid only in the first perturbation order, but nevertheless they show a right way. Really, to obtain a nontrivial 1/N-expansion, e.g., for the bulk polaron, we redefine the coupling constant in accordance with Eq.(12) and consider expressions

$$\tilde{E}^{(3)}(\alpha) = \lim_{N\to\infty} \frac{3}{N} E^{(N)}\left(\alpha \frac{2N}{3\sqrt{\pi}} \frac{\Gamma(N/2)}{\Gamma(\frac{N-1}{2})}\right),$$

$$\tilde{m}^{(3)}(\alpha) = \lim_{N\to\infty} m^{(N)}\left(\alpha \frac{2N}{3\sqrt{\pi}} \frac{\Gamma(N/2)}{\Gamma(\frac{N-1}{2})}\right). \tag{13}$$

By definition, the functions under the limit sign at N=3 are nothing else than the exact energy and mass of the bulk polaron. Evidently, they can be expanded in inverse powers of N. So, Eq.(13) gives us the leading approximation of the 1/N-expansion. What are the properties of $\tilde{E}^{(3)}(\alpha)$ and $\tilde{m}^{(3)}(\alpha)$? With the help of Eq.(11) it is easy to find the first terms of perturbation series:

$$\tilde{E}^{(3)}(\alpha) = -\alpha - \alpha^2 \frac{2}{3}\left(\frac{1}{8} - \frac{1}{3\pi}\right) + O(\alpha^3),$$

$$\tilde{m}^{(3)}(\alpha) = 1 + \frac{\alpha}{6} + \alpha^2 \frac{4}{3}\left(\frac{1}{8} - \frac{1}{3\pi}\right) + O(\alpha^3). \tag{14}$$

In the theory of bulk polaron such expansions have been obtained by Haga[8] for the energy and by Höhler and Müllensiefen[9] for the effective mass. It has been shown by Saitoh[10] that these expansions arise from the Feynman type variational approximation with arbitrary quadratic trial action. The coincidence of the first terms of perturbation series for $\tilde{E}^{(3)}(\alpha)$, $\tilde{m}^{(3)}(\alpha)$ and approximate expressions by Saitoh can be scarcely accidental. It seems, we have the reason to suggest that $\tilde{E}^{(3)}(\alpha)$ and $\tilde{m}^{(3)}(\alpha)$ coincide with the Saitoh results at any value of α.

In other words, we believe the Saitoh result to be the leading approximation of the 1/N-expansion. If it is really the case, then the 1/N-expansion is indeed suitable to describe the polaron properties in the whole range of the coupling constant. In particular, at large α when the Saitoh approximation gives the well-known Feynman results, we have

$$\tilde{E}^{(3)}(\alpha) \simeq -\frac{\alpha^2}{3\pi}, \quad \tilde{m}^{(3)}(\alpha) \simeq \frac{16\alpha^4}{81\pi^2},$$

rather close to the exact results. It follows then that the multidimensional polaron characteristics in the strong-coupling regime

$$E^{(N)}(\alpha) \simeq -A_N \alpha^2, \quad m^{(N)}(\alpha) \simeq M_N \alpha^4$$

should behave at large N as follows

$$A_N \simeq \frac{1}{2N^2}, \quad M_N \simeq \frac{4}{N^6}. \tag{15}$$

Predictions (15) are straightforward consequences of our analysis of the perspectives for the 1/N-expansion.

It is clear that in a similar way one can construct the first approximation of the 1/N-expansion for the polaron of arbitrary dimensionality: one has only to introduce appropriate factors into arguments and functions under the limit sign in Eq.(13). Functions $\tilde{E}^{(N)}(\alpha)$ and $\tilde{m}^{(N)}(\alpha)$ thus obtained will satisfy the same scaling laws (12). Therefore it is easy to obtain an analogous expansion for the polaron at any given N directly from Eq.(13).

Our analysis provides the answer to the question why the variational methods by Feynman and Saitoh are so good. It turned out that the latter is asymptotically exact at large N.

To conclude, we would like to stress once more that it will be very useful and interesting to invent a regular procedure of the 1/N-expansion which would give us an opportunity to calculate corrections to the leading approximation.

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Received by Publishing Department
on June 30, 1986.

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Теория возмущений для многомерного полярона

В рамках диаграммной техники исследуется оптический полярон в N-мерном пространстве с целью построения теории возмущений для таких характеристик N-мерного полярона, как энергия основного состояния, эффективная масса, среднее число фононов. Найдены первые два члена разложений в ряд теории возмущений энергии основного состояния и эффективной массы полярона. Обсуждаются возможности 1/N-разложения, которое способно дать новый метод исследования свойств полярона в режимах слабой и сильной связи.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1986

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Perturbation Theory for the Multidimensional Polaron

The optical polaron in N-dimensional space is investigated in the framework of diagrammatic approach. The goal of this work is to construct the perturbation theory for such characteristics of the N-dimensional polaron as the ground state energy, effective mass and average number of phonons. The first two terms of perturbation series for the ground state energy and effective mass are obtained. The perspectives of the 1/N-expansion which can provide a new method for investigation of polaron properties in both weak and strong coupling regimes are discussed.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Preprint of the Joint Institute for Nuclear Research. Dubna 1986