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991/91

E2-90-535

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SOME REMARKS ON THE POLARON THEORY

*To be published in the Proceedings of the Workshop on "Advances in Theoretical Physics", Vietri sul Mare, Italy, October 23 - 27, 1990. См

Сноска

1990

I. Approximation by variational principle

I,1) Polaron at rest

In this paper we shall consider the hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{\sqrt{V}} \sum_{(f)} \mathcal{U} \left(b_f e^{ifx} + b_f^+ e^{-ifx} \right) + \sum_{(f)} \omega_f b_f^+ b_f .$$

Here

$$f = \vec{f} = \left(\frac{2\pi n_1}{\mathcal{L}}, \frac{2\pi n_2}{\mathcal{L}}, \frac{2\pi n_3}{\mathcal{L}} \right); \quad n \text{– integers}, \quad \mathcal{L}^3 = V$$

$$x = \vec{r}, \quad p = -i \frac{\partial}{\partial x} ;$$

ω_f and $\mathcal{U}_f^+$ are supposed to be radially symmetric with respect to f :

$$\mathcal{U}_f = \mathcal{U}_{|f|}, \quad \omega_f = \omega_{|f|}$$

b_f, b_f^+ – bose amplitudes.

State vector Φ corresponding to the lowest energy is defined by

$$\langle \Phi^* H \Phi \rangle = \min = \mathcal{E} \tag{I}$$

$$\langle \Phi^* \Phi \rangle = 1 .$$

To obtain an approximation we shall now construct the trial state vectors to insist them into relation (I).

Put:

$$b_f = C_f + a_f ; \quad b_f^+ = C_f^* + a_f^+ , \tag{2}$$

where C_f, C_f^* are c-numbers and a_f, a_f^+ bose amplitude. Introduce vacuum state vector Φ for a_f, a_f^+ operators:

$$\langle \Phi_v^* \Phi_v \rangle = 1 \qquad a_f \Phi_v = 0 ; \quad \Phi_v^* a_f^+ = 0 \tag{3}$$

and construct trial state vector Φ :

$$\Phi = \varphi(x)\,\Phi_v \quad , \quad \int \varphi^*(x)\,\varphi(x)\,d_f = 1. \tag{4}$$

Here function $\varphi(x)$ and c-numbers C_f are to be determined by the variation principle:

$$\Lambda(\varphi; \cdots C_f \cdots) = min, \tag{5}$$

where

$$\Lambda(\varphi; \cdots C_f \cdots) = \int \langle \Phi_v^* \varphi^*(x) H \varphi(x) \Phi_v \rangle\, dx$$

and therefore

$$\Lambda = \int \varphi^*(x)\left\{\frac{p^2}{2m} + \frac{1}{\sqrt{V}}\sum_{(f)} \mathcal{U}_f \left(c_f e^{ifx} + c_f^* e^{-ifx}\right) + \sum_{(f)} \omega_f c_f^* c_f\right\}\varphi(x)\,dx.$$

Because of the minimal property of Λ with respect to C_f we have

$$\frac{\partial \Lambda}{\partial C_f} = 0 \quad , \quad \frac{\partial}{\partial C_f^*}\Lambda = 0 \tag{6}$$

and therefore

$$C_f^* = -\frac{\mathcal{U}_f}{\omega_f\sqrt{V}}\int e^{ifx}\varphi^*(x)\varphi(x)\,dx = C_f^*(\varphi)$$

$$C_f = -\frac{\mathcal{U}_f}{\omega_f\sqrt{V}}\int e^{-ifx}\varphi^*(x)\varphi(x)\,dx = C_f(\varphi).$$

We see from (5) that the expression

$$\Lambda(\varphi) = \Lambda(\varphi; \dots C_f(\varphi) \dots C_f^*(\varphi) \dots)$$

must have the minimal property with respect to $\varphi(x)$ and thus:

$$\delta_\varphi \Lambda(\varphi) = 0. \tag{7}$$

We have

$$\Lambda(\varphi) = \int \varphi^*(x)\left\{\frac{p^2}{2m} + U(x;\varphi)\right\}\varphi(x)\,dx, \tag{8}$$

where

$$U(x;\varphi) = \frac{1}{\sqrt{V}}\sum_{(f)} \mathcal{U}_f \left(c_f(\varphi)e^{ifx} + c_f^*(\varphi)e^{-ifx}\right) + \sum_{(f)} \omega(f)\, c_f^+(\varphi)\, c_f(\varphi). \tag{9}$$

From (6) it follows that:

$$\int \varphi^*(x)\left\{\delta U(x,\varphi)\right\}\varphi(x)\,dx = 0$$

and we have from (7)

$$\delta_\varphi \Lambda(\varphi) = \int (\delta\varphi^*(x))\left\{\frac{p^2}{2m} + U(x,\varphi)\right\}\varphi(x)\,dx + \int \varphi^*(x)\left\{\frac{p^2}{2m} + U(x,\varphi)\right\}\delta\varphi(x)\,dx = 0.$$

Here

$$\int (\delta\varphi^*(x))\,\varphi(x)\,dx + \int \varphi^*(x)\,\delta\varphi(x)\,dx = 0.$$

Therefore:

$$\left\{\frac{p^2}{2m} + U(x,\varphi)\right\}\varphi(x) = E\,\varphi(x). \tag{IO}$$

We see from (8) that:

$$E = \Lambda(\varphi).$$

Hence in order to verify the minimal principle:

$$\Lambda(\varphi) = min$$

we must find the solution of (IO) for which

$$E = E_0$$

will be minimal.

