Perturbation theory for the one-dimensional optical polaron

P. A. Khomyakov*
Department of Theoretical Physics, Belarussian State University, Fr. Skarina av. 4, Minsk 220080, Republic of Belarus
(Received 21 August 2000; revised manuscript received 28 November 2000; published 27 March 2001)

The one-dimensional optical polaron is treated on the basis of 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 eighth order of perturbation theory. The effective mass of an electron is obtained up to sixth order of perturbation theory. The radius of convergence of the series obtained is estimated.

DOI: 10.1103/PhysRevB.63.1534XX PACS number(s): 71.38.−k, 03.65.Ge, 73.21.−b

I. INTRODUCTION

Nowadays there is continuing interest in low-dimensional structures.[1–6] The one-dimensional polaron problem is relevant in semiconductor physics, where with state-of-the-art nanolithography it has become possible to confine electrons in one direction[7] (quantum wires) and in linear conjugated organic polymer conductors.[8] A treatment of the polaron problem in quantum dots can be found in Refs. 4 and 5.

There is much theoretical work where the polaron problem is investigated by means of perturbation theory (PT).[9–15] The series of perturbation theory is useful for verifying approximate nonperturbative methods in the weak-coupling limit.[16–20] PT for the N-dimensional polaron was developed in Ref. 9, where the perspective of $1/N$ expansions is discussed. The technique of $1/N$ expansion was developed later for the optical polaron in Ref. 21. Up to now the first three terms of the weak-coupling expansion for the ground-state energy of the bulk polaron have been calculated[10] (see also Refs. 11–13), as well as two terms of the surface polaron energy[9] and three terms of the wire polaron energy.[6,15] An investigation of the convergence of the PT series for 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 one to evaluate any term of the PT, in principle. The ground-state energy of the one-dimensional polaron is calculated up to eighth order of PT by using this technique. The radius of convergence of the PT series is estimated by means of the Cauchy-Hadamard criterion with respect to the calculated terms of the series.

In Sec. II the matrix diagrammatic technique is developed. In Sec. III the results obtained 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[14,19]

$$H=\frac{p^2}{2}+\sum_k \omega_k a_k^\dagger a_k+\sum_k (V_k^* a_k^\dagger e^{-ikx}+V_k a_k e^{ikx}), \tag{1}$$

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

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

$$H'=U^{-1}HU, \tag{2}$$

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

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

where P is a c number representing the total system momentum, we obtain the Schrödinger equation (SE) for Eq. (1) in the form

$$(H_0+H_1)|\Psi'\rangle=E|\Psi'\rangle,$$

$$H_0=\frac{1}{2}\left(P-\sum_k k a_k^\dagger a_k\right)^2+\sum_k a_k^\dagger a_k, \tag{5}$$

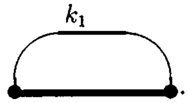
$$H_1=\sum_k V_k(a_k^\dagger+a_k).$$

Let us use the conventional perturbation theory[23] for the SE Eq. (5) in the Fock basis, where H_0 is the unperturbed Hamiltonian. Thus, if the zero approximation of the vector state $|\Psi'\rangle$ is the vacuum state of the 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 the odd terms of PT are equal to zero, $E_0^{(1)}=E_0^{(3)}=\cdots=0$. The second order of the PT is[9]

$$E_0^{(2)}=\left\langle H_1\frac{1}{h_0}H_1\right\rangle=\frac{2^{1/2}\alpha}{2\pi}\int_{-\infty}^{\infty}\frac{dk_1}{E_0^{(0)}-\frac{1}{2}(P-k_1)^2-1}, \tag{6}$$

where $h_0=E_0^{(0)}-H_0$ and $\langle 0|\cdots|0\rangle\rightarrow\langle\cdots\rangle$. This term is defined by one connected diagram

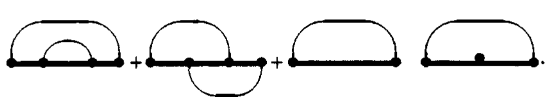


The thick line corresponds to electron propagation with momentum $P-k_1$. The thin line corresponds to propagation of a virtual phonon with momentum k_1. The bold points on the thick electron line correspond to vertices, where a phonon is either created or annihilated. Below we shall give the Feynman rules for the connected diagrams represented in the matrix form. The number of diagrams increases in the next orders of PT: two connected diagrams in the fourth order, ten connected diagrams in the sixth order, 74 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 residue theory. This can be seen from Eq. (10) below. Thus, there is a technical problem in generating and evaluating all diagrams in the higher orders.

