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1/N-EXPANSION FOR THE FROHLICH POLARON

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1. Introduction

An electron in an ionic crystal generates in its neighborhood a domain of a local deformation of a medium, thus creating a quasiparticle, a polaron. Among the whole number of polaron models a simple but rather nontrivial model described by the Fröhlich Hamiltonian is well known. May be, it is the unique model of a particle interacting with a quantized field which allows both the expansion in a standard series of perturbation theory and the strong coupling expansion in inverse powers of the coupling constant. It is why the Fröhlich polaron model has been used readily by theorists exercising in the development of various schemes of approximate calculations. On the other hand, the interest in this model is stimulated by the physical reasons. Up to now the theory of the Fröhlich polaron can be considered as a well developed field of solid state physics. The investigations have been done extensively for various quantities characterizing a one-polaron system: self-energy and effective mass, mobility, optical absorption coefficient and so on. The list of papers on the subject is huge and we refer the reader to recent review articles [1,2].

However, much less attention has been paid to studying many-polaron systems which are rather important. In particular, the problem of a two-polaron bound state (bipolaron) attracted attention recently, which was caused by attempts of explaining the high-temperature superconductivity. According to the proposed bipolaronic mechanism of superconductivity, the bipolarons of a high enough density undergo the Bose-Einstein condensation, which results in a superconductivity state [3].

To study the polaron properties, and especially its bound states, one needs a good scheme of approximate calculations which would allow one to compute the polaron characteristics with a high accuracy. While investigating the Fröhlich polaron the path integral method has been widely used. In terms of path integrals a representation can be obtained for the partition function Z_{int}, which contains all the effects of electron-phonon interaction. For an optical Fröhlich polaron at rest in an N-dimensional space, Z_{int} can be written in the form

$$Z_{int} = \int\limits_{x(0)=x(\beta)} \frac{\mathcal{D}x}{\text{const}} e^{S}, \quad S = -\frac{1}{2}\int_0^\beta ds\,\dot{x}^2(s) + \frac{\alpha}{2\sqrt{2}}\iint_0^\beta \frac{ds_1\, ds_2}{|x(s_1)-x(s_2)|} G_{12},$$

$$G_{ij} = \frac{\mathrm{ch}(\beta/2-|s_i-s_j|)}{\mathrm{sh}(\beta/2)}. \qquad (1.1)$$

Here α is the coupling constant of electron-phonon interaction, $\beta=\omega/k\theta$, θ is the temperature of the system, and ω is the LO-phonon frequency. The normalization constant in the path integral (1.1) is determined by the condition $Z_{int}(\alpha=0) = 1$. In the limit of zero temperatures ($\beta \Rightarrow \infty$) we have $Z_{int} \approx \exp[-\beta E(\alpha)]$, where $E(\alpha)$ is the energy of the polaron ground-state. For calculating it, a number of methods have been developed among which a very popular is the Feynman variational method [4]) that gives an upper bound $E_F(\alpha)$ on $E(\alpha)$ valid throughout the whole range of variation of the coupling constant $\alpha \geq 0$. The method is based on the Jensen inequality and the known quadratic approximate action

$$S_F = -\frac{1}{2}\int_0^\beta ds\,\dot{x}^2(s) - \frac{C}{2}\iint_0^\beta ds_1\, ds_2\, e^{-W|s_1-s_2|}\,[x(s_1)-x(s_2)]^2, \qquad (1.2)$$

where C and W are variational parameters. An essential development of the Feynman method has been proposed by Saitoh [5]): he has changed the function $C\exp(-W|s_1-s_2|)$ in the approximating action (1.2) to an arbitrary function $p(|s_1-s_2|)$ over which variation is carried out. Thus, the Saitoh method gives the best upper bound that can be obtained with the quadratic action. To illustrate this, one may compare the Saitoh results with those obtained in the scope of the straight-

-forward generalization of the Feynman method when

$$p(|s_1-s_2|) = \sum_{i=1}^{n} C_i \exp(-W_i|s_1-s_2|).$$

The calculations have been performed at $n=2$ in ref. 6 and at $n=3$ in ref. 7.

Both the Feynman and Saitoh (all the more so) methods failed to provide an analytic approximate expression for the polaron energy. However, it is possible to construct the weak- and the strong coupling expansions of the form:

$$E(\alpha) = \sum_{n\geq 1} E_n \alpha^n, \qquad (1.3a)$$

$$E(\alpha) = \sum_{n\geq 1} A_n \alpha^{2-n}, \quad A_{2k+1} = 0. \qquad (1.3b)$$

The numerical values of the first few expansion coefficients in (1.3) for the Feynman and Saitoh approximations will be reported later. Now we stress that estimates obtained by Feynman and Saitoh methods are rather close to each other and work well enough in the whole range of the values of the coupling constant α. For example, the value of the leading term of strong coupling expansion (1.3b) (which is the same for both the approximations) differs from the exact value only by 2.2%. The weak coupling expansions exactly reproduces the first coefficient E_1, but the next coefficient E_2 noticeably differs from the exact one (more than by 20%). As is well known, physically significant values of α (say from 3 to 10) correspond to the intermediate coupling regime. To reproduce the polaron characteristics in that regime with more adequacy, one should construct a scheme of subsequent approximations which will work in the whole range of the coupling constant values and will allow one to calculate corrections to the leading term.

