

ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ
ДУБНА



K-66

24/II-75
E2 - 8540

655/2-75

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INVESTIGATION OF POLARON MODEL
BY FUNCTIONAL INTEGRATION METHOD

1975

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**INVESTIGATION OF POLARON MODEL
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Submitted to *TMO*

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A polaron model is of great interest for physicists during many recent years. First it is due to its simplicity as an example of interaction of a particle with a quantized field and, second, it is obviously interesting problem from the viewpoint of modelling of physical processes. Just with this model being concerned N. Bogolubov has formulated his canonical transformations^{/1/}, which have made it possible to construct a consistent scheme of subsequent approximations with exact account of the conservation laws. Because of growing hopes for this model as applied to strong interactions this model became very popular recently.^{/2/} A special attention has been paid to properties of invariance of a system relative to a definite group of transformations that is nontrivial in theories with strong coupling.

In the paper the polaron model is studied by integrating in the functional space. Note that an analogous problem was solved by R. Feynman^{/3/}. However, he did not take into account the momentum conservation law in his calculations and as a result the effective mass of polaron appeared to be written *brevi manu*.

In the present paper the effective mass is calculated by the Bogolubov canonical transformations and approximate continual

integration. The results thus obtained are slightly different from those of ref.^{/3/}.

1. First recall some results of paper^{/4/} devoted to study of the Green function of a system defined by the Hamiltonian

$$H = -\frac{1}{2M} \Delta_r + g \sum_{\mathbf{k}} (A_{\mathbf{k}} e^{i\vec{\mathbf{k}}\vec{\mathbf{z}}} b_{\mathbf{k}} + A_{\mathbf{k}}^* e^{-i\vec{\mathbf{k}}\vec{\mathbf{z}}} b_{\mathbf{k}}^{\dagger}) + \frac{1}{2} \sum_{\mathbf{k}} \omega_{\mathbf{k}} (b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + b_{\mathbf{k}} b_{\mathbf{k}}^{\dagger}). \quad (1.1)$$

Here $b_{\mathbf{k}}^{\dagger}, b_{\mathbf{k}}$ are the creation and annihilation operators of quanta of a scalar field with a wave vector $\vec{\mathbf{k}}$, and

$$[b_{\mathbf{k}}, b_{\mathbf{k}'}^{\dagger}] = \delta_{\mathbf{k}\mathbf{k}'}$$

and $A_{\mathbf{k}}$ are the Fourier components of the source density.

By using the Bogolubov canonical transformation^{/1/}

$$\begin{aligned} b_{\mathbf{k}} &\rightarrow Z_{\mathbf{k}} = e^{i\vec{\mathbf{k}}\vec{\mathbf{z}}} b_{\mathbf{k}}, \\ b_{\mathbf{k}}^{\dagger} &\rightarrow Z_{\mathbf{k}}^{\dagger} = e^{-i\vec{\mathbf{k}}\vec{\mathbf{z}}} b_{\mathbf{k}}^{\dagger}, \\ [Z_{\mathbf{k}}, Z_{\mathbf{k}'}^{\dagger}] &= \delta_{\mathbf{k}\mathbf{k}'}, \\ -i\vec{\nabla}_r &\rightarrow \vec{\mathcal{P}} - \sum_{\mathbf{k}} \vec{\mathbf{k}} Z_{\mathbf{k}}^{\dagger} Z_{\mathbf{k}}, \end{aligned} \quad (1.2)$$

it is possible to reduce the system Hamiltonian to the form

$$H = \frac{1}{2M} (\vec{\mathcal{P}} - \sum_{\mathbf{k}} \vec{\mathbf{k}} Z_{\mathbf{k}}^{\dagger} Z_{\mathbf{k}})^2 + \frac{1}{2} \sum_{\mathbf{k}} \omega_{\mathbf{k}} (Z_{\mathbf{k}}^{\dagger} Z_{\mathbf{k}} + Z_{\mathbf{k}} Z_{\mathbf{k}}^{\dagger}) + g \sum_{\mathbf{k}} (A_{\mathbf{k}} Z_{\mathbf{k}} + A_{\mathbf{k}}^* Z_{\mathbf{k}}^{\dagger}). \quad (1.3)$$

Here $\vec{\mathcal{P}}$ is the total momentum of the system:

$$\vec{\mathcal{P}} = -i\vec{\nabla}_r + \sum_{\mathbf{k}} \vec{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} \quad (1.4)$$

and due to the translational invariance $[\vec{S}, H]=0$ it may be considered to be c-number.

