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POLARON GROUND STATE ENERGY IN THE STRONG COUPLING LIMIT

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1 Introduction

The polaron problem describing an interaction between the electron and the phonon field is valuable as a nontrivial model in quantum field theory, and therefore, it has been studied by many investigators [1-14]. Among the methods applied to the subject there is Feynman's path integral approach [1] based on a certain choice of a trial action in the polaron partition function. In the strong coupling regime, a variational method [2] applied to this problem gives an upper bound of the polaron self-energy. But a variational approach does not allow one to know how close is the obtained estimation to the true energy and does not give a recipe how to calculate the next contributions. The second order corrections to Feynman's variational estimation of the polaron self-energy has been calculated in [3] and the obtained result was not close enough to the exact solution found numerically [4,5].

In this paper, we present an improved estimation for the optical polaron ground state energy at large coupling constant α , using the general method of representation of functional integrals in the strong coupling regime [6]. It is shown that the leading term reproduces Feynman's variational solution. We introduce a diagrammatic representation to calculate the next corrections to the leading term of polaron self-energy. This way,we have obtained explicitly corrections due to strong connected graphs. We have also found the next contribution to energy from some more complicated graphs to be a relatively small. Our estimation of polaron ground state energy in the strong coupling limit is in good agreement with the frequently quoted exact solution [4,5].

2 Ground State Energy of the Polaron

The ground state energy $E(\alpha)$ of the Frölich polarons is defined by the expression

$$E(\alpha) = -\lim_{\beta\to\infty}\frac{1}{\beta}\ln Z_\beta(\alpha)\,, \tag{2.1}$$

$$Z_\beta(\alpha) = N_o\int\limits_{\mathbf{r}(0)=\mathbf{r}(\beta)}\delta\mathbf{r}\,\exp\left\{-\frac{1}{2}\int\limits_0^\beta ds\,\dot{\mathbf{r}}^2(s) + \frac{\alpha}{\sqrt{8}}\iint\limits_0^\beta dt\,ds\,\frac{\exp\{-|s-t|\}}{|\mathbf{r}(t)-\mathbf{r}(s)|}\right\}. \tag{2.2}$$

Our aim is to get the behaviour of the function $E(\alpha)$ for $\alpha\to\infty$. We apply the method described in the previous paper [6] to the functional integral (2.2). The integral can be written in the form

$$Z_T(\alpha) = N_o \int\limits_{\mathbf{r}(-T)=\mathbf{r}(T)} \delta\mathbf{r}\, \exp\left\{ -\frac{1}{2} \iint\limits_{-T}^{T} dt\, ds\, \mathbf{r}(t)\, D_o^{-1}(t,s)\, \mathbf{r}(s) + \alpha\, U[\mathbf{r}] \right\}, \tag{2.3}$$

where

$$T = \frac{\beta}{2}, \qquad D_o^{-1}(t,s) = -\frac{\partial^2}{\partial t^2}\delta(t-s),$$

and

$$\alpha\, U[\mathbf{r}] = \frac{\alpha}{\sqrt{8}} \iint\limits_{-T}^{T} dt\, ds\, e^{-|t-s|} \int \frac{d\mathbf{k}}{2\pi^2\, \mathbf{k}^2} e^{i\mathbf{k}(\mathbf{r}(t)-\mathbf{r}(s))}, \tag{2.4}$$

$$E(\alpha) = -\lim_{T\to\infty} \frac{1}{2T} \ln Z_T(\alpha). \tag{2.5}$$

The Green function $D_o(t,s)$ satisfying the periodic boundary conditions is

$$D_o(t,s) = -\frac{1}{2}|t-s| - \frac{t\,s}{T} \quad \xrightarrow[T\to\infty]{} \quad D_o(t-s) = -\frac{1}{2}|t-s|,$$

$$\tilde{D}_o(k) = \int\limits_{-\infty}^{+\infty} dx\, e^{ikx}\, D_o(x) = \frac{1}{2}\left[\frac{1}{(k+i0)^2} + \frac{1}{(k-i0)^2}\right]. \tag{2.6}$$