In our paper [8]) we have considered weak coupling expansions for a multidimensional polaron and have suggested a connection between the Saitoh estimates and expansions in inverse powers of the number N of the space dimensions. We adduced arguments in favor of that the Saitoh result coincides with the leading term of the $1/N$-expansion. At present our conjecture is confirmed. In 1987 we reported the first results on the $1/N$-expansions for the Fröhlich polaron[9]. Here we construct a regular self-consistent scheme which allows us to obtain the $1/N$-expansion from the path integrals and to calculate corrections to the leading term. Besides we answer the question why the Feynman and Saitoh variational methods work rather well, the latter turns out to be asymptotically exact in the limit of large N.

The paper is organized as follows. In Sec.2 we derive the general formulae for the $1/N$-expansion. Then we investigate the leading term in Sec.3 and the first correction to it in Sec.4. In Sec.5 the results obtained are used for the approximate calculation of the coefficients of weak- and strong coupling expansions. Appendices contain details of calculations.

2. General approach to the 1/N-expansion

Proceeding from eq. (1.1) for Z_{int} with the redefined coupling constant

$$\alpha = 2\sqrt{2}\, N^{3/2} a, \tag{2.1}$$

we obtain the following expansion for the polaron energy:

$$E^{(N)}(\alpha) = N\,\varepsilon_0(a) + \varepsilon_1(a) + O(1/N)\ , \tag{2.2}$$

where index N denotes the number of the space dimensions. This redefinition is not an innovation: we used a similar transformation in ref. 10 while constructing the $1/N$-expansion for an anharmonic oscillator, which allowed us to reproduce both the perturbation theory and the strong coupling limit.

Next, we make use of the Feynman representation[11] for a continual δ-function:

$$\mathcal{F}\,[\,|x(s_1)-x(s_2)|^2] = \int\mathcal{D}\sigma\int\left(\frac{\mathcal{D}p}{2\pi}\right)\,\mathcal{F}\,[\sigma]\,\exp\left\{i\int\!\!\int_0^\beta ds_1\,ds_2\;p(s_1,s_2)\right.$$
$$\left.[\sigma(s_1,s_2)-|x(s_1)-x(s_2)|^2]\right\}\ , \tag{2.3}$$

where $\mathcal{F}$ is a functional, and unlike the standard formulae, the path integration here is performed over functions of two variables $p(s_1,s_2)$ and $\sigma(s_1,s_2)$. If we apply relations (2.3) to (1.1), the integral over the vector function $x(s)$ will turn into an N-th power of a similar integral over one of its components $x(s)$. As a result, we get the representation

$$Z_{int} = \int\mathcal{D}\sigma\int\left(\frac{\mathcal{D}p}{2\pi}\right)\,e^{S'},\quad S' = i\int\!\!\int_0^\beta ds_1\,ds_2\;p\sigma + aN^{3/2}\int\!\!\int_0^\beta ds_1\,ds_2\;G_{12}/\sqrt{\sigma} +$$
$$N\ln\left\{\int_{x(0)=x(\beta)}\frac{\mathcal{D}x}{\mathrm{const}}\exp\left[-\frac{1}{2}\int_0^\beta ds\,\dot{x}^2(s) - i\int\!\!\int_0^\beta ds_1\,ds_2\,p(s_1,s_2)[x(s_1)-x(s_2)]^2\right]\right\}, \tag{2.4}$$

where G_{12} is defined by eq. (1.1). Changing the variables of path integration

$$(\sigma,\ p) \Rightarrow (y,\ z)\ ,$$

$$\sigma = N\,\Sigma + i\sqrt{N}\,\Sigma\,y\ ,\qquad p = -i\,P - iz/(\sqrt{N}\,\Sigma)\ , \tag{2.5}$$

where functions $\Sigma(s_1,s_2)$ and $P(s_1,s_2)$ are defined by the equations for a stationary point $\delta S'/\delta\sigma = \delta S'/\delta p = 0$, we arrive at the system of equations:

$$P(s_1,s_2) = \frac{a}{2\Sigma^{3/2}(s_1,s_2)}\,G_{12}\ ,\quad \Sigma(s_1,s_2) = \langle[x(s_1)-x(s_2)]^2\rangle\ . \tag{2.6}$$

Here use was made of the notation for the averaging of a functional over a one-dimensional Gaussian action:

$$\langle\mathcal{F}\rangle = \int_{x(0)=x(\beta)}\frac{\mathcal{D}x}{\mathrm{const}}\mathcal{F}[x]\exp\left\{-\frac{1}{2}\int_0^\beta ds\,\dot{x}^2(s) - \int\!\!\int_0^\beta ds_1\,ds_2\,P(s_1,s_2)[x(s_1)-x(s_2)]^2\right\}. \tag{2.7}$$

with such a normalization that averaging of a constant does not change its value (for instance, $\langle 1\rangle = 1$). Inserting (2.5) into (2.4) and using notation (2.7), we arrive at the representation

$$Z_{int} = \exp(NS_0)\int\mathcal{D}y\int\left(\frac{\mathcal{D}z}{2\pi}\right)\exp\tilde{S}\ . \tag{2.8}$$