The Green function of the system given by the equation

$$(H - E)G = 1 \quad (1.5)$$

is represented as a continual integral. As its expectation value in ref. /4/ there has been found the expression:

$$\langle G \rangle = -i \int_0^{\tau} d\tau' e^{-i\tau'(\mathcal{E} - \vec{S}^2/2\mu - \omega)} \int \frac{\delta \vec{v}}{\text{const.}} e^{-i \int_0^{\tau'} \vec{v}^2(\tau) d\tau} \exp\left\{-g^2 \sum_{\kappa} |A_{\kappa}|^2 \int_0^{\tau} ds_1 \int_0^{s_1} ds_2 e^{i \int_{s_2}^{s_1} [\omega_{\kappa} - \vec{k}\vec{S}/\mu + \vec{k}\vec{v}(\tau)\sqrt{2/\mu}]}\right\} \quad (1.6)$$

where

$$\mathcal{E} = E - \frac{1}{2} \sum_{\kappa} \omega_{\kappa}.$$

From (1.6) it is seen that as $\tau \rightarrow \infty$ for the system energy $\mathcal{E}(\vec{S})$ one has the representation

$$e^{i\tau[\mathcal{E}(\vec{S}) - \vec{S}^2/2\mu]} = \int \frac{\delta \vec{v}}{\text{const.}} e^{-i \int_0^{\tau} \vec{v}^2(\tau) d\tau} \exp\left\{-g^2 \sum_{\kappa} |A_{\kappa}|^2 \int_0^{\tau} ds_1 \int_0^{s_1} ds_2 e^{i(\omega_{\kappa} - \vec{k}\vec{S}/\mu)(s_1 - s_2)} e^{i\sqrt{2/\mu} \vec{k} \int_{s_2}^{s_1} \vec{v}(\tau) d\tau}\right\} \quad (1.7)$$

To simplify our consideration we make a new change in eq. (1.7) in the following form

$$\begin{aligned} \tau &\rightarrow i\tau, \\ s_{1,2} &\rightarrow i s_{1,2}, \\ \vec{v}(i\tau) &\rightarrow i\vec{v}(\tau). \end{aligned} \quad (1.8)$$

As a result we obtain

$$e^{-\tau [G(\vec{S}) - \vec{S}^2/2\mu]} = \int_{\text{const}} \frac{d\vec{v}}{e} e^{-\int_0^{\vec{v}} \vec{v}^2(\gamma) d\gamma} \exp\left\{g^2 \sum_{\kappa} |A_{\kappa}|^2\right\} \quad (1.9)$$

$$\int_0^{\tau} \int_0^{S_1} \int_0^{S_2} dS_1 dS_2 e^{-(\omega_{\kappa} - \vec{k}\vec{S}/\mu)(S_1 - S_2) - i\sqrt{2/\mu} \vec{k} \int_0^{\vec{v}} \vec{v}(\gamma) d\gamma} \Big|_{\vec{v}} = \int \frac{d\vec{v}}{e} e^{g^2 L[\vec{v}]}$$

The integration variable \vec{v} in (1.9) represents, up to a factor, itself the velocity of motion along the Feynman trajectory. To obtain the velocity \vec{v}_0 appropriate to the classical trajectory it is necessary to solve the equation $\frac{\delta S[\vec{v}]}{\delta \vec{v}} = 0$.

Allowing for that in the case of polaron

$$\omega_{\kappa} = \omega, \quad g^2 \sum_{\kappa} |A_{\kappa}|^2 = \frac{\omega\sqrt{\omega} \alpha}{2\sqrt{2} \pi^2 \sqrt{\mu}} \int \frac{d\vec{k}}{R^2} \Theta(L - \kappa) \quad (1.10)$$

we obtain for the velocity \vec{v}_0

$$\vec{v}_0(\gamma) = -i \frac{\omega^{3/2} \alpha}{4\pi^2 \mu} \int_0^{\tau} dS_1 \int_0^{S_2} dS_2 e^{-\omega(S_1 - S_2)} \int \frac{d\vec{k}}{R^2} \vec{k} \Theta(L - \kappa) \cdot e^{\vec{k}\vec{S}(S_1 - S_2)/\mu - i\sqrt{2/\mu} \int_0^{\vec{v}} \vec{k} \vec{v}_0(\gamma') d\gamma'}$$
(1.11)

In formulas (1.10) and (1.11) we have introduced a cut-off on the upper limit of the modulus of the integration momentum \vec{k} in order to remove the divergences arising in (1.11) at coinciding S_1 and S_2 .