Because of our particular choice for the trial state vectors (4) it is clear that

$$E_0 \geq \mathcal{E}. \tag{11}$$

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It is to be noted that the equation (IO) was first obtained by Landau and Pekar by other way as all the mass of the moving polaron. In our paper of 1950 on the adiabatic approximation we have received these formulae as a first approximation. //

Remark also that

$$E_0 = \min \Lambda(\varphi) = \min_{\varphi} \; \min_{c} \Lambda(\varphi; \cdots c_f \cdots) \leqq$$
$$\leqq \min_{\varphi} \Lambda(\varphi, \ldots 0 \ldots) = \min_{\varphi} \int \varphi^*(x) \frac{p^2}{2m} \varphi(x)\, dx = 0 .$$

Thus:

$$\mathcal{E} \leq E_0 \leqq 0 . \tag{11'}$$

Suppose now that the equation (IO) has such solution

$$\varphi = \varphi_0(x) ; \quad E = E_0$$

that the associated linear equation

$$\left\{ \frac{p^2}{2m} + U(x; \varphi_0) \right\} \varphi(x) = E \varphi(x) \tag{12}$$

has, for $E = E_0$, a unique (apart from the arbitrary constant) solution $\varphi = \varphi_0$. For its other eigenvalues $E_n > E_0$.

As from (9)

$$\overset{*}{U}(x; \varphi) = U(x; \varphi)$$

we can take φ_0 to be real.

Let us further remark that

$$U(x; \varphi) = -\frac{2}{V} \sum_{(f)} \frac{\mathcal{U}_f^2}{\omega_f} \left\{ \int e^{-i(fx)} \varphi^*(x) \varphi(x)\, dx \right\} e^{ifx} +$$
$$+ \frac{1}{V} \sum_{(f)} \frac{\mathcal{U}_f^2}{\omega_f} \left| \int e^{-i(fx)} \varphi^*(x) \varphi(x)\, dx \right|^2$$

and hence:

$$U(x, \varphi) = -\int K(x-y) \varphi^*(y) \varphi(y)\, dy +$$
$$+ \frac{1}{2} \int K(x-y) \varphi^*(x) \varphi(x) \varphi^*(y) \varphi(y)\, dx\, dy .$$

where

$$K(x) = \frac{2}{V} \sum_{(f)} \frac{\mathcal{U}_f^2}{\omega_f} e^{ifx} = \frac{2}{(2\pi)^3} \int \frac{\mathcal{U}_f^2}{\omega_f} e^{ifx}\, df .$$

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As

$$\frac{\mathcal{U}_f^2}{\omega_f}$$

is radially symmetrical with respect to f the expression $K(x)$ is a radially symmetrical function of x :

$$K(x) = \mathcal{K}(|x|) .$$

Therefore if a $\varphi(x)$ is radially symmetrical, then

$$U(x; \varphi)$$

also possesses this property.

Thus, in the considered situation the operator

$$\frac{p^2}{2m} + U(x; \varphi)$$

conserves the property of radial symmetry.

We may hence consider the radially symmetrical solutions of (IO).

We suppose that one of them $\varphi_0(x)$ corresponds to the lowest possible value of the energy E_0 .

It is to be stressed that if $\varphi(x)$ is a solution of the equation (IO) then $\varphi(x+\xi)$ will also satisfy this equation for arbitrary constant ξ .

Such translation may be considered as a translation of coordinate system in (x)-space by fixing the zero-point anywhere in space.

We thus see that we are in the degeneracy situation and so our averages computed by means of $\varphi_0(x)$ are what is called the quasi-averages.

Fix somehow the zero point origin of the coordinate system then

$$\varphi_0(x) = f(|x|)$$

is fully determined and so is also

$$U(x; \varphi_0) = U(|x|)$$

Therefore the linear equation (12)

$$\left\{ \frac{p^2}{2m} + U(|x|) \right\} \varphi(x) = E \varphi(x)$$

is no more translationally invariant and we may suppose that its solution

$$\Psi(x) = \varphi_0(x) = f(|x|)$$

for $E = E_0$ is unique, apart from the arbitrary constant multiplying $\Psi(x)$.

I,2) The case of moving polaron

Here we have to deal with the problem of minimum

$$\bar{H} = \langle \Phi^* H \Phi \rangle = min \; ; \quad \langle \Phi^* \Phi \rangle = 1 \tag{I}$$

with the supplementary conditions:

$$\vec{p}\,\Phi = (\vec{p} + \sum_{(f)} \vec{f} B_f^+ B_f)\,\Phi ,$$

$\vec{P}$ being the total momentum (integral of motion).

Applying the usual procedure we have to minimize:

$$\bar{H} + \vec{\lambda}\,\vec{I} = min , \tag{2}$$

where

$$\vec{I} = \langle \Phi^* \{ \vec{P} - \vec{p} - \sum_{(f)} \vec{f} B_f^+ B_f \} \Phi \rangle$$

and after finding the corresponding solution we must determine multipliers $\vec{\lambda}$ from the condition:

$$I = 0.$$

To find an approximation we shall use the same method as in the previous case. Instead of arbitrary state vectors Φ we insert in (2) the special set of state vectors the same as in (4,1).

We thus obtain the approximate variational principle:

$$\Lambda_\lambda (\varphi; \dots c_f \dots) = min = E_\lambda , \tag{3}$$

where

$$\Lambda_\lambda = \langle \Phi_\vartheta^* \varphi^* (H - \vec{\lambda}\vec{\mathcal{J}}) \varphi \Phi_\vartheta \rangle$$

$$\vec{\mathcal{J}} = \vec{P} - \vec{p} - \sum \vec{f} B_f^+ B_f . \tag{4}$$

After determining φ C_f we connect $\vec{\lambda}$ and $\vec{P}$ by the relation:

$$\vec{I}_\lambda = \langle \Phi_\vartheta^* \varphi \vec{\mathcal{J}} \varphi \Phi_\vartheta \rangle = 0 . \tag{5}$$

We see that E_λ is our approximation for the energy of polaron with the total momentum $\vec{P}$.

We also remark that

$$\frac{\partial E_\lambda}{\partial \vec{P}} = \lambda . \tag{5'}$$

Hence $\vec{\lambda}$ is the average velocity of polaron.