The factorized term that gives a contribution leading in $1/N$, does not depend on the integration variables $y(s_1,s_2)$ and $z(s_1,s_2)$:

$$S_0 = \iint_0^{\beta} ds_1\, ds_2\; P\Sigma + \alpha \iint_0^{\beta} ds_1\, ds_2\; G_{12}/\sqrt{\Sigma} + \ln I\,, \qquad (2.9)$$

$$I = \int_{x(0)=x(\beta)} \frac{\mathcal{D}x}{\text{const}} \exp\left\{ -\frac{1}{2}\int_0^{\beta} ds\; \dot{x}^2(s) - \iint_0^{\beta} ds_1\, ds_2 P(s_1,s_2)[x(s_1)-x(s_2)]^2 \right\}.$$

The normalization constant for I is determined from the condition $I_{|P=0} = 1$. Recall that functions $P(s_1,s_2)$ and $\Sigma(s_1,s_2)$ are solutions to eq. (2.6).

All the corrections to the leading term of the $1/N$-expansion enter into the action $\tilde{S}$:

$$\tilde{S} = i \iint_0^{\beta} ds_1\, ds_2\; zy - \frac{\alpha}{2} \iint_0^{\beta} ds_1\, ds_2\; y^2 A[y]\; G_{12}/\sqrt{\Sigma} +$$

$$+ N \ln \left\langle \exp\left\{ -\frac{1}{\sqrt{N}} \iint_0^{\beta} ds_1\, ds_2\; z\, B_{12}[x]/\Sigma \right\} \right\rangle , \qquad (2.10)$$

where

$$A[y] = \frac{2+Y}{Y(1+Y)^2}\,, \qquad Y = \left(1 + i\frac{y}{\sqrt{N}}\right)^{1/2},$$

$$B_{12}[x] = [x(s_1)-x(s_2)]^2 - \langle [x(s_1)-x(s_2)]^2 \rangle . \qquad (2.11)$$

Subscripts in the functional $B_{12}[x]$ denote the dependence on arguments s_1 and s_2. Since $A[y] = 3/4 + O(1/\sqrt{N})$ and $\langle B_{12} \rangle = 0$ by definition (2.11), then the first nonvanishing term of the $1/N$-expansion of $\tilde{S}$ will be of an order of $O(N^0)$. Neglecting higher-order terms, from eq. (2.10) we obtain the representation in which the Gaussian quadrature over the function $y(s_1,s_2)$ can be calculated. As a result, we have

$$Z_{int} = \exp(NS_0)\int(\mathcal{D}z/\sqrt{\pi})\exp S_1\,, \quad S_1 = -\iint_0^{\beta} ds_1\, ds_2\, z^2(s_1,s_2) +$$

$$+ \frac{3\alpha}{8} \iiiint_0^{\beta} ds_1\, ds_2\, ds_3\, ds_4\, [z]_{12} [z]_{34} (\Sigma_{23}+\Sigma_{14}-\Sigma_{13}-\Sigma_{24})^2, \qquad (2.12)$$

where

$$\Sigma_{ij} = \Sigma(s_i,s_j), \qquad [z]_{ij} = z(s_i,s_j)\; \Sigma_{ij}^{-3/4}\; G_{ij}^{1/2} . \qquad (2.13)$$

Formula (2.12) is derived straightforwardly; note only that there use has been made of the relationship:

$$\langle B_{12} B_{34} \rangle = \langle [x(s_1)-x(s_2)]^2\, [x(s_3)-x(s_4)]^2 \rangle - \qquad (2.14)$$

$$- \langle [x(s_1)-x(s_2)]^2 \rangle \langle [x(s_3)-x(s_4)]^2 \rangle = \frac{1}{2}(\Sigma_{23} + \Sigma_{14} - \Sigma_{13} - \Sigma_{24})^2,$$

which follows from the definition (2.7). The obtained formulae (2.9) and (2.12) allow us to compute the first two terms of the $1/N$- expansion (2.2) for the ground-state energy of the Fröhlich polaron.

3. The leading term of 1/N-expansion

From eq. (2.6) it follows that the functions $P(s_1,s_2)$ and $\Sigma(s_1,s_2)$ depend on the difference of their arguments:

$$P = P(|s_1 - s_2|), \qquad \Sigma = \Sigma(|s_1 - s_2|) .$$

The Gaussian path integral in eq. (2.9) is computed by the following method [12,5]. The integration variable $x(s)$ and function P are expanded in Fourier series in the interval $[0,\beta]$:

$$P(|s_1 - s_2|) = \sum_n p_n \exp[i2\pi n(s_1 - s_2)/\beta], \quad p_n^* = p_{-n} = p_n\,,$$

$$x(s) = \sum_n x_n \exp(i2\pi ns/\beta)\,, \qquad x_n^* = x_{-n} \qquad (3.1)$$

and then the path integration reduces to the conventional multiple integration over independent variables **Re** x_n $(n \geq 0)$ and **Im** x_n $(n > 0)$. Introducing the notation

$$\Xi_n = \beta^3 (p_0 - p_n)/(\pi n)^2\,, \qquad (3.2)$$

we then obtain from (2.9)

$$I = \prod_{n>0} \frac{1}{1+\Xi_n}\,, \quad S_0 = -\sum_{n>0} \ln(1+\Xi_n) + 3\sum_{n>0} \Xi_n/(1+\Xi_n) . \qquad (3.3)$$

