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ON THE GENERAL PATH INTEGRAL APPROACH TO POLARON PROBLEM

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As is known, the two quantitatively different pictures arise when describing the motion of an electron in the ion crystal. In the first case, when electron is in a weak interaction with the ion lattice of the crystal, its motion is just the same as the motion of the free zone electron with the energy shifted down relative to the bottom of the conduction band, and the effective mass is replaced by the renormalized one [1] (weak coupling polaron). In the other limit case, when electron is in the strong interaction with the ion crystal, there arises a whole number of different self-consistent states of electron and lattice each having its own effective mass and radius [2-4] (strong coupling polaron).

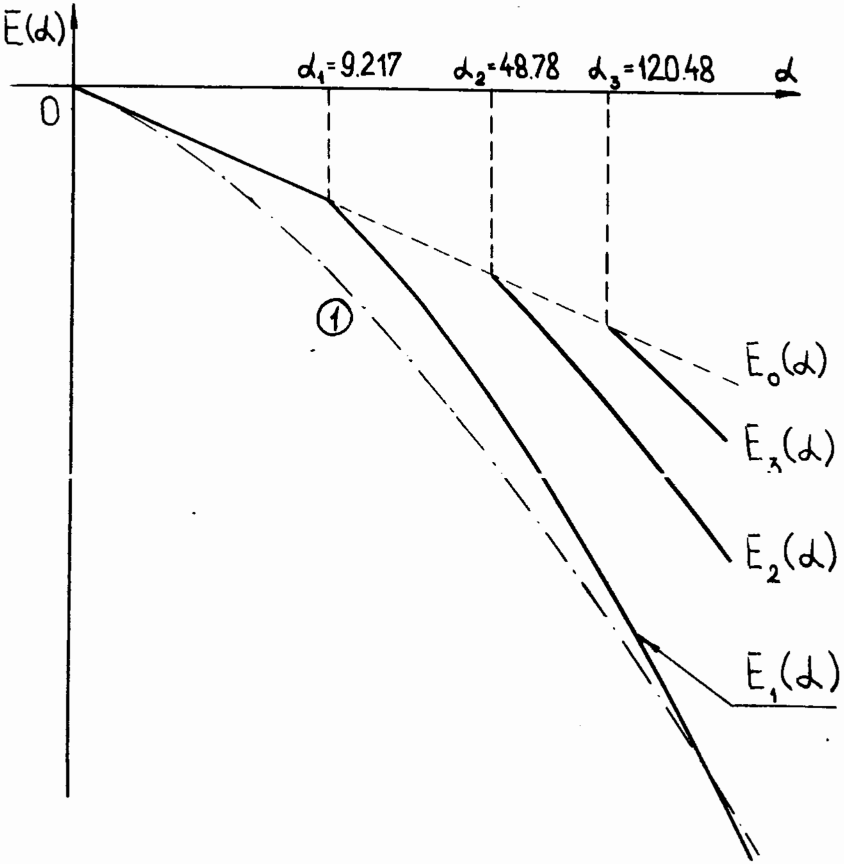
Although in both limit cases the motion of electron in the ion crystal is described by means of the Pekar-Fröhlich Hamiltonian, each of them requires its special method of research. For example, in the strong coupling theory the special form of adiabatic perturbation theory was worked out [2,4], in which the translational degeneracy was removed still before the expansion in perturbation series. For the present time one succeeded in connecting the two described pictures in the framework of Feynman's variational approach in which the smooth upper estimate to the polaron ground state energy was obtained for all values of the electron-phonon coupling constant α (see the figure).

In this connection the paper [6] can be mentioned in which thermodynamical quantities are calculated by a special reduction of the problem to the calculation of mean quantities of T-products. An approach, developed in [6] is more convenient for concrete calculations than the use of path integrals [5]. It seems to us that it gives also some advantages in carrying out general demonstrations concerning the choice of approximating Hamiltonians (in [6] it has been illustrated by the linear model of Bogolubov), analysis of the behaviour of the polaron in external fields and so on.