By averaging in (4),(5) over Φ_ϑ we get:

$$\Lambda_\lambda = \int \varphi^*(x) \Big\{ \frac{p^2}{2m} - \vec{\lambda}\vec{p} + \frac{1}{\sqrt{V}} \sum_{(f)} \mathcal{U}_f (C_f e^{ifx} + C_f^+ e^{-ifx}) + \sum_{(f)} (\omega_f - \vec{\lambda}\vec{f}) C_f^+ C_f \Big\} \varphi(x)\, dx + \vec{\lambda}\vec{P}$$

$$\vec{I}_\lambda = \vec{P} - \int \varphi^*(x)\, \vec{p}\, \varphi(x)\, dx - \sum_{(f)} \vec{f} C_f^+ C_f .$$

Because of

$$\frac{\partial \Lambda_\lambda}{\partial C_f} = 0 , \quad \frac{\partial \Lambda_\lambda}{\partial C_f^+} = 0 ,$$

we obtain

$$C_f = -\frac{1}{\sqrt{V}} \frac{\mathcal{U}_f}{\omega_f - \vec{f}\vec{\lambda}} \int e^{-ifx} \varphi^*(x) \varphi(x)\, dx ,$$

$$C_f = -\frac{1}{\sqrt{V}} \frac{\mathcal{U}_f}{\omega_f - \vec{f}\vec{\lambda}} \int e^{ifx} \varphi^*(x) \varphi(x)\, dx$$

and

$$\Lambda_\lambda = \int \varphi^*(x) \Big\{ \frac{p^2}{2m} - \vec{\lambda}\vec{p} - \frac{1}{V} \sum_{(f)} \mathcal{U}_f^2 \Big\{ \frac{1}{\omega_f + \vec{f}\vec{\lambda}} + \frac{1}{\omega_f - \vec{f}\vec{\lambda}} \Big\} e^{-ifx} \varphi^*(x)\varphi(x)\, dx + \frac{1}{V} \sum_{(f)} \mathcal{U}_f^2 \frac{\left| \int e^{-ifx} \varphi^*(x)\varphi(x)\, dx \right|^2}{\omega_f - \vec{f}\vec{\lambda}} \Big\} \varphi(x)\, dx + \vec{\lambda}\vec{P}$$

Or:

$$\Lambda_\lambda = \int \varphi^*(x) \Big\{ \frac{p^2}{2m} - \vec{\lambda} p^2 - \frac{2}{V} \sum_{(f)} \mathcal{U}_f^2 \frac{\omega_f}{\omega_f^2 - (\vec{f}\vec{\lambda})^2} e^{ifx} \int e^{-ifx} \varphi^*(x)\varphi(x)\, dx + \frac{1}{V} \sum_{(f)} \mathcal{U}_f^2 \frac{\omega_f}{\omega_f^2 - (\vec{f}\vec{\lambda})^2} \left| \int e^{-ifx} \varphi^*(x)\varphi(x)\, dx \right|^2 \Big\} \varphi(x)\, dx + \vec{\lambda}\vec{P} . \tag{6}$$

We also have:

$$I_{\lambda}=\vec{P}-\int\varphi^{*}(x)\vec{p}\varphi(x)dx-\sum_{(f)}\frac{1}{V}\mathcal{U}_f^2\,\frac{\vec{f}}{(\omega_f-\vec{f}\vec{\lambda})^2}\left|\int e^{-ifx}\varphi^{*}(x)\,\varphi(x)dx\right|^2 = \tag{7}$$

$$=\vec{P}-\int\varphi^{*}(x)\vec{p}\varphi(x)dx-\sum_{(f)}\frac{2}{V}\,\frac{\vec{f}(\vec{f}\vec{\lambda})\,\omega_f}{(\omega_f^2-(\vec{f}\vec{\lambda})^2)^2}\left|\int e^{-ifx}\varphi^{*}(x)\varphi(x)dx\right|^2.$$

Minimizing Λ_{λ} with respect to φ we get the equation:

$$\left\{\frac{p^2}{2m}-\vec{\lambda}p^2-\frac{2}{V}\sum_{(f)}\frac{\mathcal{U}_f^2\,\omega_f}{\omega_f^2-(\vec{f}\vec{\lambda})^2}\,e^{ifx}\int e^{-ifx}\varphi^{*}(x)\varphi(x)\,dx\right. +$$
$$\left.+\frac{1}{V}\sum_{(f)}\frac{\mathcal{U}_f^2\omega_f}{\omega_f^2-(\vec{f}\vec{\lambda})^2}\left|\int e^{-ifx}\varphi^{*}(x)\varphi(x)dx\right|^2\right\}\varphi(x)=E_{\lambda}\,\varphi(x)\,. \tag{8}$$

It is useful to introduce the function $\theta\,(x)$ by putting:

$$\varphi(x)=e^{im\vec{\lambda}\vec{x}}\,\theta(x)\,. \tag{9}$$

Then (6),(7),(8) become:

$$\Lambda_{\lambda}=\int\theta^{*}(x)\left\{\frac{p^2}{2m}-\frac{m\lambda^2}{2}+U_{\lambda}(x\,;\theta\right\}\theta(x)\,dx+\vec{\lambda}\,\vec{P} \tag{10}$$

$$\left\{\frac{p^2}{2m}-\frac{m\lambda^2}{2}-U_{\lambda}(x;\theta)\right\}\theta(x)=(E_{\lambda}-\vec{\lambda}\,\vec{P})\theta(x) \tag{11}$$

$$I_{\lambda}=\vec{P}-m\vec{\lambda}-\int\theta^{*}(x)p\,\theta(x)\,dx\;-$$
$$-\frac{2}{V}\sum\frac{\vec{f}(\vec{f}\vec{\lambda})\mathcal{U}_f^2\omega_f}{(\omega_f^2-(\vec{f}\vec{\lambda})^2)^2}\left|\int e^{-ifx}\theta^{*}(x)\theta(x)dx\right|^2, \tag{12}$$

where

$$U_{\lambda}(x;\theta)=-\frac{2}{V}\sum_{(f)}\frac{\mathcal{U}_f^2\,\omega_f}{\omega_f^2-(\vec{f}\vec{\lambda})^2}\,e^{ifx}\int e^{-ifx}\theta^{*}(x)\theta\,(x)\,dx\;+$$
$$+\frac{1}{V}\sum_{(f)}\frac{\mathcal{U}_f^2\omega_f}{(\omega_f-(\vec{f}\vec{\lambda})^2)^2}\left|\int e^{-ifx}\theta^{*}(x)\,\theta(x)\,dx\right|^2. \tag{13}$$

Denote by θ_{λ} the solution of the equation (11) corresponding to the lowest value of E_{λ} .