Equations (2.6) acquire the form

$$\Sigma(\xi) = \frac{\beta}{\pi^2}\sum_{n>0} \frac{1-\cos(2\pi n\xi/\beta)}{n^2\,(1+\Xi_n)}\,,$$

$$\Xi_n = \frac{\alpha\beta^2}{2\pi^2 n^2}\int_0^\beta d\xi \, \frac{1-\cos(2\pi n\xi/\beta)}{\Sigma^{3/2}(\xi)} \frac{\mathrm{ch}(\beta/2-\xi)}{\mathrm{sh}(\beta/2)}. \tag{3.4}$$

Equations (3.3,4) are similar to the equations derived by Saitoh [5], and may be used for estimating the free energy of a polaron at finite temperatures. In the limit of zero temperatures they may be simplified if we change summation over n to integration over $x = 2\pi n/\beta$, for instance,

$$\ln I = -\sum_{n>0} \ln(1+\Xi_n) = -\sum_{n>0} \ln\left[1+ \frac{\beta^2}{\pi^2 n^2}\int_0^\beta d\xi \, P(\xi) \, (1-\cos \frac{2\pi n\xi}{\beta})\right] \Rightarrow$$

$$\Rightarrow -\frac{\beta}{2\pi}\int_0^\infty dx \, \ln\left[1 + \frac{4}{x^2}\int_0^\infty d\sigma \, P(\sigma) \, (1 - \cos x\sigma)\right] .$$

Remembering that $S_0 \approx -\beta\varepsilon_0(\alpha)$ when $\beta \Rightarrow \infty$, we obtain instead of (2.9) and (3.3) the following expression

$$\varepsilon_0(\alpha) = -\int_0^\infty d\xi \, P(\xi) \, \Sigma(\xi) - 2\alpha \int_0^\infty \frac{d\xi}{\sqrt{\Sigma(\xi)}} e^{-\xi} +$$

$$+ \frac{1}{2\pi}\int_0^\infty dx \, \ln\left[1 + \frac{4}{x^2}\int_0^\infty d\sigma \, P(\sigma) \, (1-\cos x\sigma)\right] . \tag{3.5}$$

Then from the equation for the stationary point $\delta\varepsilon_0/\delta P = \delta\varepsilon_0/\delta\Sigma = 0$ we get, instead of (2.6), the following relations

$$P(\xi) = \alpha \, \Sigma^{-3/2}(\xi) \, e^{-\xi} ,$$

$$\Sigma(\xi) = \frac{2}{\pi}\int_0^\infty dx \, \frac{1 - \cos x\xi}{x^2 + 4 \int_0^\infty d\sigma \, P(\sigma) \, (1-\cos x\sigma)} . \tag{3.6}$$

Using them, from (3.5) we get the equations

$$\varepsilon_0(\alpha) = -\alpha \int_0^\beta \frac{d\xi}{\sqrt{\Sigma(\xi)}} e^{-\xi}(3-2\xi), \quad d\varepsilon_0(\alpha)/d\alpha = -\alpha \int_0^\beta \frac{d\xi}{\sqrt{\Sigma(\xi)}} e^{-\xi} , \tag{3.7a}$$

$$\Sigma(\xi) = \frac{2}{\pi}\int_0^\infty dx \, \frac{1 - \cos x\xi}{x^2 + 4\alpha \int_0^\infty d\sigma \, e^{-\sigma} \, \Sigma^{-3/2}(\sigma) \, (1-\cos x\sigma)} , \tag{3.7b}$$

whose solution provides the leading term $\varepsilon_0(\alpha)$ of the $1/N$-expansion. It is clear that eq. (3.7) may be solved only numerically, and therefore we will consider the limits of weak and strong coupling. Calculations are described in Appendix A, and we here present only the results. In the case of weak coupling we have:

$$\varepsilon_0(\alpha) = \sum_{n\geq 1}\alpha^n \tilde{E}_n , \qquad \tilde{E}_1 = -2\sqrt{\pi} ,$$

$$\tilde{E}_2 = -\pi + 8/3 , \qquad \tilde{E}_3 = \sqrt{\pi}\,(-\frac{5\pi}{3} + \frac{544}{15} - 18\sqrt{3}). \tag{3.8}$$

In the strong coupling regime we obtain the expansion:

$$\varepsilon_0(\alpha) = -4\alpha^2 - (\ln 2 + 1/4) + \mathcal{O}(1/\alpha^2) . \tag{3.9}$$

4. The first correction

Now let us turn to the expression

$$Z_1 = \int (\mathcal{D}z/\sqrt{\pi}) \exp S_1 , \tag{4.1}$$

where S_1 is defined by eq. (2.12). The first correction to the leading term may be found as follows:

$$\varepsilon_1(\alpha) = \lim_{\beta\Rightarrow\infty} (-\frac{1}{\beta} \ln Z_1) . \tag{4.2}$$