From (1.11) it follows that \vec{v}_0 can be represented in the form

$$\vec{v}_0 = -i \frac{\vec{S}}{\sqrt{2\mu}} f(\gamma) \quad (1.12)$$

As we are interested in the effective mass m^* so we are searching for $G(\vec{S})$ up to the terms \vec{S}^2 :

$$g(\vec{Q})|_{\vec{Q} \rightarrow 0} = \epsilon_0 + \frac{\vec{Q}^2}{2m} + \dots \quad (1.13)$$

Therefore it suffices for us to calculate $f_0(z) = f(z)|_{\vec{Q} \rightarrow 0}$. Substituting (1.12) into (1.11), taking the limit $\vec{Q} \rightarrow 0$ and integrating over \vec{k} we get:

$$f_0(z) = 2C \int_0^\tau ds_1 \int_0^z ds_2 e^{-\omega(s_1 - s_2)} \left[s_1 - s_2 - \int_{s_2}^{s_1} f_0(z) dz \right], \quad (1.14)$$

where

$$C = \frac{\omega^{3/2} \alpha L^3}{9\sqrt{2} \pi \rho^{3/2}} \quad (1.15)$$

Making change in (1.11) in the following way: $\vec{v} \rightarrow \vec{v} \cdot \vec{v}$.

we obtain

$$e^{-\tau[\epsilon(\vec{Q}) - \vec{Q}^2/2m]} = e^{\frac{\vec{Q}^2/2m \cdot \int_0^\tau f_0(z) dz}{\text{const.}} e^{-\int_0^\tau v^2 dz}} \cdot \exp \left\{ i \frac{\sqrt{2}}{\rho} \vec{Q} \int_0^\tau f_0(z) \vec{v}(z) dz + \frac{\omega^{3/2} \alpha}{4\sqrt{2} \pi^2 \rho} \int_0^\tau ds_1 ds_2 e^{-\omega|s_1 - s_2|} \int \frac{d\vec{k}}{k^2} \theta(L-k) e^{i\vec{k} \cdot \vec{Q} [s_1 - s_2 - \int_{s_2}^{s_1} f_0(z) dz]} / \rho - i \sqrt{2}/\rho \vec{k} \int_{s_2}^{s_1} \vec{v}(z) dz \right\}. \quad (1.16)$$

Changing the velocity integration by the Feynman path integration with the use of the variable substitution $\vec{v} \rightarrow \vec{x}$, where

$$\vec{x}(z) = \sqrt{2} \int_0^z \vec{v}(z) dz, \quad (1.17)$$

we rewrite (1.16) in the form

$$\begin{aligned}
 e^{-\tau[\mathcal{E}(\vec{Q}) - \vec{Q}^2/2\mu]} &= e^{\vec{Q}^2/2\mu} \int_0^{\tau} f_0^2(\nu) d\nu \int \frac{\delta \vec{x}}{\text{const.}} e^{-\frac{1}{2} \int_0^{\nu} \vec{x}^2(\nu) d\nu} \\
 \exp\left\{i \frac{\vec{Q}}{\sqrt{\mu}} \int_0^{\tau} f_0(\nu) \vec{x}(\nu) d\nu + \frac{\omega^{3/2} \alpha}{4\sqrt{2} \pi^2 \sqrt{\mu}} \int_0^{\tau} ds_1 ds_2 e^{-\omega|s_1 - s_2|} \right. \\
 &\quad \left. \int \frac{\delta \vec{x}}{R^2} e^{i \vec{K} \cdot \vec{Q} [s_1 - s_2 - \int_{s_2}^{s_1} f_0(\nu) d\nu]} / \mu \right. \\
 &\quad \left. \Theta(L - \kappa) e^{-i \vec{K} [\vec{x}(s_1) - \vec{x}(s_2)] / \sqrt{\mu}} \right\} \\
 &= e^{\vec{Q}^2/2\mu} \int_0^{\tau} f_0^2(\nu) d\nu \int \frac{\delta \vec{x}}{\text{const.}} e^{\mathcal{S}[\vec{x}]} \quad (1.18)
 \end{aligned}$$

2. In the previous section we have found the representation (1.18) which together with eq. (1.14) enables one to calculate the ground energy level \mathcal{E}_0 and polaron effective mass m .

