Perturbation theory for the one-dimensional optical polaron

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The one-dimensional optical polaron is treated on the basis of the perturbation theory in the weak coupling limit. A special matrix diagrammatic technique is developed. It is shown how to evaluate all terms of the perturbation theory for the ground-state energy of a polaron to any order by means of this technique. The ground-state energy is calculated up to the eighth order of the perturbation theory. The effective mass of an electron is obtained up to the sixth order of the perturbation theory. The radius of convergence of the obtained series is estimated.

I. INTRODUCTION

Nowadays there is a stable interest in low-dimensional structures. The one-dimensional polaron problem is relevant in semiconductor physics, where with state-of-the-art nano-lithography it has become possible to confine electrons in one direction (quantum wires) and in linear conjugated organic polymer conductors. The treatment of the polaron problem in quantum dots can be found in Ref.

Now there are a lot of theoretical works, where the polaron problem is investigated by means of the perturbation theory (PT). The series of the perturbation theory is useful for verifying the approximate nonperturbative methods in the weak-coupling limit. The PT for the N-dimensional polaron has been developed in Ref., where the perspectives of $1/N$-expansions are discussed. The technique of $1/N$-expansions has been developed later for the optical polaron in Ref. Up to now the first three terms of the weak-coupling expansion for the ground-state energy of the bulk polaron have been calculated (see also), as well as two terms for the surface polaron energy and three terms of the wire polaron energy. The investigation of the

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convergence of the PT series of the bulk polaron can be found in Ref. 22.

In this paper the matrix diagrammatic technique is developed for an optical large polaron. This technique permits to evaluate any term of the PT, in principle. The ground-state energy of the one-dimensional polaron is calculated up to the eighth order of the PT by using the developed technique. The radius of convergence of the PT series is estimated by means of Cauchy-Hadamar’s criterion with respect to the calculated terms of the series.

In Section II the matrix diagrammatic technique is developed. In Section III the obtained results for the ground-state energy and the effective mass of an electron are given. The radius of convergence of the PT series is also estimated.

II. THE MATRIX DIAGRAMMATIC TECHNIQUE FOR THE POLARON PROBLEM
IN THE WEAK COUPLING LIMIT

The Hamiltonian of the one-dimensional optical large polaron is given by

\[ H = \frac{p^2}{2} + \sum_k \omega_k a_k^+ a_k + \sum_k \left( V_k^* a_k^+ e^{-ikx} + V_k a_k e^{ikx} \right), \tag{1} \]

where \( \omega_k \) is a frequency of a phonon with momentum \( k \), for the optical polaron \( \omega_k = \omega \) does not depend on \( k \) and \( V_k = 2^{1/4}(\alpha/L)^{1/2} \); \( p, x \) are the momentum and space operators of an electron; \( a_k^+, a_k \) are the creation and annihilation operators of a phonon with momentum \( k \); \( L \) is a normalized length; \( \alpha \) acts as a coupling constant of the electron-phonon interaction. Our units are such that \( \hbar, \omega \) and the electron mass are unity. Below we shall make usual simplifying assumption, such that the crystal lattice acts like a dielectric medium. It means that we can replace a sum \( \sum_k \) by an integral \( L \int d\mathbf{k}/2\pi \).

Let us consider the weak coupling limit \( \alpha \ll 1 \) for the polaron with the Hamiltonian (1). After doing Lee-Low-Pines transformation

\[ H' = U^{-1} H U, \tag{2} \]

\[ |\Psi\rangle = U |\Psi'\rangle, \tag{3} \]

\[ U = \exp \left[i (P - \sum_k ka_k^+ a_k) x \right], \tag{4} \]

where \( P \) is a c-number representing the total system momentum, we obtain the Shrödinger equation for Eq. (1) in the next form
\[(H_0 + H_1)|\Psi'\rangle = E|\Psi'\rangle,\]
\[H_0 = \frac{1}{2}(P - \sum_k k a_k^+ a_k)^2 + \sum_k a_k^+ a_k,\]
\[H_1 = \sum_k V_k \left(a_k^+ + a_k\right).\]

Let us use the conventional perturbation theory for the SE Eq. (5) in the Fock basis, where $H_0$ is an unperturbed Hamiltonian. Thus, if the zero-approximation of the vector state $|\Psi'\rangle$ is a vacuum state of a phonon field $|0\rangle$ then the ground-state energy of $H_0$ is given by $E^{(0)}_0 = \langle 0|H_0|0\rangle = P^2/2$.