The scheme of calculations is obvious in the weak coupling regime. While expanding the integrated expression in eq. (4.1) in powers of the second term of the action (2.12), the path integral is calculated easily. Then one should use the expansion of $\Sigma(\xi)$ in powers of α (see Appendix A). The result in the first two orders is as follows:

$$\varepsilon_1(\alpha) = -(3\sqrt{\pi}/2)\alpha - (88/5-21\pi/4)\alpha^2 + \mathcal{O}(\alpha^3) . \tag{4.3}$$

The calculations are more complicated in the strong coupling regime, and here we limit ourselves to the first correction to the leading term of the order of α^2. It follows from the formula (A.6,8) of Appendix A that at large α the function Σ has the form:

$$\Sigma(s_1,s_2) = [1 - \exp(-16\alpha^2|s_1 - s_2|)]/16\alpha^2. \qquad (4.4)$$

Substituting (4.4) into (2.12) and performing the scaling $s_i \Rightarrow s_i/16\alpha^2$, $z \Rightarrow 16\alpha^2 z$, we get the action S_1 in a simplified form

$$\tilde{S}_1 = -\iint_0^b ds_1\, ds_2\, z^2(s_1,s_2) + \frac{3}{16b}\iiiint_0^b ds_1\, ds_2\, ds_3\, ds_4\, z(s_1,s_2) z(s_3,s_4)(e_{23}+e_{14}-e_{13}-e_{24})^2,$$

$$e_{ij} = \exp(-|s_i - s_j|)\ ,\ b = 16\alpha^2\beta. \qquad (4.5)$$

The calculations, described in Appendix B, give the result:

$$\varepsilon_1(\alpha) = -\ \alpha^2\ (19-4\sqrt{10}) + O(\alpha^0). \qquad (4.6)$$

5. The 1/N-expansion as a source of approximations

Expansion (2.2) gives the origin to various approximations. Since the series in powers of $1/N$ is truncated, the polaron energy $E(\alpha)$ cannot be determined exactly. So certain approximations can be made, differing from each other in terms of higher order in $1/N$. We will proceed as follows. The expression

$$E^{(m)}(\alpha) = \frac{m}{N} E^{(N)}\left[\alpha N \frac{\Gamma(N/2)\Gamma(m/2-1/2)}{\Gamma(m/2)\Gamma(N/2-1/2)}\right] \qquad (5.1)$$

becomes an identity if we put $m=N$ (the index denotes the number of space dimensions). We shall first expand the r.h.s. of eq.(5.1) in a series in powers of $1/N$, and then we shall set $m=N$, thus obtaining an approximate expression for the energy of an N-dimensional polaron. The argument of the function $E^{(N)}$ in (5.1) is chosen so that already in the leading approximation in $1/N$, the first coefficient of the weak coupling expansion will be reproduced exactly. This coefficient has the form

$$E_1 = -\frac{\sqrt{\pi}\ \Gamma(m/2-1/2)}{2\ \Gamma(m/2)}. \qquad (5.2)$$

Using (2.2) we get from (5.1):

$$E^{(m)}(\alpha) = m\ \varepsilon_0(\alpha) + \frac{m}{N}\ \varepsilon_1(\alpha) + O(1/N^2). \qquad (5.3)$$

Here we should take into account also the modification of eq.(2.1) owing to the scaling of the argument of the function $E^{(N)}(\alpha)$:

$$\alpha = \frac{\alpha}{2\sqrt{2}\ N^{3/2}}\frac{N}{m}\frac{\Gamma(N/2)}{\Gamma(N/2-1/2)}\ \frac{\Gamma(m/2-1/2)}{\Gamma(m/2)} =$$

$$= \alpha_0(1 - 3/4N - 7/32N^2 + \ldots), \qquad (5.4)$$

where

$$\alpha_0 = \alpha\ \frac{\Gamma(m/2-1/2)}{4m\ \Gamma(m/2)}. \qquad (5.5)$$

Inserting (5.4) into (5.3) we finally get

$$E^{(N)}(\alpha) = N\ \varepsilon_0(\alpha_0) + [\varepsilon_1(\alpha_0) - \frac{3}{4}\ \alpha_0\varepsilon_0'(\alpha_0)] + O(1/N), \qquad (5.6)$$

where we take $m = N$.

Using the formulae (3.8,9) and (4.3,6) we may write the first coefficients of the weak coupling expansion:

$$E_1 = -\frac{\sqrt{\pi}\ \Gamma(N/2-1/2)}{2\ \Gamma(N/2)}, \qquad (5.7)$$

$$E_2 = -\left(\frac{\Gamma(N/2-1/2)}{4N\ \Gamma(N/2)}\right)^2 [N(\pi-8/3) + (108/5 - 27\pi/4) + O(1/N)],$$

$$E_3 = -\left(\frac{\Gamma(N/2-1/2)}{4N\ \Gamma(N/2)}\right)^3 [N\ \sqrt{\pi}\ (5\pi/3 - 544/15 + 18\sqrt{3}) + O(N^0)]\ .$$