As in the previous paragraph we suppose that the linear equation associated with (11)

$$\left\{\frac{p^2}{2m}-\frac{m\lambda^2}{2}+\vec{\lambda}\vec{P}+U_{\lambda}(x;\theta_{\lambda})\right\}\theta(x)=E\,\theta(x) \tag{14}$$

for $E=E_{\lambda}$ has unique (apart from the arbitrary constant)

$$\theta(x)=\theta_{\lambda}(x)\,.$$

Because

$$U_{\lambda}^{*}(x\,;\theta)=U_{\lambda}(x\,;\theta)\,,$$

we see that $\theta_{\lambda}(x)$ may be chosen to be real;

$$\theta_{\lambda}^{*}(x)=\theta_{\lambda}(x)\,. \tag{15}$$

In this situation we have:

$$\int\theta_{\lambda}^{*}(x)\vec{p}\,\theta_{\lambda}(x)dx=-i\int\theta_{\lambda}(x)\frac{\partial}{\partial x}\,\theta_{\lambda}(x)dx=-\frac{i}{2}\int\frac{d\,\theta_{\lambda}^2(x)}{dx}dx=0$$

and therefore we get from (5),(12)

$$\vec{P}=m\vec{\lambda}+\frac{2}{V}\sum_{(f)}\frac{\vec{f}(\vec{f}\vec{\lambda})\mathcal{U}_f^2\omega_f}{(\omega_f^2-(\vec{f}\vec{\lambda})^2)^2}\left|\int e^{-ifx}\theta^2(x)dx\right|^2.$$

We shall now proceed to the calculation of the effective mass of the polaron. To this end we must find the expressions for E_{λ} , $\vec{P}$ leaving only the terms of order λ^2 in E_{λ} and of order λ in P .

Expand U_{λ} , $\vec{P}$ in powers of λ (considered as sufficiently small) leaving only the principal term.

We obtain:

$$\vec{P}=m\vec{\lambda}+\frac{2}{V}\sum_{(f)}\frac{\vec{f}(\vec{f}\vec{\lambda})}{\omega_f^2}\mathcal{U}_f^2\left|\int e^{-ifx}\,\theta_{\lambda}^2(x)\,dx\right|^2+\lambda^3\cdots \tag{16}$$

$$U_{\lambda}(x,\theta)=U(x,\theta)-\frac{2}{V}\sum_{(f)}\frac{\mathcal{U}_f^2(\vec{f}\vec{\lambda})^2}{\omega_f^3}e^{ifx}\int e^{-ifx}\theta^2(x)\,dx\;+$$

$$+\frac{1}{V}\sum_{(f)}\frac{\mathcal{U}_f^2(\vec{f}\vec{\lambda})^2}{\omega_f^3}\left|\int e^{-ifx}\theta^2(x)dx\right|^2+\lambda^4\ldots \tag{17}$$

Then, from (11) we get:

$$\Big\{\frac{p^2}{2m}+U(x;\theta_\lambda)-\frac{m\lambda^2}{2}+\vec{\lambda}\vec{p}-\frac{2}{V}\sum_{(f)}\frac{\mathcal{U}_f^2(\vec{f}\vec{\lambda})^2}{\omega_f^3}e^{ifx}\int e^{-ifx}\theta_\lambda^2(x)dx+ \tag{18}$$

$$+\frac{1}{V}\sum_{(f)}\frac{\mathcal{U}_f^2(\vec{f}\vec{\lambda})^2}{\omega_f^3}\left|\int e^{-ifx}\theta_\lambda^2(x)dx\right|^2+\lambda^4\ldots-E_\lambda\Big\}\theta_\lambda(x)=0.$$

Noting that:

$$\left\{\frac{p^2}{2m}+U(x,\varphi_0)-E_0\right\}\varphi_0(x)=0 \tag{19}$$

we may remark that the difference between $\varphi_0(x)$ and closest to it $\theta_\lambda(x)$, $\varphi_0(x)-\theta_\lambda(x)$ tends to zero when $\lambda\to 0$.

Then, neglecting in (16) the terms which tend to zero more rapidly than λ , we obtain

$$\vec{p}=m\vec{\lambda}+\frac{2}{V}\sum_{(f)}\frac{\vec{f}(\vec{f}\vec{\lambda})}{\omega_f^3}\mathcal{U}_f^2\left|\int e^{-ifx}\varphi_0^2(x)dx\right|^2.$$

Or, because of radial symmetry of $\mathcal{U}_f^2/\omega_f^3$ and $\varphi_0^2(x)$;

$$\vec{p}=M\vec{\lambda}, \tag{20}$$

where

$$M=m+\frac{2}{3V}\sum_{(f)}\frac{f^2\mathcal{U}_f^2}{\omega_f^3}\left|\int e^{-ifx}\varphi_0^2(x)dx\right|^2. \tag{21}$$

From (5) it follows

$$\frac{\partial E_\lambda}{\partial\vec{p}}=\vec{\lambda}\ ;\quad \frac{\partial E}{M\partial\vec{\lambda}}=\vec{\lambda}$$

and therefore:

$$E_\lambda=\frac{1}{2}M\lambda^2+E_0. \tag{22}$$

We thus have completed the calculation of the effective mass of the polaron (21), or taking the limit

$$M=m+\frac{2}{3(2\pi)^3}\int\frac{f^2\mathcal{U}_f^2}{\omega_f^3}\left|\int e^{-ifx}\varphi_0^2(x)dx\right|^2dx. \tag{23}$$

II) Adiabatic approximation

We assume here that

$$\mathcal{U}_f=\frac{\varepsilon}{\sqrt{2}}A_f\ ,\qquad \omega_f=\varepsilon^2\nu_f \tag{I}$$

where ε is a small parameter.