We want to find the limit in (2.5). Therefore we shall consider that $T = \beta/2$ is asymptotically large. In this limit the Green functions are translationally invariant, i.e.

$$D_o(t,s) = D_o(t-s), \qquad D(t,s) = D(t-s).$$

The interaction function $\bar{U}[\mathbf{b}]$ in equation (2.15) in [6] can be written

$$\bar{U}[\mathbf{b}] = \frac{1}{\sqrt{8}} \iint\limits_{-T}^{T} dt\, ds\, e^{-|t-s|} \int \frac{d\mathbf{k}}{2\pi^2\, \mathbf{k}^2} \exp\left\{ i\mathbf{k}\,(\mathbf{b}(t) - \mathbf{b}(s)) - \mathbf{k}^2 F(t-s) \right\}, \tag{2.7}$$

where

$$F(t-s) \equiv D(0) - D(t-s).$$

Now let us consider equations (2.16) in [6]. We choose $\mathbf{b}(s) = 0$ as a solution of the first equation because this seems to be natural as it follows from the explicit form of the integral (2.2). Then, we obtain

$$\Sigma_{ij}(t-s) = \delta_{ij}\cdot\Sigma(t-s) = \frac{\delta^2\, \bar{U}\,[\mathbf{b}]}{\delta\, b_i(t)\, \delta\, b_j(s)}\Big]_{b=0} =$$

$$= \frac{\delta_{ij}}{6\sqrt{2\pi}} \left[\delta(t-s) \int\limits_{-\infty}^{\infty} \frac{dx\, e^{-|x|}}{F^{3/2}(x)} - \frac{e^{-|t-s|}}{F^{3/2}(t-s)} \right], \tag{2.8}$$

and

$$\tilde{\Sigma}(k) = \int\limits_{-\infty}^{\infty} ds\, e^{iks}\cdot\Sigma(s) = \frac{1}{3\sqrt{2\pi}} \int\limits_{0}^{\infty} dt\, e^{-t}\cdot\frac{1-\cos(kt)}{F^{3/2}(t)}. \tag{2.9}$$

The second constraint equation in (2.16) in [6] has the following form :

$$\tilde{D}(k) = \tilde{D}_o(k) - \tilde{D}_o(k)\,\alpha\,\tilde{\Sigma}(k)\,\tilde{D}(k),$$

and

$$\tilde{D}(k) = \frac{1}{\tilde{D}_o^{-1}(k) + \alpha\,\tilde{\Sigma}(k)}. \tag{2.10}$$

Finally, we obtain for the function $F(s)$ the following equation :

$$F(s) = \int\limits_{0}^{\infty} \frac{dk}{\pi}\cdot\frac{1-\cos(ks)}{k^2 + \alpha\,\tilde{\Sigma}(k)}, \tag{2.11}$$

where $\tilde{\Sigma}(k)$ is defined in (2.9).

The energy $E_o(\alpha)$ which is defined by W_o in the representation (2.18) in the paper [6] becomes

$$E_o(\alpha) = -\frac{3}{2\pi}\int\limits_{0}^{\infty} dk\left[\ln\left(k^2\,\tilde{D}(k)\right) - k^2\,\tilde{D}(k) + 1\right] - \frac{\alpha}{\sqrt{2\pi}}\int\limits_{0}^{\infty}\frac{dt\,\exp(-t)}{\sqrt{F(t)}}. \tag{2.12}$$

The representation for the polaron functional integral looks as ($T = \beta/2$ is asymptotically large)

$$Z_T(\alpha) = e^{-2T\,E_o(\alpha)}\, J_T(\alpha), \tag{2.13}$$

$$J_T(\alpha) = N \int\limits_{\mathbf{r}(-T)=\mathbf{r}(T)} \delta\mathbf{r}\,\exp\left\{ -\frac{1}{2}\iint\limits_{-T}^{T} dt\, ds\, \mathbf{r}(t)\, D^{-1}(t-s)\,\mathbf{r}(s) + \alpha\,\bar{U}_2[\mathbf{r}] \right\}, \tag{2.14}$$

where

$$\bar{U}_2[\mathbf{r}] = \frac{1}{\sqrt{8}} \iint\limits_{-T}^{T} dt\, ds\, e^{-|t-s|} \int \frac{d\mathbf{k}}{2\pi^2\,\mathbf{k}^2} e^{-\mathbf{k}^2 F(t-s)}$$

$$:e^{i\mathbf{k}(\mathbf{r}(t)-\mathbf{r}(s))} - 1 + \frac{\mathbf{k}^2}{6}[\mathbf{r}(t) - \mathbf{r}(s)]^2 : . \tag{2.15}$$