The coefficient E_1 is determined exactly as we should like it to be. In the strong coupling limit for the first coefficients of the expansion (1.3b) we get:

$$A_0 = -\left(\frac{\Gamma(N/2-1/2)}{4N\ \Gamma(N/2)}\right)^2 [4N + (13-4\sqrt{10}) + O(1/N)]\ .$$

$$A_2 = -\ N\ (\ln 2 + 1/4) + O(N^0) \qquad (5.8)$$

It follows from eqs. (5.7,8) that in the leading approximation the polaron energy depends on N so that the scaling law (5.1) is valid at arbitrary m and N. In the Feynman approximation that fact has been noticed at first by Devreese et

Table 1

First coefficients of the weak- and strong coupling expansions for the polaron ground-state energy

	Feynman method	1/N-expansion: leading term	+ correction	Exact result
		$N = 3$ (bulk polaron)		
$-E_1$	1	1	1	1
$-E_2$	$\frac{1}{81} =$ 1.2346 10^{-2}	$\frac{1}{12}-\frac{2}{9\pi} =$ 1.2598 10^{-2}	$-\frac{5}{48}+\frac{17}{45\pi} =$ 1.608373 10^{-2}	$\ln(1+\frac{3\sqrt{2}}{4}) - \frac{\sqrt{2}}{2} =$ 1.59196 10^{-2}
$-E_3$	$8(7\sqrt{7}-18)/3^8 =$ 634366 10^{-3}	$\frac{5}{216}-\frac{68}{135\pi}+\frac{\sqrt{3}}{4\pi} =$ .6465 10^{-3}	?	.806070048 10^{-3}
$-A_0$	$\frac{1}{3\pi} =$ .06103	$\frac{1}{3\pi}$	$\frac{25-4\sqrt{10}}{36\pi} =$ .109206	.108513
$-A_2$	$3\ln 2+\frac{3}{4} =$ 2.829	$3\ln 2+\frac{3}{4}$	?	2.836
		$N = 2$ (surface polaron)		
$-E_1$	$\pi/2 =$ 1.5708	$\pi/2$	$\pi/2$	$\pi/2$
$-E_2$	$\frac{\pi^2}{216} =$ .045693	$\pi(\frac{\pi}{32}-\frac{1}{12}) =$ .046626	$\frac{\pi}{32}(\frac{122}{15}-\frac{19\pi}{8}) =$ .065978	.063973966
$-E_3$	$\frac{\pi^3(7\sqrt{7}-18)}{2904} =$ .555485 10^{-2}	$\frac{\pi^2}{32}(\frac{5\pi}{24}-\frac{68}{15}+\frac{9\sqrt{3}}{4}) =$ .563784 10^{-2}	?	.0074
$-A_0$	$\frac{\pi}{8} =$ .3927	$\frac{\pi}{8}$	$\frac{\pi(21-4\sqrt{10})}{64} =$ .4099	.4047
$-A_2$	$2\ln 2 + .5 =$ 1.886294	$2\ln 2 + .5$	?	?

al.[13]. It is clear now that this is not accidental but is connected with the exact expression for the coefficient E_1 .

Numerical results obtained with the help of eqs. (5.7,8) are presented in Table 1. A few comments are needed. In the first column there are presented results obtained by the Feynman method. Note that coefficients of the weak- and strong coupling expansions for the Feynman polaron were found in our paper [14] up to the E_{12} and A_{10}. The coefficient E_2 for the bulk polaron coincides in the leading order (2-nd column) with the Saitoh result which reproduces, in its turn, the value obtained many years ago by Haga [15] who has used completely different approach. In the same approximation the coefficient A_0 for the bulk polaron coincides with the well-known result by Feynman (and Saitoh).

In the last column there are presented few known exact results. For the bulk polaron the exact analytical expression for E_2 has been obtained by Röseler [16], and the value of E_3 has been computed in our paper [17] (see also ref. 14). Coefficients A_0 and A_2 were calculated by Miyake [18]. For the surface polaron coefficients E_2 and A_0 were calculated in refs. 19, 20 and E_3 - in ref. 21.

Comparing the approximate results with the exact ones we notice that the correction of order $O(N^0)$ substantially improves the approximations. Indeed, for the bulk polaron the values of the coefficients E_2 and A_0 , given in the 3-rd column, differ from the exact ones only by 1% and 0.6% , respectively. Naturally, the more is the value of N, the better are our approximations. Note also that the first correction leads to lower estimates, whereas the leading term of the $1/N$-expansion provides an upper bound.

6. Conclusion

A couple of conclusion remarks are to the point. We established the connection of the $1/N$-expansion with the variational methods for the particular model of the optical Fröhlich polaron. It can also be shown that an analogous connection between these methods exists in quantum mechanics when the ground-state energy is computed for a particle in a potential field [22]. Besides, it is natural to expect that there is a certain relation between the $1/N$-expansion and the diagrammatic technique which allows us to construct standard perturbation theory. That technique for a polaron was developed in our paper [17]. It can be shown that the leading term of the $1/N$-expansion is associated with a planar approximation when electron propagators are expanded in powers of products of momenta of different phonons.