Our hamiltonian takes the form:

$$\mathcal{H}=\frac{p^2}{2m}+\varepsilon\frac{1}{V}\sum_{(f)}\frac{A_f}{\sqrt{2}}(b_fe^{ifx}+b_f^+e^{-ifx})+\varepsilon^2\sum_{(f)}\nu_f b_f^+b_f.$$

Introduce like previously (I) the new bose-amplitudes

$$b_f=c_f+a_f\ ;\quad c_f=\frac{u_f}{\varepsilon}\ ;\quad u_f=-\frac{A_f}{(\sqrt{2V})\nu_f}\int e^{-i(fx)}\varphi_0^2(x)dx, \tag{2}$$

where $\varphi_0(x)$ is the same as in (I,1).

Then:

$$\mathcal{H}=\Gamma+\varepsilon\Big\{\frac{1}{\sqrt{2V}}\sum_{(f)}A_f(a_fe^{ifx}+a_f^+e^{-ifx}) \tag{3}$$

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$$+\varepsilon^2\sum_{(f)}\nu_f a_f^+a_f,$$

where

$$\Gamma=\frac{p^2}{2m}+U(x;\varphi_0). \tag{4}$$

The first order approximation hamiltonian may be obtained by dropping in (3) the terms of the order $\varepsilon,\varepsilon^2$.

In this approximation we have the same equation which was obtained in (I,1) by using the variational principle.

Here

$$\Phi=\varphi_0(x)\Phi_v.$$

Because

$$a_f^+ a_f \Phi_v = 0,$$

we see that as the first order hamiltonian we also may take:

$$H_0 = \Gamma + \varepsilon^2 \sum_{(f)} \nu_f a_f^+ a_f = \Gamma + \sum_{(f)} \omega_f a_f^+ a_f . \tag{5}$$

The inclusion here of the ε^2-order term clearly does not change the result:

$$\begin{aligned} \Phi &= \varphi_0(x)\Phi_v \\ \Gamma \varphi_0(x) &= E_0 \varphi_0(x). \end{aligned} \tag{6}$$

Taking into account (21,I,2) we see that in our first approximation the effective mass of the polaron is given by the relation:

$$\begin{aligned} M = m + \frac{1}{\varepsilon^4 3(2\pi)^3} \int \frac{f^2 A_f^2}{\nu_f^3} \left| \int e^{-ifx} \varphi_0^2(x) dx \right|^2 df \sim \\ \sim \frac{1}{\varepsilon^4 3(2\pi)^3} \int \frac{f^2 A_f^2}{\nu_f^3} \left| \int e^{-ifx} \varphi_0^2(x) dx \right|^2 df . \end{aligned} \tag{7}$$

Let us now consider the second approximation.
Write

$$H = H_0 + \varepsilon H_1 \tag{8}$$

$$H_0 = \Gamma + \sum_{(f)} \omega_f a_f^+ a_f ; \quad H_1 = \frac{1}{\sqrt{V}} \sum_{(f)} (a_f e^{ifx} + a_f^+ e^{-ifx}) \frac{A_f}{\sqrt{2}} + \sum_{(f)} \nu_f (u_f^* a_f + u_f a_f^+)$$

and put in the equation for the state vector

$$H\Phi = E\Phi$$

the expansions:

$$\begin{aligned} \Phi &= \Phi_0 + \varepsilon \Phi_1 + \varepsilon^2 \Phi_2 + \cdots ; \quad \Phi_0 = \varphi_0(x) \Phi_v \\ E &= E_0 + \varepsilon \Delta_1 + \varepsilon^2 \Delta_2 + \cdots \end{aligned} \tag{9}$$

Then:

$$(H_0 + \varepsilon H_1)(\Phi_0 + \varepsilon \Phi_1 + \varepsilon^2 \Phi_2 + \cdots) = (E_0 + \varepsilon \Delta_1 + \varepsilon^2 \Delta_2 + \cdots)(\Phi_0 + \varepsilon \Phi_1 + \varepsilon \Phi_2 + \cdots) .$$

To satisfy this equation we take:

$$\begin{aligned} (H_0 - E_0)\Phi_0 &= 0 \\ (H_0 - E_0)\Phi_1 &= \Delta_1 \Phi_0 - H_1 \Phi_0 \\ (H_0 - E_0)\Phi_2 &= \Delta_2 \Phi_0 + \Delta_1 \Phi_1 - H_1 \Phi_1 . \end{aligned} \tag{10}$$

Let us observe that in virtue of (2),(8):

$$\int \varphi_0(x) H_1 \varphi_0(x) dx = 0 . \tag{11}$$

Hence

$$\langle \Phi_0^* H_1 \Phi_0 \rangle = 0$$

or

$$\langle \Phi_0^* (H_0 - E_0) \Phi_1 \rangle = 0 = \Delta_1 - \langle \Phi_0 H_1 \Phi_0 \rangle .$$

We thus have

$$\begin{aligned} \Delta_1 &= 0 \\ (H_0 - E_0)\Phi_1 &= -H_1 \Phi_0 \end{aligned}$$

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that is:

$$(\Gamma - E_0 + \sum_{(f)} \omega_f a_f^+ a_f)\Phi_1 = -H_1 \Phi_0 =$$

$$= -\frac{1}{\sqrt{2V}} \sum A_f a_f e^{-ifx} \varphi_0(x) \Phi_v + \sum_{(f)} \nu_f u_f a_f^+ \varphi_0(x) \Phi_v .$$