The functions $D(t)$ and $F(t)$ are defined by equations (2.7) and (2.11). It should be stressed that the representation (2.15) is completely equivalent to the initial representation (2.2) for asymptotically large $T \to \infty$.

3 The Strong Coupling Limit

In the section, we obtain the representation for the ground state energy of an optical polaron at asymptotically large α. Let us consider the functional integral (2.14). In formulas (2.14) and (2.15) we introduce new variables

$$\mathbf{k} \equiv \sqrt{\mu}\,\mathbf{p}, \qquad t \equiv \frac{u}{\mu}, \qquad s \equiv \frac{v}{\mu}, \qquad \mathbf{r}(t) \equiv \frac{\mathbf{r_o}(u)}{\sqrt{\mu}} \tag{3.1}$$

where μ is a parameter depending on α. Then all our formulas become

$$\begin{aligned} J_\Lambda(\alpha) = \; & N \int \delta\mathbf{r_o} \exp\Bigg\{ -\frac{1}{2} \iint\limits_{-\Lambda/2}^{\Lambda/2} du\,dv\, \mathbf{r_o}(u) \frac{1}{\mu^3} D^{-1}\left(\frac{u-v}{\mu}\right) \mathbf{r_o}(v) \\ & + \frac{\alpha}{\sqrt{8}} \iint\limits_{-\Lambda/2}^{\Lambda/2} du\,dv\, \frac{\exp(-|u-v|/\mu)}{\mu^{3/2}} \int \frac{d\mathbf{p}}{2\pi^2\,\mathbf{p}^2} \exp\left\{-\mathbf{p}^2 \mu F\left(\frac{u-v}{\mu}\right)\right\} \\ & : \exp\{i\mathbf{p}(\mathbf{r_o}(u) - \mathbf{r_o}(v))\} - 1 + \frac{\mathbf{p}^2}{6} [\mathbf{r_o}(u) - \mathbf{r_o}(v)]^2 : \Bigg\}. \end{aligned} \tag{3.2}$$

where $\Lambda \equiv 2T\mu$. Now let us consider equation (2.11) where we introduce

$$\mu F\left(\frac{u}{\mu}\right) = \mu^2 \int\limits_0^\infty \frac{dp}{\pi} \cdot \frac{1-\cos(pu)}{\mu^2 p^2 + \alpha\,\tilde{\Sigma}(\mu p)},$$

$$\tilde{\Sigma}(\mu p) = \frac{1}{3\sqrt{2\pi}} \int\limits_0^\infty dt\, e^{-t} F^{-3/2}(t)\,(1 - \cos(\mu p t)). \tag{3.3}$$

Our basic assumption to be justified is that the parameter μ increases as $\alpha \to \infty$.

One can see that equations (3.3) have the limit as $\mu \to \infty$ if

$$F(t) = \frac{1}{\mu} \Phi(\mu t). \tag{3.4}$$

Then, we have

$$\begin{aligned} \Phi(u) &= \int\limits_0^\infty \frac{dp}{\pi} \cdot \frac{1-\cos(pu)}{p^2 + (\alpha/\mu^2)\,\tilde{\Sigma}(\mu p)}, \\ \tilde{\Sigma}(\mu p) &= \frac{\mu^{3/2}}{3\sqrt{2\pi}} \int\limits_0^\infty dt\, e^{-t} \Phi^{-3/2}(\mu t)\,(1 - \cos(\mu p t)), \\ & \underset{\mu\to\infty}{\longrightarrow} \frac{\mu^{3/2}}{3\sqrt{2\pi}\,\Phi^{3/2}(\infty)}, \end{aligned} \tag{3.5}$$

and so

$$\Phi(u) = \int\limits_0^\infty \frac{dp}{\pi} \cdot \frac{1-\cos(pu)}{p^2+1} = \frac{1}{2}(1 - e^{-|u|}), \tag{3.6}$$

where the parameter μ is chosen in such way that

$$\frac{\alpha}{\mu^2} \frac{\mu^{3/2}}{3\sqrt{2\pi}} \frac{1}{\Phi^{3/2}(\infty)} = 1.$$