Note that the action $\mathcal{S}[\vec{x}]$ is quadratical with respect to \vec{x} due to separating out of the motion along the classical trajectory. This makes it possible to approximate the action $\mathcal{S}[\vec{x}]$ by a new action $\mathcal{S}'[\vec{x}]$ extracted from \mathcal{S} by means of quadratical terms. Expanding \mathcal{S} over $\vec{x}(\nu)$ we thus obtain (in the limit $\vec{Q} \rightarrow 0$):

$$\mathcal{S}'[\vec{x}] = -\frac{1}{2} \int_0^{\tau} \vec{x}^2(\nu) d\nu - \frac{C}{2} \int_0^{\tau} ds_1 ds_2 e^{-\omega|s_1 - s_2|} [\vec{x}(s_1) - \vec{x}(s_2)]^2, \quad (2.1)$$

where C is determined by (1.15).

Now the relation (1.18) can be rewritten in the form

$$\begin{aligned}
 e^{-\tau[\mathcal{E}(\vec{Q}) - \vec{Q}^2/2\mu]} &= e^{\vec{Q}^2/2\mu} \int_0^{\tau} f_0^2(\nu) d\nu \int \frac{\delta \vec{x}}{\text{const.}} e^{\mathcal{S}'} e^{\mathcal{S} - \mathcal{S}'} \\
 &\approx e^{\vec{Q}^2/2\mu} \int_0^{\tau} f_0^2(\nu) d\nu \int \frac{\delta \vec{x}}{\text{const.}} e^{\mathcal{S}'} \cdot e^{\langle \mathcal{S} - \mathcal{S}' \rangle} \quad (2.2)
 \end{aligned}$$

where

$$\langle S - S' \rangle = \int \frac{\delta \vec{x}}{\text{const}} e^{S'} (S - S') / \int \frac{\delta \vec{x}}{\text{const}} e^{S'} \quad (2.3)$$

We stress that the functional averaging is transferred to exponent that makes it possible to calculate approximately the functional integral (1.18).

To calculate $\langle S - S' \rangle$ we make use of the results of ref.^[3]

$$\langle e^{-i \vec{k} [\vec{x}(s_1) - \vec{x}(s_2)] / \sqrt{\mu}} \rangle = e^{-\vec{k}^2 F(1s_1 - s_2) / 2\mu V^2}$$

$$\langle [\vec{x}(s_1) - \vec{x}(s_2)]^2 \rangle = \frac{3}{V^2} F(1s_1 - s_2); \quad (2.4)$$

$$V^2 = \omega^2 + \frac{4c^2}{\omega}, \quad \int \frac{\delta \vec{x}}{\text{const}} e^{S'} \approx e^{-3\tau(V-\omega)/2}$$

$$F(\epsilon) = \omega^2 \epsilon + \frac{V^2 - \omega^2}{V} (1 - e^{-V\epsilon})$$

Expanding $\langle S - S' \rangle$ over \vec{S} we obtain, with the use of (2.4) in the limit of large τ :

$$\langle S - S' \rangle \approx \tau \left[\frac{3c}{V\omega} + \frac{\omega^{3/2} \times V}{\sqrt{\pi}} \int_0^\infty d\epsilon e^{-\omega\epsilon} F^{-1/2}(\epsilon) \right] + \frac{3^2}{2\mu} \frac{\omega^{3/2} \times V^3}{6\sqrt{\pi}} \int_0^\infty d s_1 d s_2 e^{-\omega|s_1 - s_2|} \left[|s_1 - s_2 - \int_{s_2}^{s_1} f_0(x/\mu) dx \right]^2 F^{-3/2}(|s_1 - s_2|) \quad (2.5)$$

As a result we have the following formulas for energy and effect^{2/} mass $m \vec{x}$:

$$G_0 = \frac{3}{4} \frac{(V-\omega)^2}{V} - \frac{\omega^{3/2} \times V}{\sqrt{\pi}} \int_0^\infty d\epsilon e^{-\omega\epsilon} F^{-1/2}(\epsilon) \quad (2.6)$$

^{2/} Formula (2.6) has been derived in paper^[3].