Let us now expand Φ_1 in Fourier series in eigenfunctions

$$(\Gamma - E_n)\varphi_1(x) = 0_{\, n \geq 0} \quad ; \quad \int \varphi_1^*(x) \varphi_m(x) dx = \begin{cases} 1, & n = m \\ 0, & n \neq m \end{cases} . \tag{12}$$

Noting that according with (11):

$$\int \varphi_0(x) H_1 \Phi_0 dx = 0$$

we obtain

$$\Phi_1 = -\frac{1}{\sqrt{2V}} \sum_{n>0} \varphi_n(x) \sum_{(f)} \frac{A_f \int e^{-ifx} \varphi_n(x) \varphi_0(x) dx}{E_n - E_0 + \omega_f} a_f^+ \Phi_v . \tag{13}$$

We further have:

$$(H_0 - E_0)\Phi_2 = \Delta_2 \Phi_0 - H_1 \Phi_1 .$$

But

$$<\Phi_0^*(H_0 - E_0)\Phi_2> = 0$$

and it follows that

$$\Delta_2 = <\Phi_0^* H_1 \Phi_1> . \qquad (14)$$

Remark now that is virtue of (12)

$$\int \varphi_1(x) \sum_{(f)} (\nu_f u_f a_f^+ + \nu_f u_f^* a_f)\varphi_n(x)\,dx = 0 .$$

Therefore

$$\Delta_2 = -\frac{1}{2V}\sum_{(f)}\sum_{(n>0)} \frac{|\int e^{-ifx}\varphi_n^*(x)\varphi_0(x)\,dx|^2}{E_n - E_0 + \omega_f} .$$

Our approximation for the minimal energy of polaron will be

$$E_{appr.} = E_0 - \frac{\varepsilon^2}{2V}\sum_{(f)}\sum_{(n>0)} \frac{|\int e^{-ifx}\varphi_n^*(x)\varphi_0(x)\,dx|^2}{E_n - E_0 + \omega_f} . \qquad (15)$$

We have mentioned that

$$E_0 \geqslant \mathcal{E} ,$$

where

$$\mathcal{E} = \min \frac{<\Phi^* H \Phi>}{<\Phi^* \Phi>}$$

is the lowest energy of the polaron at rest.

But now we cannot be sure that also $E \geqslant \mathcal{E}$.

So we shall construct the other approximation $\mathcal{E}$ which posseses this property and has the same order of exactitude as E.

Put

$$\Phi_2 = \Phi_0 + \varepsilon \Phi_1$$

$$\mathcal{E}_{appr.} = \frac{<\Phi_2^* H \Phi_2>}{<\Phi_2^* \Phi>} = E_0 + \frac{<\Phi_2^*(H - E_0)\Phi_2>}{<\Phi_2^* \Phi_2>} . \qquad (16)$$

Then of course:

$$\mathcal{E} \geqslant \mathcal{E} . \qquad (17)$$

Denoting $H - E_0 = H'$, $H_0' = H_0 - E_0$

We have:

$$<\Phi_a^* H' \Phi_a> = <\Phi_0^* H_0' \Phi_0> + \varepsilon<\Phi_0^* H_0' \Phi_1> + \varepsilon<\Phi_1^* H_0' \Phi_0> + \varepsilon<\Phi_0^* H_1 \Phi_0> +$$
$$+ \varepsilon^2<\Phi_0^* H_1 \Phi_1> + \varepsilon^2<\Phi_1^* H_1 \Phi_0> + \varepsilon^2<\Phi_1^* H_0' \Phi_1> + \varepsilon^3<\Phi_1^* H_1 \Phi_1> \qquad (18)$$

$$<\Phi_0^* \Phi_0> + \varepsilon<\Phi_0^* \Phi_1> + \varepsilon<\Phi_1^* \Phi_0> + \varepsilon^2<\Phi_1^* \Phi_1> = <\Phi_a^* \Phi_a> . \qquad (19)$$

But we see that

$$<\Phi_0^* \Phi_1> = 0 , \quad <\Phi_1^* \Phi_0> = 0$$

$$<\Phi_0^* H_0^* \Phi_0> = 0 , \; <\Phi_0^* H_1 \Phi_0> = 0 , \; <\Phi_1^* H_0' \Phi_0> = 0 , \; <\Phi_0^* H_0' \Phi_1> = 0 .$$

Note that:

$$<\Phi_\nu^* \alpha_1 \alpha_2 \alpha_3 \Phi_{\nu'}> = 0 , \quad \text{where } \alpha_j = a_j \text{ or } a_j^+ .$$

Hence

$$<\Phi_1^* H_1 \Phi_1> = 0 .$$

We thus may write:

$$<\Phi_a^* H' \Phi_a> = \varepsilon^2<\Phi_0^* H_1 \Phi_1> + \varepsilon^2<\Phi_1^* H_1 \Phi_0> + \varepsilon^2<\Phi_1^* H_0' \Phi_1> \qquad (20)$$

$$<\Phi^* \Phi> = 1 + \varepsilon^2<\Phi_1^* \Phi_1> . \qquad (21)$$

From (8),(11),(12),(13) follows:

$$<\Phi_1^* H_1 \Phi_0> = <\Phi_0^* H_1 \Phi_1> = -\frac{1}{2V}\sum_{n>0}\sum_{(f)} A_f^2 \frac{|\int e^{-ifx}\varphi_n^*(x)\varphi_0(x)\,dx|^2}{E_n - E_0 + \omega_f}$$

$$<\Phi_1^* H_0' \Phi_1> = \frac{1}{2V}\sum_{n>0}\sum_{(f)} A_f^2 \frac{E_n + \omega_f - E_0}{(E_n - E_0 + \omega_f)^2} \left|\int e^{-ifx}\varphi_n^*(x)\varphi_0(x)\,dx\right|^2$$

$$<\Phi_1^* \Phi_1> = \frac{1}{2V}\sum_{n>0}\sum_{(f)} \frac{A_f^2}{(E_n - E_0 + \omega_f)^2} \left|\int e^{-ifx}\varphi_n^*(x)\varphi_0(x)\,dx\right|^2 .$$