Formula (3.6) leads to $\Phi(\infty) = 1/2$ and

$$\mu = \frac{4\,\alpha^2}{9\pi}. \tag{3.7}$$

Thus, we get

$$\begin{aligned} F(t) &= \frac{1}{2\mu}(1 - \exp(-\mu|t|)), \qquad D(t) = \frac{1}{2\mu}\exp(-\mu|t|), \\ D^{-1}(t-s) &= \left(-\frac{\partial^2}{\partial t^2} + \mu^2\right)\delta(t-s). \end{aligned} \tag{3.8}$$

Let us introduce a new operator

$$\mathcal{D}^{-1}(u-v) \equiv \frac{1}{\mu^3} D^{-1}\left(\frac{u-v}{\mu}\right) = \left(-\frac{\partial^2}{\partial u^2} + 1\right)\delta(u-v).$$

Substituting these formulas into (3.2) we obtain

$$I_\Lambda(\mu) = \int d\sigma \exp\{U_\mu[\mathbf{r_o}]\} \equiv \langle \exp U_\mu[\mathbf{r_o}] \rangle \tag{3.9}$$

where we introduce a Gaussian measure

$$d\sigma = N\,\delta\mathbf{r_o} \exp\left\{-\frac{1}{2}\int\limits_{-\Lambda/2}^{\Lambda/2} du\,[\dot{\mathbf{r}}_\mathbf{o}^2(u) + \mathbf{r_o}^2(u)]\right\}, \tag{3.10}$$

$$\int d\sigma\, 1 = 1.$$

and an interaction function

$$\begin{aligned} U_\mu[\mathbf{r_o}] = \; & \frac{3}{2}\sqrt{\frac{\pi}{2}} \iint\limits_{-\Lambda/2}^{\Lambda/2} du\,dv\, G_\mu(u-v) \int \frac{d\mathbf{p}}{2\pi^2\,\mathbf{p}^2} \exp\left\{-\frac{\mathbf{p}^2}{2} + \mathbf{p}^2\mathcal{D}(u-v)\right\} \\ & : e^{i\mathbf{p}(\mathbf{r_o}(u) - \mathbf{r_o}(v))} - 1 + \frac{\mathbf{p}^2}{6}[\mathbf{r_o}(u) - \mathbf{r_o}(v)]^2 : \end{aligned} \tag{3.11}$$

Here, we introduce the notation

$$G_\mu(x) \equiv \frac{\exp\{-|x|/\mu\}}{2\mu} = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \cdot \frac{\exp(-ikx)}{1+\mu^2 k^2},$$

$$\mathcal{D}(x) \equiv \frac{\exp\{-|x|\}}{2} = \int_{-\infty}^{\infty} \frac{dq}{2\pi} \cdot \frac{\exp(-iqx)}{1+q^2}, \tag{3.12}$$

obeying the equation

$$\int_{-\infty}^{\infty} dt\, \mathcal{D}^{-1}(x-t)\,\mathcal{D}(t-y) = \delta(x-y). \tag{3.13}$$

Let us consider the ground state energy of the optical polaron defined by formula (2.1) in the form

$$E(\alpha) = E_o(\alpha) - \mu\cdot\varepsilon(\mu) \tag{3.14}$$

where

$$\varepsilon(\mu) = \lim_{\Lambda\to\infty} \frac{1}{\Lambda} \ln I_\Lambda(\mu). \tag{3.15}$$

For asymptotically large $\alpha \to \infty$, substituting (3.8) into (2.12) we get

$$E_o(\alpha) = -\frac{\alpha^2}{3\pi} + O(1) \tag{3.16}$$

It is known [1,5] that in the strong coupling limit

$$\lim_{\mu\to\infty} \varepsilon(\mu) = \varepsilon$$

where ε is a constant.