$$\frac{M}{m} = 1 - \frac{1}{\tau} \int_0^{\tau} f_0^2(z) dz - \frac{\omega^{3/2} \alpha V^2}{6 \sqrt{\pi}} \frac{1}{\tau} \int_0^{\tau} ds_1 ds_2 e^{-\omega |s_1 - s_2|}$$

$$[s_1 - s_2 - \int_{s_1}^{s_2} f_0(z) dz]^2 F^{-3/2}(|s_1 - s_2|). \quad (2.7)$$

Note that in (2.7) the limit $\tau \rightarrow \infty$ should be taken. When doing so, only large arguments of the function $f_0(z)$ will be important.

Let us calculate the function $f_0(z)$ for $\tau \rightarrow \infty$ and large z by eq. (1.14). As one can easily see, in this limit the main contribution comes from the region $s_1 \sim s_2 \sim z$. Then we have

$$f_0(z) \approx 2C [1 - f_0(z)] \int_z^{\tau} ds_1 \int_0^z ds_2 e^{-\omega(s_1 - s_2)} \quad (s_1 - s_2) \rightarrow$$

$$\rightarrow [1 - f_0(z)] \frac{4C}{\omega^3} \quad (2.8)$$

whence

$$f_0(z) = \frac{1}{1 + \omega^3/4C} = 1 - \frac{\omega^2}{V^2} \quad (2.9)$$

Substituting (2.9) into (2.7) and taking the limit $\tau \rightarrow \infty$ we arrive finally at the expression

$$\frac{M}{m} = \frac{\omega^2(2V^2 - \omega^2)}{V^4} - \frac{\omega^{11/2} \alpha}{3\sqrt{\pi} V} \int_0^{\infty} d\epsilon \epsilon^2 e^{-\omega \epsilon} F^{-3/2}(\epsilon). \quad (2.10)$$

The parameter V is obtained by minimizing \mathcal{E}_0 . At large coupling constants α the parameter V is large^{3/2}:

$$V = \frac{4\alpha^2}{9\pi} \omega. \quad (2.11)$$

In this case $F(\epsilon) = V$ and (2.10) reduces to the following expression

$$\frac{m}{m_0} = \frac{2\omega^2}{V^2} - \frac{2\alpha}{3\sqrt{\pi}} \left(\frac{\omega}{V}\right)^{5/2} \quad (2.12)$$

After substituting (2.11) into (2.12) we have

$$\frac{m}{m_0} = \frac{16}{81\pi^2} \alpha^4 = 202 (\alpha/10)^4, \quad (2.13)$$

i.e., the expression from ref. ^{13/}

It is interesting to note that if one considers the parameter C in eq. (1.14) to be different from C in the approximating functional S' and denotes it as C' then formula (2.10) is modified in the following way:

$$\frac{m}{m_0} = 1 - \frac{1}{(1 + \omega^2/4C')^2} - \frac{\omega^{3/2} \alpha^{1/2} V^2}{3\sqrt{\pi} (1 + 4C'/\omega^2)^2} \int_0^\infty dC' C'^2 e^{-\omega C'} F^{-3/2}(C'), \quad (2.14)$$

which after substitution of (2.11) gives the expression

$$\frac{m}{m_0} = 1 - \frac{1}{(1 + \omega^2/4C')^2} - \frac{16\alpha^4}{81\pi^2} \frac{1}{(1 + 4C'/\omega^2)^2} \quad (2.15)$$

It is easy to be convinced of that the minimal value of the effective mass is achieved at the following

$$C' = \omega^2 \frac{8}{81\pi^2} \alpha^4 \quad (2.16)$$

and equals

$$\frac{m}{m_0} = \frac{64\alpha^4}{243\pi^2} = 269 (\alpha/10)^4 \quad (2.17)$$

Here we would like to note that the result of ref. ^{13/} is between the values (2.17) and (2.13)

$$\frac{m}{m_0} = 232 (\alpha/10)^4 \quad (2.18)$$

To complete the paper we stress that the above developed scheme for calculation of the polaron effective mass is based on the momentum conservation law that gives it strictness and consistency.

The authors are sincerely grateful to N.N.Bogolubov, R.N.Faustov, V.A.Matveev, A.N.Sissakian and A.N.Tavkhelidze for interest in the work and useful comments.

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Received by Publishing Department
on January 17, 1975.