1. In paper [7]* a generalized path-integral approach to the polaron ground state energy has been proposed. The generalization consists in that a trial model where the electron interacts with a second particle by means of an arbitrary potential $v(\vec{r},\vec{r}')$ (and not a harmonic one as in Feynman's approach [5]) is used for variational calculations. The trial action in this case is given by the formula

$$S_0[\vec r, \vec r'] = \frac{1}{2}\int_0^\beta \dot{\vec r}^{\,2}(\tau)\,d\tau + \frac{m'}{2}\int_0^\beta \dot{\vec r}'^{\,2}(\tau)\,d\tau + V_0[\vec r, \vec r'], \quad (1)$$

$$V_0[\vec r, \vec r'] = \int_0^\beta v\,[\vec r(\tau) - \vec r'(\tau)]\,d\tau .$$



The upper bound to the polaron ground state energy E vs. the coupling constant α. Curve 1 schematically represents Feynman's result [5], and curves $E_0(\alpha) = -\alpha$, $E_1(\alpha) = -0.1085\,\alpha^2$, $E_2(\alpha) = -0.0205\,\alpha^2$, $E_3(\alpha) = -0.0083\,\alpha^2$, respectively, represent results obtained from the solution of the extremization problem for the functional $\Phi[\mu, u]$ (2).

In (1) the translational invariance of the initial problem with the Pekar-Fröhlich Hamiltonian is taken into account and the units are used for which $\hbar = m = \omega = 1$; ω and m being the frequency of longitudinal optical phonons and mass of electron, respectively. The resulting inequality for the polaron ground state energy E is [7]:

$$E \le \Phi[\mu, u] = \frac{1}{2\mu}\int |\nabla u|^2 d\vec r - \frac{\alpha}{\sqrt{2}\mu}\iint d\vec r\, d\vec r' \,\frac{|u(\vec r)|^2\,|u(\vec r')|^2}{|\vec r - \vec r'|} \times$$
$$\times\,(1 - e^{-C|\vec r - \vec r'|}), \quad (2)$$

where α is the constant of coupling strength, $C = \frac{\sqrt{2\mu}}{\sqrt{1-\mu}}$ and $\mu = \frac{m'}{1+m'}$ is the reduced mass of the two particle trial system. In (2) μ and the wave function of the electron $u(\vec r)$ are treated as variational parameters. We can see, that $\Phi[\mu, u]$ in (2) can be considered as a modified expression for the Bogolubov-Pekar-Tyablikov functional [2-4], into which it turns when $\mu = 1$ (the strong coupling case). The principal moment here is that in the limit $\mu \to 0$ $\Phi[\mu, u]$ leads to the correct expression for the ground state polaron energy $E_0 = -\alpha$ in the weak coupling case (see below).

In order to obtain the best upper estimate to E, functional $\Phi[\mu, u]$ must be minimized with respect to $\mu \in [0, 1]$ and $u(\vec r)$ with the condition:

$$\int |u(\vec r)|^2 d\vec r = 1. \quad (3)$$

The condition $\delta[\Phi - \mathcal{E}\int |u(\vec r)|^2 d\vec r] = 0$ leads to the equation [7]:

$$\left\{-\frac{1}{2\mu}\nabla^2 - \frac{\alpha\sqrt{2}}{\mu}\int d\vec r' \,\frac{|u(\vec r')|^2}{|\vec r - \vec r'|}\,(1 - e^{-C|\vec r - \vec r'|})\right\} u(\vec r) = \mathcal{E} u(\vec r) \quad (4)$$

and the conditions $\frac{\partial \Phi}{\partial \mu} = 0$ and $\frac{\partial}{\partial t}\Phi[\mu, t^{3/2} u(t\vec r)]|_{t=1} = 0$ give the following relation for μ:

$$\mu = \frac{4T}{T - \mathcal{E}}, \quad (5)$$

where $T = \frac{1}{2\mu} \int d\vec{r}\, |\nabla u|^2$. The total energy E is related to T and to the eigenvalue $\mathcal{E}$ by the expression $E = \frac{1}{2}(\mathcal{E} + T)$.

The solutions of this problem are the sets $\mu, \mathcal{E}, u(\vec{r})$ satisfying (3)-(5). It is not difficult to see that the following exact solutions hold for all α: a) $\mu_0 = 0$; $\mathcal{E}_0 = -2\alpha$; $u_0(\vec{r}) =$ const. This solution gives $E_0(\alpha) = -\alpha$ b) $\mu_n = 1$, $\mathcal{E} = \mathcal{E}_n$, $u = u_n(\vec{r})$, where $\mathcal{E}_n$, $u_n(\vec{r})$ are the solutions of the Pekar equations

$$\{ -\frac{1}{2}\nabla^2 - \alpha\sqrt{2} \int d\vec{r}\,' \frac{|u_n(\vec{r}\,')|^2}{|\vec{r} - \vec{r}\,'|} \} u_n(\vec{r}) = \mathcal{E}_n u_n(\vec{r}). \qquad (6)$$