It is easy to verify that all odd terms of the PT are equal to zero $E^{(1)}_0 = E^{(3)}_0 = \ldots = 0$. The second order of the PT is

\[E^{(2)}_0 = \langle H_1 \frac{1}{h_0} H_1 \rangle = \frac{2^{1/2} \alpha}{2\pi} \int_{-\infty}^{\infty} \frac{dk_1}{E^{(0)}_0 - \frac{1}{2}(P - k_1)^2 - 1},\]

where $h_0 = E^{(0)}_0 - H_0$ and $\langle 0|\ldots|0\rangle \rightarrow \langle \ldots \rangle$, this term is defined by one connected diagram (see Eq1.eps). The thick line corresponds to an electron propagation with momentum $P - k_1$. The thin line corresponds to a propagation of a virtual phonon with momentum $k_1$, a bold point on the thick electron line corresponds to a vertex, where one phonon either creates or annihilates. Below we shall give the Feynman rules for the connected diagrams represented in the matrix form. The quantity of the diagrams increases in the next orders of the PT: two connected diagrams in the forth order, ten connected diagrams in the sixth order, seventy-four connected diagrams in the eighth order and so on. There are also unconnected diagrams. These diagrams can be evaluated by differentiating the energy terms, which are the sums of the corresponding connected diagrams, with respect to $E^{(0)}_0$ (see below). Note that all multidimensional integrals corresponding to the diagrams are evaluated by the residue theory. It can be seen from (10). Thus, there is a technical problem to generate and evaluate all diagrams in the higher orders.

Now we shall show how to build the matrix diagrammatic technique which permits us to generate all connected diagrams by means of any modern system of computer algebra (SCA). Any connected diagram can be represented in the $n$-th order of the PT by using $n/2$ by $(n - 1)$ matrix $[|N||]$, where $n$ is an even number. For example, let us consider the energy term of the forth order $(n = 4)$. It has the following form

\[E^{(4)}_0 = \langle H_1 \left(\frac{1}{h_0} H_1\right)^3 \rangle + \frac{1}{2} \frac{\partial}{\partial E^{(0)}_0} \left[\langle H_1 \frac{1}{h_0} H_1 \rangle\right]^2.\]
This term is defined by a sum of two connected and one unconnected graphical diagrams (see Eq2.eps). These diagrams can be written in the following matrix form

\[ E_0^{(4)} = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix} + (1) \frac{\partial (1)}{\partial E_0^{(0)}}, \]  

(8)

where \( i \)-th row of \( \|N\| \) describes a history of propagation of \( i \)-th phonon with momentum \( k_i \) \((i = 1, 2 \ldots n/2)\). And \( j \)-th matrix column shows a distribution of phonons after passing \( j \)-th vertex, where one phonon either creates or annihilates \((j = 1, 2 \ldots n − 1)\). The value of \( N_{ij} = 1 \) or 0 corresponds to the existence or absence of \( i \)-th phonon between \( j \)-th and \((j + 1)\)-th vertex respectively. The generation of all connected diagrams for the \( n \)-th order is realized by selecting \( n/2 \) by \( n − 1 \) matrixes with respect to the next rules

\[
N_{ij} = 0 \text{ or } 1, \quad \sum_{i=1}^{n/2} N_{ij} \neq 0, \quad \sum_{j=1}^{n-1} N_{ij} \neq 0,
\]

\[
\sum_{i=1}^{n/2} N_{i1} = 1, \quad \sum_{i=1}^{n/2} N_{in-1} = 1,
\]

\[
\sum_{j=1}^{n-1} |N_{ij+1} − N_{ij}| = 1.
\]  

(9)

We have to keep only one arbitrary matrix among matrixes which are transformed into each other by permutating matrix rows. Thus, the whole set of connected diagrams can be got in the matrix form by means of any SCA. Using the graphical diagrammatic technique it is easy to find the next rule for our matrix diagrammatic technique

\[
\|N\| \leftrightarrow \left(\frac{2^{1/2} \alpha}{2\pi}\right)^{n/2} \int_{-\infty}^{+\infty} dk_1 \ldots \int_{-\infty}^{+\infty} dk_{n/2} \prod_{j=1}^{n-1} \left[ E_0^{(0)} - \frac{1}{2} (P - \sum_{i=1}^{n/2} N_{ij} k_i)^2 - \sum_{i=1}^{n/2} N_{ij} \right]^{-1}.
\]  

(10)