Using the definition (3.7) we finally obtain

$$E(\alpha) = -\frac{\alpha^2}{3\pi}\left(1+\frac{4}{3}\varepsilon\right) + O(1). \tag{3.17}$$

Calculating $I_\Lambda(\mu)$ in (3.15) as $\alpha\to\infty$ we find the desired parameter ε. We stress here that μ enters only into the function $G_\mu(x)$.

4 High Order Corrections to $E_o(\alpha)$

The parameter ε is expected commonly [1,3-5] to be small. Expanding the exponential in (3.15) we get a perturbation series in the general term

$$\ll U_\mu^n \gg = \prod_{i=1}^{n} \int \frac{dk_i}{1+\mu^2 k_i^2} R(k_1,\ldots,k_n), \tag{4.1}$$

where $\ll \ldots \gg$ denotes only the connected part proportional to Λ due to the logarithm in (3.15) and

$$R(k_1,\ldots,k_n) = \left(\frac{3}{\sqrt{32\pi^3}}\right)^n \prod_{i=1}^{n} \iint_{-\Lambda/2}^{\Lambda/2} du_i dv_i \exp[-ik_i(u_i-v_i)] \int \frac{d\mathbf{p}_i}{\mathbf{p}_i^2} e^{-\mathbf{p}_i^2/2}\, S\cdot Q, \tag{4.2}$$

$$S \equiv \prod_{j=1}^{n} \exp\{\mathbf{p}_j^2 \mathcal{D}(u_j - v_j)\} = 1 + \ldots,$$

$$Q \equiv \prod_{l<m}^{n} \exp\{-\mathbf{p}_l\mathbf{p}_m [\mathcal{D}(u_l-u_m) + \mathcal{D}(v_l-v_m) - \mathcal{D}(u_l-v_m) - \mathcal{D}(u_m-v_l)]\}.$$

In (4.2) we have used the definitions

$$<\mathbf{r}_{oi}(u)\,\mathbf{r}_{oj}(v)> = \delta^{ij}\mathcal{D}(u-v),$$

$$<:\exp[i\mathbf{p}\mathbf{r}_o(u)]::\exp[i\mathbf{q}\mathbf{r}_o(v)]:> = \exp\{-\mathbf{p}\mathbf{q}\mathcal{D}(u-v)\}. \tag{4.3}$$

First, we will factorize out these terms of R which give finite nonvanishing contributions to (4.1) as $\mu\to\infty$. One can see in (4.1) that these terms must have the next form

$$R_{finite}(k_1,\ldots,k_n) \sim \Lambda\,\delta(k_1)\ldots\delta(k_n). \tag{4.4}$$

Expanding S in a power series in $\mathcal{D}(u_j - v_j)$ and taking into account (3.12) one finds that only the term

$$S_{finite} = 1 \tag{4.5}$$

obeys the requirement (4.4). It is a more complicated task to pick out parts in Q contributing to (4.4) and we will do this later using diagrammatic representations for (4.1).

Using a symmetry $u \leftrightarrow v$ in U_μ and taking into account (4.5) we rewrite (3.11)

$$U_\mu[\mathbf{r}_o] = V[\mathbf{r}_o] + W[\mathbf{r}_o], \tag{4.6}$$

where

$$\begin{aligned} V[\mathbf{r}_o] &\equiv \frac{3}{2}\sqrt{\frac{\pi}{2}} \iint_{-\Lambda/2}^{\Lambda/2} du\,dv\, G_\mu(u-v) \int d\mathcal{P}\,[2 : e^{i\mathbf{p}\mathbf{r}_o(u)} - 1 + \frac{\mathbf{p}^2}{6}\mathbf{r}_o{}^2(u) :] \\ &= 3\sqrt{\frac{\pi}{2}} \int_{-\Lambda/2}^{\Lambda/2} du \int d\mathcal{P} \sum_{n\geq 2} \frac{(-1)^n}{(2n)!} : (\mathbf{p}\mathbf{r}_o(u))^{2n} : \\ &= \sum_{n\geq 2} a_n \int_{-\Lambda/2}^{\Lambda/2} du\, V_{2n}(u), \end{aligned} \tag{4.7}$$