Note also that the $1/N$-expansion is applicable for estimating the energy of a bound state of two or more polarons. Earlier [23] we evaluated the ground state energy of a bipolaron and its effective mass within the Feynman method. In the same manner we estimated the energy of a bound state of n polarons in a recent paper [24]. Application of the $1/N$-expansion can essentially improve those estimates. This makes possible a more detailed investigation of the polaron contribution to a mechanism of HTSC.

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Appendix A

At small values of α the function $\Sigma(\xi)$ is of the form:

$$\Sigma(\xi) = \Sigma_0(\xi) + \alpha\,\Sigma_1(\xi) + \alpha^2\,\Sigma_2(\xi) + \dots , \qquad (A.1)$$

and the integral equation (3.7b) is rewritten as follows:

$$\Sigma(\xi)=\sum_{k\geq 0}(-\alpha)^k\int_0^\infty \prod_{m=1}^{k}[ds_m e^{-s_m}\,\Sigma^{-3/2}(s_m)]\,f_{k+1}(\xi,s_1,\dots,s_k). \qquad (A.2)$$

We introduce the notation:

$$f_k(s_1,\dots,s_k) = \frac{2^{2k-1}}{\pi}\int_0^\infty \frac{dx}{x^{2k}}\prod_{m=1}^{k}(1-\cos xs_k) , \qquad (A.3)$$

from which it follows that

$$f_1(s) = s,$$

$$f_2(s_1,s_2) = \frac{2}{3}[-s_1^3 - s_2^3 + \frac{1}{2}(s_1+s_2)^3 + \frac{1}{2}|s_1-s_2|^3],$$

$$f_3(s_1,s_2,s_3) = \frac{2}{15}[s_1^5 + s_2^5 + s_3^5 - \frac{1}{2}(s_1+s_2)^5 - \frac{1}{2}|s_1-s_2|^5 -$$
$$- \frac{1}{2}(s_1+s_3)^5 - \frac{1}{2}|s_1-s_3|^5 - \frac{1}{2}(s_3+s_2)^5 - \frac{1}{2}|s_3-s_2|^5 + \frac{1}{4}(s_1+s_2+s_3)^5 +$$
$$+ \frac{1}{4}|s_1+s_2-s_3|^5 + \frac{1}{4}|s_1-s_2+s_3|^5 + \frac{1}{4}|-s_1+s_2+s_3|^5], \text{ etc.} \qquad (A.4)$$

Substituting (A.1) into (A.2), we find $\Sigma_k(\xi)$ and the weak coupling expansion of the coefficient $\varepsilon_0(\alpha)$ which is defined by eq. (3.7a):

$$\varepsilon_0(\alpha) = \sum_{n\geq 1}\alpha^n\,\check{E}_n ,$$

$$\check{E}_1 = -2\int_0^\infty ds\, e^{-s}\, f_1^{-1/2}(s) = -2\sqrt{\pi} ,$$

$$\check{E}_2 = -\frac{1}{2}\iint_0^\infty \prod_{m=1}^{2}[ds_m e^{-s_m}\, f_1^{-3/2}(s_m)]\, f_2(s_1,s_2) = -\pi + 8/3 ,$$

$$\check{E}_3 = \iiint_0^\infty \prod_{m=1}^{3}[ds_m e^{-s_m}\, f_1^{-3/2}(s_m)]\,[\frac{1}{3} f_3(s_1,s_2,s_3) -$$
$$- \frac{3}{4} f_2(s_1,s_2)f_2(s_1,s_3)/f_1(s_1)] = \sqrt{\pi}\,(-\frac{5\pi}{3} + \frac{544}{15} - 18\sqrt{3}). \qquad (A.5)$$

Let us consider now the strong coupling regime. The solution of the integral equation (3.7b) is suggested to be of the form:

$$\Sigma(\xi) = [\Phi(\xi)+\Psi(\alpha^2\xi)\exp(-\gamma\alpha^2\xi)]/\alpha^2, \qquad (A.6)$$

$$\Phi(\xi) = \Phi_0[1+\Phi_1(\xi)/\alpha^2+O(1/\alpha^4)], \quad \Psi(\xi) = \Psi_0[1+O(1/\alpha^2)].$$

Substituting (A.6) into eq.(3.7a) for $\varepsilon_0(\alpha)$, we get the coefficients of the strong coupling expansion:

$$\varepsilon_o(a) = \tilde{A}_0 a^2 + \tilde{A}_2 + O(1/a) \qquad \tilde{A}_0 = -1/\sqrt{\Phi_0}\,, \qquad (A.7)$$

$$\tilde{A}_2 = \sqrt{\Phi_0}\{\frac{1}{2}\int_0^\infty d\xi\; e^{-\xi}(3-2\xi)\Phi_1(\xi) - 3\int_0^\infty d\xi\; [(1+e^{-\gamma\xi}\;\Psi_0/\Phi_0)^{-1/2} - 1]\}.$$

Substitution of eq. (A.6) into eq. (3.7b) gives us:

$$\Phi_0 = \gamma^{-1} = -\Psi_0 = 1/16\,,$$
$$\Phi_1(\xi) = (\xi + 4\;ln2 - 1)/16\,. \qquad (A.8)$$