Any diagram represented in the matrix form corresponds to an analytical expression. So that in accordance with the rule we have for \( (8) \)

\[
(1) \leftrightarrow \frac{2^{1/2} \alpha}{2\pi} \int_{-\infty}^{+\infty} dk_1 \left[ E_0^{(0)} - \frac{1}{2} (P - k_1)^2 - 1 \right]^{-1},
\]

\[
\begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 0 \end{pmatrix} \leftrightarrow \frac{2 \alpha^2}{(2\pi)^2} \int_{-\infty}^{+\infty} dk_1 \int_{-\infty}^{+\infty} dk_2 \left[ E_0^{(0)} - \frac{1}{2} (P - k_1)^2 - 1 \right]^{-1} \prod_{j=1}^{n-1} \left[ E_0^{(0)} - \frac{1}{2} (P - k_j)^2 - 1 \right]^{-1},
\]

\[
\begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix} \leftrightarrow \frac{2 \alpha^2}{(2\pi)^2} \int_{-\infty}^{+\infty} dk_1 \int_{-\infty}^{+\infty} dk_2 \left[ E_0^{(0)} - \frac{1}{2} (P - k_1)^2 - 1 \right]^{-1} \prod_{j=1}^{n-1} \left[ E_0^{(0)} - \frac{1}{2} (P - k_2)^2 - 1 \right]^{-1}.
\]
In order to summarize all unconnected diagrams in the n-th order we can use the general structure of the conventional perturbation theory series. Note that the term of the PT

$$E_0^{(n)c} = \langle H_1 \left( \frac{1}{\hbar_0} H_1 \right)^{n-1} \rangle,$$

contains all connected diagrams. This term does not contain unconnected diagrams at all. The other terms of n-th order $E_0^{(n)n}$ contain unconnected diagrams modifying the powers of the corresponding electron propagators in the previous orders. If the dependence of $E_0^{(s)c}(s < n)$ on $E_0^{(0)}$ will be conserved explicitly then $E_0^{(n)n}$ can be represented as a function of $E_0^{(s)c}$ and their derivatives. For example, $E_0^{(n)n}$ is written for some particular cases as follows

$$E_0^{(4)n} = E_2 E'_2,$$

$$E_0^{(6)n} = \frac{1}{2!} (E_2)^2 E''_2 + E_2 (E'_2)^2 + (E_2 E_4)',$$

$$E_0^{(8)n} = E_2 (E'_2)^3 + 3 \frac{1}{2!} (E_2)^2 E'_2 E''_2 + \frac{1}{3!} (E_2)^3 E'''_2$$

$$+ E_4 (E'_2)^2 + 2 \frac{1}{2!} E_2 E'_2 E_4 + (E_2 E_6)' + E_4 E'_4$$

$$+ 2 E_2 E'_2 E'_4 + \frac{1}{2!} (E_2)^2 E''_4,$$

where $E_n = E_0^{(n)c}$ and a prime denotes a derivative with respect to $E_0^{(0)}$. All integrals (10) are evaluated analytically by means of the residue theory without expanding them in powers of $P$.

Then the effective mass of an electron is defined by the next formula

$$\frac{1}{2m^*} = \left. \frac{\partial^2 E_0}{\partial P^2} \right|_{P=0}.$$  

We should like to note that the suggested matrix diagrammatic technique is acceptable for any N-dimensional optical large polaron, but the rule (10) has to be generalized with respect to the Feynman rules for N- dimensional polaron.

### III. RESULTS

Let us carry out an asymptotic expansion of the ground-state energy up to the eighth order of the PT. At first, it is necessary to generate and evaluate all connected diagrams for the corresponding orders with respect to the conditions (9) and rule (10). At second, we have to summarize obtained diagrammatic terms and unconnected diagrammatic terms defined by Eq. (12)-(14).
Thus, the polaron ground-state energy up to the eighth order is \( E_0(P) = \sum_{n=0}^{8} E_0^{(n)}(P) \), where the energy terms are defined by

\[
E_0^{(0)}(P) = \frac{P^2}{2}, \tag{16}
\]

\[
E_0^{(2)}(P) = -\frac{2^{1/2}}{(2-P^2)^{1/2}} \alpha = -\alpha - \frac{P^2}{4} \alpha + o(P^4), \tag{17}
\]

\[
E_0^{(4)}(P) = -\left[ \frac{P^2(P^2 - 4) + 6}{(2-P^2)^{3/2}(4-P^2)^{1/2}} - \frac{P^2(P^2 - 3) + 4}{(2-P^2)^2} \right] \alpha^2
- \left( \frac{3\sqrt{2}}{4} - 1 \right) \alpha^2 + \frac{P^2}{32}(8 - 5\sqrt{2}) \alpha^2 + o(P^4), \tag{18}
\]

\[
E_0^{(6)}(P) = -\left( 5 - \frac{63}{8\sqrt{2}} + \frac{1}{16}\sqrt{\frac{4931}{3} - 1102\sqrt{2}} \right) \alpha^3
- \frac{P^2}{2} \left( -\frac{15}{4} + \frac{163}{32\sqrt{2}} + \frac{1}{96}\sqrt{\frac{98593}{6} - 11472\sqrt{2}} \right) \alpha^3 + o(P^4), \tag{19}
\]

\[
E_0^{(8)}(P) = -\left( \frac{442369}{15456} - \frac{218861}{7728\sqrt{2}} + \frac{151925}{2208\sqrt{3}} - \frac{261335}{2208\sqrt{6}} \right) \alpha^4 + o(P^2). \tag{20}
\]