Therefore (20),(21) give:

$$<\Phi_\alpha^* H'\Phi_\alpha> = +\frac{\varepsilon^2}{2V}\sum_{n>0}\sum_{(f)}\frac{A_f^2}{(E_n-E_0+\omega_f)^2}\{(E_n+\omega_f-E_0) -$$

$$- 2(E_n-E_0+\omega_f)\}\left|\int e^{-ifx}\varphi_n^*(x)\varphi_0(x)\,dx\right|^2 =$$

$$= -\frac{\varepsilon^2}{2V}\sum_{n>0}\sum_{(f)}\frac{A_f^2}{E_n-E_0+\omega_f}\left|\int e^{-ifx}\varphi_n^*(x)\varphi_0(x)\,dx\right|^2$$

$$<\Phi_\alpha^*\Phi_\alpha> = 1+\frac{\varepsilon^2}{2V}\sum_{n>0}\sum_{(f)}\frac{A_f^2}{(E_n-E_0+\omega_f)^2}\left|\int e^{-ifx}\varphi_n^*(x)\varphi_0(x)\,dx\right|^2 .$$

So that taking into account the definition (16) of $\mathcal{E}_{eff}$ we finally obtain:

$$\mathcal{E}_{appr.} = \frac{-\frac{\varepsilon^2}{2V}\sum_{n>0}\sum_{(f)}\frac{A_f^2}{E_n-E_0+\omega_f}\left|\int e^{-ifx}\varphi_n^*(x)\varphi_0(x)dx\right|^2}{1+\frac{\varepsilon^2}{2V}\sum_{n>0}\sum_{(f)}\frac{A_f^2}{(E_n-E_0+\omega_f)^2}\left|\int e^{-ifx}\varphi_n^*(x)\varphi_0(x)dx\right|^2} + E_0 . \qquad (22)$$

From (15) and (22) follows that the difference $\mathcal{E} - E$ is of the order ε^4.

Therefore the values of $\mathcal{E}_{appr.}$, $E_{appr.}$ have the same order of exactness (of the order ε^2).

Note now that in the energy interval $E_0 < E_n < \infty$ some E_n may belong ($V \to \infty!$) to the continuous spectrum and so, the summation over $n>0$ may also contain integrals.

In order to get rid of $\varphi_n(x)$, E_n in our formulae (15),(22) let us introduce the function $\Psi_f(x)$ defined by the equation:

$$(\Gamma - E_0+\omega_f)\,\Psi_f(x) = \left(e^{-ifx} - \int e^{-ifx}\varphi_0^2(x)dx\right)\varphi_0(x) . \qquad (23)$$

We have:

$$\Psi_f(x) = \sum_{n>0}\varphi_n(x)\frac{\int e^{-ifx}\varphi_n^*(x)\varphi_0(x)dx}{E_n-E_0+\omega_f} .$$

Then:

$$\int \Psi_f^*(x)\Psi_f(x)\,dx = \sum_{n>0}\frac{\left|\int e^{-ifx}\varphi_n^*(x)\varphi_0(x)dx\right|^2}{(E_n-E_0+\omega_f)^2}$$

$$\int \Psi_f(x)e^{ifx}\varphi_0^*(x)\,dx = \sum_{n>0}\frac{\left|\int e^{-ifx}\varphi_n^*(x)\varphi_0(x)dx\right|^2}{E_n-E_0+\omega_f}$$

and we see that our approximations (15),(22) for the lowest energy ~~of~~ the polaron may be put in the form:

$$E_{appr.} = E_0 - \varepsilon^2\frac{1}{2V}\sum_{(f)}A_f^2\int\Psi_f(x)\,e^{ifx}\varphi_0(x)\,dx \qquad (24)$$

$$\mathcal{E}_{appr.} = E_0 - \frac{\frac{\varepsilon^2}{2V}\sum_{(f)}A_f^2\int\Psi_f(x)e^{ifx}\varphi_0(x)dx}{1+\frac{\varepsilon^2}{2V}\sum_{(f)}A_f^2\int\Psi_f^*(x)\Psi_f(x)dx} . \qquad (25)$$

Consider now a special case when

$$U(x,\varphi) = 0$$

$$\Gamma = \frac{p^2}{2m}, \quad \varphi_0(x) = \frac{1}{\sqrt{V}}, \quad E_0 = 0 .$$

We see that here $\varphi_0(x)$ is normalized only for finite volume V.

From (23) we get

$$\Psi_f(x) = \frac{e^{-ifx}}{\sqrt{V}\left(\frac{f^2}{2m}+\omega_f\right)}, \quad f \neq 0, \quad \Psi_0(x) = 0 .$$

Therefore

$$\int\Psi_f(x)\,e^{ifx}\varphi_0(x)\,dx = \frac{1}{\frac{f^2}{2m}+\omega_f}\cdot\frac{1}{V}\int dx = \frac{1}{\frac{f^2}{2m}+\omega_f}$$

and

$$E_{appr.} = -\frac{\varepsilon^2}{2V}\sum_{(f\neq 0)}\frac{A_f^2}{\frac{f^2}{2m}+\omega_f} . \qquad (26)$$

Hence in the limit $V \to \infty$

$$E_{appr.} = -\frac{\varepsilon^2}{2(2\pi)^3} \int \frac{A_f^2}{\frac{f}{2m} + \omega_f} \, df . \tag{26'}$$

We have thus obtained the usual formula for the lowest energy of the polaron, in the ε^2-approximation, for the weak coupling case.

So, our results are valid not only in adiabatic but also in weak coupling case.

Suppose now that $\Psi_f(x), \varphi_0(x)$ may be defined in the whole space (x), (f), tend sufficiently rapidly to zero at infinity and it is possible to pass to the limit $V \to \infty$ directly in (24), (25).