Then it follows from eqs. (A.7,8) that

$$\tilde{A}_0 = -4\,, \qquad \tilde{A}_2 = -\;ln2 - 1/4\,. \qquad (A.9)$$

Appendix B

To compute the path integral (4.1) with the action (4.5), we use the method of Sec. 3. Shifting the arguments in (4.5) $s_i \Rightarrow s_i + b/2$, we represent functions e_{ij} and $z(s_i, s_j)$ as Fourier series in the interval $[-b/2, b/2]$:

$$z(s_i, s_j) = \sum_{nm} z(n,m)\; \exp[i2\pi(ns_i + ms_j)/b], \qquad (B.1)$$

$$e_{ij} = \sum_n \sigma_n \exp[i2\pi n(s_i - s_j)/b],$$
$$\sigma_n = (b/2\pi^2)\;[n^2 + (b/2\pi)^2]^{-1}\,. \qquad (B.2)$$

The expression for σ_n is given here in the limit $b \Rightarrow \infty$. With eq.(B.2) taken into account, the combination of functions e_{ij} in eq. (4.5) can be written in the form:

$$(e_{23} + e_{14} - e_{13} - e_{24})^2 = \sum_{mnkl} Q_{mnkl}\; \exp[i2\pi(ms_1 + ns_2 + ks_3 + ls_4),$$

where a lot of components of Q_{mnkl} occurs to be equal to zero. Here we present only the obtained expression for the action $\tilde{S}_1$:

$$\tilde{S}_1 = \sum_{mn} z(n,m)z(-n,-m) + (3b/16) \sum_{mn} \sigma_n \sigma_{m-n}[z(0,m)z(-m,0) +$$

$$+ z(0,m)z(0,-m) + z(m,0)z(-m,0) + z(m,0)z(0,-m)] +$$

$$+ (3b/8) \sum_{mn} \sigma_n\sigma_m\; [z(n,m)z(-m,-n) + z(n,m)z(-n,-m)] -$$

$$- (3b/4) \sum_{mn} \sigma_n\sigma_m\; [z(n,m)z(-m-n,0) + z(n,m)z(0,-n-m)]. \qquad (B.3)$$

The path integral (4.1) is replaced by a multifold integral over independent quantities $z(n,m) = x(n,m) + iy(n,m)$. A functions $z(s_i, s_j)$ are real, the following relations take place:

$$x(n,m) = x(-n,-m)\,, \qquad y(n,m) = -\,y(-n,-m). \qquad (B.4)$$

It follows from (B.4) that independent are the quantities $x(0,0)$, $x(0,m)$ and $y(0,m)$ at $m>0$, $x(n,0)$ and $y(n,0)$ at $n>0$, $x(n,m)$ and $y(n,m)$ at $n>0$, $m \neq 0$. It is easy to rewrite the quadratic form (B.3) only as a function of independent variables, upon which integrations can be performed:

$$Z_1 = \exp\{-\sum_{\substack{m>0\\n>0}} ln(1 - \tfrac{3}{4}b\sigma_m\sigma_n) - \sum_{m>o} ln(1 - 2A_m) - \tfrac{1}{2}\sum_{m>o} ln(1 - \tfrac{3}{4}b\sigma_m^2) -$$

$$- \frac{1}{2}\; ln[1 - \frac{3}{2}\,b \sum_{m>o} \sigma_m^2 - \frac{9}{4}\,b^2 \sum_{m>o} \sigma_m^4/(1 - \frac{3}{4}\,b\;\sigma_m^2)]\}, \qquad (B.5)$$

where

$$A_m = \frac{3}{8}\,b \sum_{n>o} \sigma_n\sigma_{m+n} + \frac{3}{16}b \sum_{n>o}^{m-1} \sigma_n\sigma_{m-n}(1 + \tfrac{3}{4}b\sigma_n\sigma_{m-n})/(1 - \tfrac{3}{4}b\sigma_n\sigma_{m-n}). \qquad (B.6)$$

Note now that in the limit of zero temperatures $b \Rightarrow \infty$ summation is replaced by integration, with regard to eq. (B.2):

$$\sum_{m>o} F(\sigma_m) \Rightarrow (b/2\pi) \int_0^\infty dm\; F[2/b(m^2+1)].$$

It is easy to get, for instance,

$$\sum_{m,n\geq 0} \ln(1-\tfrac{3}{4}b\sigma_m\sigma_n) = (b/2\pi)^2 \int_0^\infty\int dm dn \ln[1-3/b(m^2+1)(n^2+1)] \Rightarrow$$

$$\Rightarrow -(3b/4\pi^2)\left[\int_0^\infty dm/(m^2+1)\right]^2 = -3b/16 . \quad (B.7)$$

Similar calculations give us

$$\sum_{m>0}\ln(1-2A_m) \Rightarrow (b/2\pi)\int_0^\infty dm \ln[1-3/2(m^2+4)] = b(\sqrt{10}/4-1). \quad (B.8)$$

Other two terms in eq. (B.5) for Z_1 are of an order of $\mathcal{O}(b^0)$ at large b and do not contribute to the polaron energy. It follows from eqs. (B.7,8) that

$$Z_1 \approx \exp[-b(4\sqrt{10}-19)/16]. \quad (B.9)$$

Taking into account the notation (4.5) and the definition (4.2), we arrive at the final result (4.6).

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