and

$$W[\mathbf{r_o}] = \frac{3}{2}\sqrt{\frac{\pi}{2}} \iint\limits_{-\Lambda/2}^{\Lambda/2} du\, dv\, G_\mu(u-v) \int d\mathcal{P} \; :(e^{i\mathbf{p}\mathbf{r_o}(u)}-1)(e^{i\mathbf{p}\mathbf{r_o}(v)}-1) - \mathbf{p}\mathbf{r_o}(u)\cdot\mathbf{p}\mathbf{r_o}(v):$$

$$= \frac{3}{2}\sqrt{\frac{\pi}{2}} \iint\limits_{-\Lambda/2}^{\Lambda/2} du\, dv\, G_\mu(u-v) \int d\mathcal{P} \sum_{l\geq 2}\sum_{m\geq 1} \frac{(-1)^{(l-m)/2}}{l!\,m!} : (\mathbf{p}\mathbf{r_o}(u))^l(\mathbf{p}\mathbf{r_o}(v))^m : \quad (4.8)$$

$$= \sum_{l\geq 2}\sum_{m\geq 1} b_{lm} \iint\limits_{-\Lambda/2}^{\Lambda/2} du\, dv\, W_{lm}(u,v)\,.$$

In (4.6)-(4.8) we have used the notation

$$d\mathcal{P} \equiv \frac{d\mathbf{p}}{2\pi^2\,\mathbf{p}^2}\exp\Big\{-\mathbf{p}^2/2\Big\}. \quad (4.9)$$

Substituting (4.7) and (4.8) into (3.9) and expanding the exponential we obtain for the parameter ε a sum of products of the functions V and W averaged with the Gaussian measure defined in (3.10). To each term in the sum here we can associate a series of diagrams built by the following rules:

- *A graph consists of two or more vertices $V_{2n}(u)$ and $W_{lm}(u,v)$.*
- *Each one-point vertex $V_{2n}(u)$ emits $2n$ numbers of $\mathbf{r_o}$ lines ,where $n \geq 2$.*
- *Each two-point vertex $W_{lm}(u,v)$ has l and m $\mathbf{r_o}$ lines entering into points u and v. The points are connected by a wavy line $G_\mu(u-v)$ defined in (3.12). We stress that the dependence $\tilde{G}_\mu(p) = (1+\mu^2p^2)^{-1}$ plays an important role in further considerations. Here $l \geq 2$, $m \geq 1$ and $l+m = 2N_o \geq 4$.*
- *All the $\mathbf{r_o}$ lines of a vertex in a graph must be connected with $\mathbf{r_o}$ lines of other vertices by the solid lines $\mathcal{D}(u,v)$. A line from a given vertex can not be coupled with another from the same vertex due to normal ordering in (4.7) and (4.8).*
- *Only connected graphs arise there according to (3.15).*

Following these rules we get graphs shown in Figs.1b-1e . In the case $\mu \to \infty$, according to (4.1) and (4.4), a finite contribution to ε is given only by the "tree" graphs shown in Fig.1d, connected "weakly" relative to wavy G_μ lines. These diagrams, which cannot be separated into a pair of disconnected subgraphs by cutting one G_μ line (Fig.1c), give a vanishing contribution proportional to $O(1/\mu)$. So we deal only with "tree" graphs in the strong coupling regime.

The "tree" structure of graphs as $\mu \to \infty$ leads to a requirement: both l and m are even for each vertex W_{lm} in a graph. Indeed, let us consider the elementary fragment shown in Fig.1f with one external G_μ line. All the V vertices in the fragment have even