As is shown in ref.[2,4], eq. (6) is asymptotically exact in the $\alpha \to \infty$ limit. All the solutions of (6) satisfy (5) in consequence of the virial theorem $E = -T$. The energies of the four lower states with $\mu = \mu_n = 1$ are[8,9]:

$$E_1(\alpha) = -0.1085\alpha^2; \qquad E_2(\alpha) = -0.0205\alpha^2; \qquad (7)$$

$$E_3(\alpha) = -0.0083\alpha^2; \qquad E_4(\alpha) = -0.0045\alpha^2.$$

We know that $E_0(\alpha)$ and $E_1(\alpha)$ are asymptotically exact expressions for the polaron ground state energy in the limiting cases $\alpha \to 0$ and $\alpha \to \infty$, respectively. If eqs. (3-5) do not have solutions with $\mu \in (0,1)$ and energy lower than E_0 and E_1 in some interval of values of α, then the polaron ground state energy from the variational estimate is simply $-\alpha$ for $\alpha < \alpha_1$ and $-0.1085\alpha^2$ for $\alpha > \alpha_1$. The value α_1 can be interpreted as "critical value α" corresponding to the first order phase transition from the free polaron state ($\alpha < \alpha_1$) to the self-localized state ($\alpha > \alpha_1$), and it is equal to 9.21.

In a recent paper [10] these results were obtained by solving equation (4) with the Ritz variational method. Here we see that no numerical work is needed to reach the same conclusions. The other two solutions (besides E_0 and E_1) obtained in[10] are not solutions of (3)-(5) but consequences of the use of the Ritz method.

From (7) there also follows the existence of a set α_n (n = 2, 3,...) of critical values of α defined by the equations

$$-\alpha_n = E_n(\alpha_n). \qquad (8)$$

For $\alpha > \alpha_2 = 48{,}78$ the first excited state is not the free one but the self consistent localized state of energy $E_2(\alpha)$, for $\alpha > \alpha_3 = 120{,}48$ the first two excited states are the self consistent localized states of energies $E_2(\alpha)$ and $E_3(\alpha)$ and so on. The full picture is schematically given in the figure.

It is necessary to point out that we discuss here the picture arising from (2) rather than how a good approximation to the polaron energy it gives. As is well known, the numerical estimate of the polaron ground state energy of Feynman's theory[5] is better except for very large α and does not show any phase transition-like behaviour. On the other band, we do not know yet whether or not other solutions of (3)-(5) with $\mu \in (0,1)$ and energy lower than E_0 and E_1 exist. These solutions, if they exist, do not arise when solving the problem by the Ritz method. Only exact numerical solution of (3)-(5) can say the last word about it.

2. From the picture described in the previous section it follows that at critical transition points such polaron characteristics as effective mass, radius and number of phonons should have jumps. The exact path integral representations for the polaron gound state effective mass m^*, radius R and for the mean number of phonons N in the cloud surrounding the electron at zero temperature are[5,11]:

$$E(\vec{u}) = E + \frac{1}{2} m^* \vec{u}^2 + \ldots = -\lim_{\beta \to \infty} \frac{1}{\beta} \ln \int_{\vec{r}(\beta) = \vec{r}(0) + \vec{u}\beta} D\vec{r}\, e^{-S[\vec{r}]}$$

$$\frac{1}{R} = \frac{4\pi}{V} \sum_{\vec{k}} \frac{1}{k^2} \int_0^\infty d\tau\, e^{-\tau} J(\vec{k}, \tau), \qquad (9)$$

$$N = \frac{2\sqrt{2}\pi\alpha}{V} \sum_{\vec{k}} \frac{1}{k^2} \int_0^\infty d\tau\, e^{-\tau}\, \tau J(\vec{k}, \tau),$$

where $S[\vec{r}]$ is the polaron action functional[5]

$$S[\vec{r}] = \frac{1}{2} \int_0^\beta d\tau\, \dot{\vec{r}}^2(\tau) - \frac{\alpha}{2^{3/2}} \int_0^\beta \int_0^\beta d\tau\, d\sigma \frac{e^{-|\tau - \sigma|}}{|\vec{r}(\tau) - \vec{r}(\sigma)|}$$

and

$$J(\vec{k}, \tau) = \lim_{\beta \to \infty} \frac{\int_{\vec{r}(0) = \vec{r}(\beta)} D\vec{r}\, e^{-S[\vec{r}] + i\vec{k}[\vec{r}(\tau_1) - \vec{r}(\tau_2)]}}{\int_{\vec{r}(0) = \vec{r}(\beta)} D\vec{r}\, e^{-S[\vec{r}]}}; \qquad \tau = |\tau_1 - \tau_2|.$$