In this situation we get:

$$E_{appr.} = E_0 - \frac{\varepsilon^2}{2(2\pi)^3} \int A_f^2 \left| \int \Psi_f(x) e^{ifx} \varphi_0(x) dx \right|^2 df \tag{26}$$

$$\mathcal{E}_{appr.} = E_0 - \frac{\frac{\varepsilon^2}{2(2\pi)^3} \int A_f^2 \left| \int \Psi_f(x) e^{ifx} \varphi_0(x) dx \right|^2 df}{1 + \frac{\varepsilon^2}{2(2\pi)^3} \int A_f^2 \left\{ \int \Psi_f^*(x) \Psi_f(x) dx \right\} df} . \tag{27}$$

Let us now make in conclusion some remarks concerning the evaluation of the integrals in (26), (27).

Consider the equation (12):

$$\left\{ \frac{p^2}{2m} + U(r) - E_0 \right\} \Psi_f(x) = \left\{ e^{-ifx} - \int e^{-ifx} \varphi_0^2(x) dx \right\} \varphi_0(r) ,$$

where

$$r = |x| , \quad \varphi_0(r) = \varphi_0(x) , \quad U(r) = U(x, \varphi_0)$$

and transform it to spherical coordinates of x, taking as z-axis in the direction of $\vec{f}$:

$$fx = \kappa r \cos\theta , \qquad \kappa = |\kappa| .$$

Then:

$$-\frac{1}{2mr} \frac{\partial^2 r \Psi_f}{\partial r^2} - \frac{1}{2mr^2} \left\{ \frac{1}{\sin\theta} \frac{\partial \left(\sin\theta \frac{\partial \Psi_f}{\partial \theta} \right)}{\partial \theta} + \frac{1}{\sin^2\theta} \frac{\partial^2 \Psi_f}{\partial \vartheta^2} \right\} +$$

$$+ U(r) \Psi_f - E_0 \Psi_f = \left\{ e^{-i\kappa r \cos} - 4\pi \int_0^\infty \varphi_0^2(r) \frac{\sin \kappa r}{\kappa} r dr \right\} \varphi_0(r) .$$

?

This linear equation is invariant with respect to ϑ and its right-hand side does not depend on ϑ.

Hence we may use the expansion

$$r \Psi_f = \Phi_0(r, \kappa) + \sum_{\ell=1}^{\infty} \Phi_\ell(r, \kappa) P_\ell(\cos\theta) . \tag{28}$$

where $P_\ell(\xi)$ are Legendre's polynomials.

Remembering that:

$$\int_0^\pi P_\ell(\cos\theta) P_{\ell'}(\cos\theta) \sin\theta \, d\theta = \begin{cases} \frac{2}{2\ell+1} , & \ell' = \ell \\ 0 & \ell' \neq \ell \end{cases}$$

$$\int_0^\pi P_\ell(\cos\theta) \sin\theta \, d\theta = 0 ,$$

obtain

$$-\frac{\partial^2 \Phi_0}{2m\partial r^2} + U(r)\Phi_0 - E_0 \Phi_0 = \left\{ 2\frac{\sin \kappa r}{\kappa r} - 4\pi \int_0^\infty \varphi_0^2(r) \frac{\sin \kappa r}{r} r dr \right\} \frac{r \varphi_0(r)}{2} \tag{29}$$

$$-\frac{\partial^2 \Phi_\ell}{2m\partial r^2} + U(r)\Phi_\ell + \frac{\ell(1+\ell)}{2mr^2} \Phi_\ell - E_0 \Phi_\ell = \frac{2\ell+1}{2} r \varphi_0(r) \int_{-1}^{1} e^{-i(\kappa r)\xi} P_\ell(\xi) d\xi .$$

We also may note that

$$-\frac{\partial^2 r \varphi_0(r)}{2m \partial r^2} + r U(r) \varphi_0(r) - E_0 r \varphi_0(r) = 0 \tag{30}$$

$$4\pi \int_0^\infty \varphi_0^2(r) r^2 dr = 1 , \quad \int_0^\infty \Phi_0(r, \kappa) \varphi_0(r) r dr = 0 .$$

Note also that

$$\int_{-1}^{1} P_\ell(\xi) e^{ia\xi} d\xi = (i)^\ell j_\ell(a) \tag{31}$$

$$j_\ell(a) = \frac{a^\ell}{2^{\ell-1} \ell!} \left(1 + \frac{\partial^2}{\partial a^2}\right)^\ell \frac{\sin a}{a}$$

$$j_\ell(-a) = (-1)^\ell j_\ell(a) .$$

Hence in order to deal only with real-valued functions put

$$\Phi_\ell = (i)^\ell j_\ell (a). \tag{32}$$

Then the equation (29) takes the form:

$$-\frac{1}{2m}\frac{\partial^2 f_\ell(r,\kappa)}{\partial r^2} - \frac{\ell(1+\ell)}{2m r^2} f_\ell(r,\kappa) + U(r) f_\ell(r,\kappa) - E_0 f(r,\kappa) = \tag{29'}$$
$$= \frac{2\ell+1}{2} r \varphi_0(r) j_\ell(\kappa r).$$

Taking into account (28),(31),(32) we finally obtain:

$$\int \Psi_f^*(x)\Psi_f(x)dx = 4\pi\int_0^\infty \Phi_0^2(r,\kappa)dr + 2\pi\sum_{\ell=1}^\infty \frac{2\ell+1}{2}\int_0^\infty f_\ell^2(r,\kappa)dr \tag{33}$$

$$\int \Psi_f(x) e^{ifx} dx = 4\pi\int_0^\infty \frac{\sin\kappa r}{\kappa}\Phi_0(r,\kappa)dr +$$
$$+ 2\pi\sum_{\ell=1}^\infty \frac{2\ell+1}{2}\int_0^\infty f_\ell(r,\kappa) j_\ell(\kappa r)\varphi_0(r) r\, dr .$$

In conclusion we wish to remark that the conditions of radial symmetry imposed here are not essential for the validity of our methods both in (I) and in (II) and were adopted in this paper only for the simplification of the final formulae.

Received by Publishing Department
on November 28, 1990.