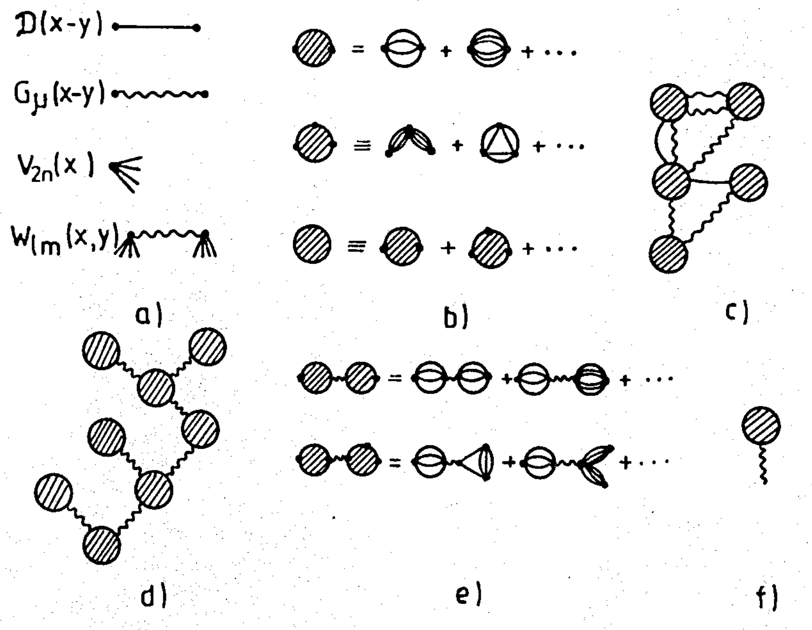

Figure 1: Diagrams giving high order corrections to $E_o(\alpha)$.

numbers of incoming lines and taking into account the circumstance that each internal $\mathcal{D}$ line ends at two vertices, we can conclude that the point with G_μ line must contain an even number of incoming $\mathbf{r_o}$ lines. This means that, for example, $m = even$ at the corresponding point of W_{lm} and thus $l = even$ immediately because of the condition $m + l = 2N_o$. Going to the "trunk" of our "tree" we see that each pair $\{l_i; m_i\}$ is even separately for all the vertices W_{l_i,m_i}.

Then, taking into account (4.7) and (4.8) we find that the sign of a "tree" graph shown in Fig.1e containing N vertices V and L vertices W is

$$sign \sim \prod_{i=1}^{N}\prod_{j=1}^{L}(-1)^{n_i+(l_j-m_j)/2}, \quad (4.10)$$

for fixed n_i, l_j and m_j. It is easy to see that the lowest simple diagrams giving an essential contribution to ε has the positive sign +1 because $n = 4$, $l = m = 2$ for them.

So the contribution of the given "tree" graph to ε can be represented as a sum of the fast-decreasing alternating series with a positive first term. The sum is positive. We have shown the positiveness of "tree" graphs.

5 Numerical Results

The first corrections to ε will be given by diagrams shown in Fig.1b. These are induced only by the interaction function $V[\mathbf{r_o}]$. Using this circumstance, we will show how one can exactly summarize these diagrams. Let us come back in $V[\mathbf{r_o}]$ to the ordinary operator product. After some transformations one can get

$$\ll e^V \gg = N_o \int \delta\mathbf{r_o} \exp\left\{ -\int_0^\Lambda dt \left[\frac{1}{2}\dot{\mathbf{r}}_o^2(t) - 3\sqrt{2}\int_0^1 ds \exp\{-s^2 \mathbf{r_o}^2(t)\} + \frac{9}{4} \right] \right\}. \tag{5.1}$$

It means that solving the Schrödinger equation

$$\left[-\frac{1}{2}\frac{d^2}{dx^2} + U(\mathrm{x}^2) \right] \cdot \Psi(\mathrm{x}) = -\varepsilon_2 \cdot \Psi(\mathrm{x}) \tag{5.2}$$

with a potential

$$U(\mathrm{x}^2) = -3\sqrt{2}\int_0^1 ds\, exp[-s^2 \cdot \mathrm{x}^2] + \frac{9}{4} \tag{5.3}$$

for the lowest eigenvalue, one can exactly find the parameter ε_2. Solving (5.2) numerically we have obtained

$$\varepsilon_2 = 0.015541(1) \tag{5.4}$$

or in other words, taking into account only the corrections caused by $V[\mathbf{r_o}]$ we get

$$E_2(\alpha) = -\frac{\alpha^2}{3\pi} \cdot 1.020721(1) = -\alpha^2 \cdot 0.108302(1)\,. \tag{5.5}$$