Since the terms \( E_0^{(6)}(P) \) and \( E_0^{(8)}(P) \) are too bulky, we have only written out their expansion in powers of momentum \( P \). Using Eq. (16)-(20) the ground-state energy of a slow-moving polaron is written as

\[
E_0(P) = \frac{P^2}{2m^*} - \alpha - 0.06066017 \alpha^2
- 0.00844437 \alpha^3 - 0.00151488 \alpha^4 + o(\alpha^5). \tag{21}
\]

The effective mass of an electron is defined by equation Eq. (13)

\[
m^* = 1 + \frac{\alpha}{2} + \frac{5 - 2\sqrt{2}}{8\sqrt{2}} \alpha^2 + \left( \frac{33}{8} + \frac{183}{32\sqrt{2}} \right) + \frac{1}{2}\sqrt{\frac{98593}{13824} - \frac{239}{24\sqrt{2}}} \alpha^3 + o(\alpha^4) \approx 1 + 0.5 \alpha
+ 0.1919417 \alpha^2 + 0.0691096 \alpha^3 + o(\alpha^4). \tag{22}
\]

Now let us compare the obtained asymptotic formula for the polaron ground-state energy with the energy obtained in the frame of the Feynman polaron theory\textsuperscript{13,21} (see Table I). For \( \alpha < 3.4 \) the asymptotic energy Eq. (21) lies lower than the Feynman variational result \( E_0^F \) with maximum deviation about 4 percent. For \( \alpha \gtrsim 5 \) formula Eq. (21) is not correct because of the radius of convergence of the series is \( R \sim 5 \) (see below). Note that the first three terms of the energy Eq. (21) coincide with the same terms from Ref.\textsuperscript{6,14}
Let us estimate the radius of convergence of the PT series for $E_0(0)$. The radius of convergence $R$ can be evaluated by Cauchy-Hadamar’s criterion\(^2\)

$$R = \lim_{n \to \infty} R_n = \lim_{n \to \infty} \left( \frac{|E_0^{(n)}|/\alpha^{n/2}}{2^{n}} \right)^{-2/n}. \quad (23)$$

It is clear from Table II that there is quite fast convergence of the sequence $\{R_n\}$ near the point $\alpha \sim 5$. So if the nonevaluated higher order energy terms conserve the existent tendency to convergence of the sequence $\{R_n\}$ then the series Eq. (21) has a finite radius of convergence $R \sim 5$.

**IV. CONCLUSION**

The main purpose of the paper is to develop the matrix diagrammatic technique for the optical large polaron problem in the weak coupling limit. The first four terms of the ground-state energy and the first three terms of the effective mass of the one-dimensional polaron are evaluated by means of this technique. The suggested technique is acceptable for any $N$-dimensional optical large polaron. The obtained results are compared with the results from the Feynman polaron theory. The radius of convergence of the PT series for the one-dimensional polaron is estimated by Cauchy-Hadamar’s criterion.

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| TABLE I. The ground-state energy $E_0(P)$. |
\[ \alpha \quad -E_F^E \quad -E_0(0) \text{ from (21)} \]

| \(\alpha\) | \(-E_F^E\) | \(-E_0(0)\) |
|---|---|---|
| 0.1 | 0.100376 | 0.100615 |
| 0.5 | 0.510063 | 0.516315 |
| 1.0 | 1.044445 | 1.070619 |
| 1.5 | 1.613146 | 1.672654 |
| 2.0 | 2.236957 | 2.334434 |
| 2.5 | 2.959682 | 3.070245 |
| 3.0 | 3.828595 | 3.896646 |
| 3.3 | 4.426768 | 4.443709 |
| 3.4 | 4.639049 | 4.635570 |
| 3.5 | 4.857770 | 4.832468 |
| 4.0 | 6.047798 | 5.898815 |
| 4.5 | 7.398112 | 7.119062 |
| 5.0 | 8.908301 | 8.518858 |

**TABLE II.** First four terms of the sequence \(\{R_n\}\)

| \(n\) | 2 | 4 | 6 | 8 | \(\infty\) |
|---|---|---|---|---|---|
| \(R_n\) | 1 | 4.060207 | 4.910708 | 5.068795 | \(R\) |