In the framework of the approximation of paper [7] $J(\vec{k}, \tau)$ is replaced by

$$J_0(\vec{k}, \tau) = e^{-\frac{1-\mu}{2} k^2 \tau} \left| \int d\vec{r}\, e^{i\mu \vec{k}\vec{r}} |u(\vec{r})|^2 \right|^2,$$

and the approximate expressions for m*, R and N are:

$$m^* = 1 + \frac{4\sqrt{2}\pi a}{3V} \sum_{\vec{k}} \frac{1}{[1 + \frac{1-\mu}{2} k^2]^3} \left| \int d\vec{r}\, e^{i\mu \vec{k}\vec{r}} |u(\vec{r})|^2 \right|^2,$$

$$\frac{1}{R} = \frac{4\pi}{V} \sum_{\vec{k}} \frac{1}{k^2[1 + \frac{1-\mu}{2} k^2]} \left| \int d\vec{r}\, e^{i\mu \vec{k}\vec{r}} |u(\vec{r})|^2 \right|^2, \tag{10}$$

$$N = \frac{2\sqrt{2}\pi a}{V} \sum_{\vec{k}} \frac{1}{k^2[1 + \frac{1-\mu}{2} k^2]^2} \left| \int d\vec{r}\, e^{i\mu \vec{k}\vec{r}} |u(\vec{r})|^2 \right|^2.$$

When $\mu = 0$ we obtain

$$m_0^* = 1 + \frac{a}{6}; \quad R_0 = \frac{1}{\sqrt{\pi}}; \quad N_0 = \frac{a}{2}.$$

When $\mu = 1$ and $E = E_1(a)$ the results are:

$$m_1^* = 1 + 0.227 a^4; \quad R_1 = \frac{3.2585}{a}; \quad N_1 = 0.2170 a^2,$$

and the corresponding jumps of these quantities at a_1 are:

$$\Delta m^* = 162.3; \quad \Delta R = 0.3535; \quad \Delta N = 13.82.$$

Analogously, by means of (10) the jumps at all the critical values a_n can be calculated.

3. As was mentioned in section 1, the picture described above rests essentially on the proposition that there are no solutions different from solutions pointed out in 1. At $\mu = 1$ $(a \to \infty)$ $\Phi[\mu, u]$ coincided with the Bogolubov-Pekar-Tyablikov functional, the extremals of which for $u(\vec{r})$ describe some states of electron in the polarization well. The question about the description of spectrum of electron in the well formed by its polarization of the crystal at intermediate coupling on the basis of (6) remains open. Whether or not it is possible to

construct the solution of (6) close to the Pekar solution at $\mu < 1$ should be elucidated by the numerical solution of the problem (3)-(5). Till now along this way no essential progress was reached and one should concern the conclusion about the possible phase transition from the picture of the weak coupling polaron to strong coupling polaron, made in ref. [10], with great care.

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Федянин В.К. и др. E17-83-645

Об обобщенном функциональном подходе к проблеме полярона

Обсуждаются некоторые точные решения вариационной задачи на экстремум для энергии основного состояния полярона, возникающей в рамках обобщенного функционального подхода /7/. В частности, анализируются возникающие в рамках этого подхода переходы при некоторых "критических" значениях константы связи α_n в автолокализованные состояния и вычисляются сопровождающие переходы скачки эффективной массы, радиуса полярона и числа возбужденных фононов.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Fedyanin V.K. et al. E17-83-645

On the General Path Integral Approach to Polaron Problem

Some exact solutions of the variational problem for the polaron ground state energy, which arises in the framework of the generalized path integral approach /7/ are discussed. In particular, phase transitions to self consistent localized states appearing in this formulation at some critical values α_n of the coupling constant are analysed, and the jumps of the effective mass, radius and mean number of phonons in the cloud surrounding the electron are calculated.

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

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