For the next correction to ε we have calculated the diagrams shown in Fig.1e. The first row of graphs gives

$$\varepsilon_3' \sim \frac{27\pi^{3/2}}{\sqrt{2}\Lambda} \int \cdots \int_{-\Lambda/2}^{\Lambda/2} dt\, ds\, dx\, dy\, G_\mu(x-y)$$

$$\cdot \prod_{i=1}^{3} \int \frac{d\mathbf{k}_i}{2\pi^2 \mathbf{k}_i^2} e^{-\mathbf{k}_i^2/2} \exp\{-\mathbf{k}_1\mathbf{k}_3 \mathcal{D}(x-t) - \mathbf{k}_2\mathbf{k}_3\mathcal{D}(y-s)\} \tag{5.6}$$

The second series of diagrams after summation gives the contribution

$$\varepsilon_3'' \sim \frac{81\pi^2}{8\Lambda} \int \cdots \int_{-\Lambda/2}^{\Lambda/2} dt\, ds\, dx\, dy\, dz\, G_\mu(t-s) \prod_{i=1}^{4} \int \frac{d\mathbf{k}_i}{2\pi^2 \mathbf{k}_i^2} e^{-\mathbf{k}_i^2/2}$$

$$\cdot \exp\{-\mathbf{k}_1\mathbf{k}_4\mathcal{D}(x-t) + \mathbf{k}_2\mathbf{k}_4\mathcal{D}(y-s) + \mathbf{k}_3\mathbf{k}_4\mathcal{D}(s-z) - \mathbf{k}_2\mathbf{k}_3\mathcal{D}(z-y)\} \tag{5.7}$$

Authors	Results
Feynman, Schultz	0.1061
Pekar	0.1088
Miyake (exact)	0.108513
Luttinger, Lu	0.1066
Marshall, Mills	0.1078
Sheng, Dow	0.1065
Smondyrev (lower bound)	0.109206
Adamowski, Gerlach	0.1085128
Feranchuk, Komarov	0.1078
Efimov, Ganbold	0.1080
Ours	0.10843

Table 1: Comparison of some results for the polaron ground state energy at large coupling (the coefficient of α^2).

In (5.6) and (5.7) we wrote only the leading first terms corresponding to main exponentials in the functions $V[\mathbf{r_o}]$ and $W[\mathbf{r_o}]$ in (4.7) and (4.8), respectively. Taking into account the necessary remaining terms and omitting details of calculations we present the final numerical result

$$\varepsilon_3 = \varepsilon_3' + \varepsilon_3'' = 0.0012(1) \tag{5.8}$$

Adding it to $E_2(\alpha)$ we finally get

$$E_3(\alpha) \leq -\frac{\alpha^2}{3\pi} 1.0219(1) = -\alpha^2 \cdot 0.10843(1)\,. \tag{5.9}$$

We propose that higher-order corrections can produce a small contribution to (5.9). Our result in (5.9) is in good agreement with the exact solution obtained by Miyake [4] and later confirmed in [5]. The relative error in energy is less than 0.07 per cent. The comparison of some results obtained by quoted authors [1-14] is shown in Table 1.

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Энергия основного состояния полярона в пределе сильной связи

Получена улучшенная оценка для энергии основного состояния полярона в области большой константы взаимодействия. Используется предложенный нами ранее метод представления функциональных интегралов в режиме сильной связи. Главный член в нашем представлении воспроизводит вариационную оценку Фейнмана. Построена диаграммная техника для учета следующих поправок к энергии. Этим путем явно получены поправки, обусловленные сильносвязными графами. Получено хорошее согласие с известными точными численными расчетами энергии полярона.

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Polaron Ground State Energy in the Strong Coupling Limit

Using the general method developed earlier for the representation of functional integrals in the strong coupling limit, we obtain an improved estimation for the polaron ground state energy at large coupling constant. It is shown, that the leading term reproduces the Feynman's variational estimation. A diagrammatic representation is suggested for the next corrections to the polaron self-energy. This way, we have obtained explicitly corrections due to the strong connected graphs. Our results are in good agreement with the often quoted exact numerical solution.

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

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