Now we shall show how to build the matrix diagrammatic technique that 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 nth order of PT by using an $n/2\times(n-1)$ matrix $||N||$, where n is an even number. For example, let us consider the energy term of fourth order ($n=4$). It has the form[23]

$$E_0^{(4)}=\left\langle H_1\left(\frac{1}{h_0}H_1\right)^3\right\rangle+\frac{1}{2}\frac{\partial}{\partial E_0^{(0)}}\left[\left\langle H_1\frac{1}{h_0}H_1\right\rangle\right]^2. \tag{7}$$

This term is defined by the sum of two connected and one unconnected graphical diagrams,[9]



These diagrams can be written in the following matrix form:

$$E_0^{(4)}=\begin{pmatrix}1&1&1\\0&1&0\end{pmatrix}+\begin{pmatrix}1&1&0\\0&1&1\end{pmatrix}+(1)\frac{\partial(1)}{\partial E_0^{(0)}}, \tag{8}$$

where the ith row of $||N||$ describes the history of propagation of the ith phonon with momentum k_i ($i=1,2,\ldots,n/2$), and the jth matrix column shows the distribution of phonons after passing the jth vertex, where one phonon is either created or annihilated ($j=1,2,\ldots,n-1$). The value of $N_{ij}=1$ or 0 corresponds to the existence or absence of the ith phonon between the jth and $(j+1)$th vertices. The generation of all connected diagrams for the nth order is realized by selecting $n/2\times n-1$ matrices with respect to the rules

$$N_{ij}=0 \text{ or } 1,\quad \sum_{i=1}^{n/2}N_{ij}\neq 0,\quad \sum_{j=1}^{n-1}N_{ij}\neq 0,$$
$$\sum_{i=1}^{n/2}N_{i\,1}=1,\quad \sum_{i=1}^{n/2}N_{i\,n-1}=1, \tag{9}$$
$$\sum_{j=1}^{n-1}|N_{ij+1}-N_{ij}|=1.$$

We have to keep only one arbitrary matrix among the matrices that are transformed into each other by permutating matrix rows. Thus, the whole set of connected diagrams can be obtained in matrix form by means of any SCA. Using the graphical diagrammatic technique[9] it is easy to find the next rule for our matrix diagrammatic technique:

$$||N||\leftrightarrow\left(\frac{2^{1/2}\alpha}{2\pi}\right)^{n/2}\int_{-\infty}^{+\infty}dk_1\cdots\int_{-\infty}^{+\infty}dk_{n/2}\times\prod_{j=1}^{n-1}\left[E_0^{(0)}-\frac{1}{2}\left(P-\sum_{i=1}^{n/2}N_{ij}k_i\right)^2-\sum_{i=1}^{n/2}N_{ij}\right]^{-1}. \tag{10}$$

Any diagram represented in the matrix form corresponds to an analytical expression. So that in accordance with the rule (10) we have for (8)

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

$$\begin{pmatrix}1&1&1\\0&1&0\end{pmatrix}\leftrightarrow\frac{2\alpha^2}{(2\pi)^2}\int_{-\infty}^{\infty}dk_1\int_{-\infty}^{\infty}dk_2\times\left[E_0^{(0)}-\frac{1}{2}(P-k_1)^2-1\right]^{-1}\times\left[E_0^{(0)}-\frac{1}{2}(P-k_1-k_2)^2-2\right]^{-1}\times\left[E_0^{(0)}-\frac{1}{2}(P-k_1)^2-1\right]^{-1},$$

$$\begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix} \leftrightarrow \frac{2\alpha^2}{(2\pi)^2}\int_{-\infty}^{\infty} dk_1 \int_{-\infty}^{\infty} dk_2 \times\left[E_0^{(0)}-\frac{1}{2}(P-k_1)^2-1\right]^{-1} \times\left[E_0^{(0)}-\frac{1}{2}(P-k_1-k_2)^2-2\right]^{-1} \times\left[E_0^{(0)}-\frac{1}{2}(P-k_2)^2-1\right]^{-1}.$$

In order to summarize all unconnected diagrams in the nth order we can use the general structure of the conventional perturbation theory series.[23] Note that the term of PT

$$E_0^{(n)c}=\left\langle H_1\left(\frac{1}{h_0}H_1\right)^{n-1}\right\rangle \qquad (11)$$

contains all connected diagrams. This term does not contain unconnected diagrams at all. The other terms of nth 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 $E_0^{(0)}$ is explicitly conserved then $E_0^{(n)n}$ can be represented as a function of $E_0^{(s)c}$ and its derivatives. For example, $E_0^{(n)n}$ is written for some particular cases as follows:

$$E_0^{(4)n}=E_2E_2', \qquad (12)$$

$$E_0^{(6)n}=\frac{1}{2!}(E_2)^2E_2''+E_2(E_2')^2+(E_2E_4)', \qquad (13)$$

$$E_0^{(8)n}=E_2(E_2')^3+3\frac{1}{2!}(E_2)^2E_2'E_2''+\frac{1}{3!}(E_2)^3E_2'''+E_4(E_2')^2 +2\frac{1}{2!}E_2E_2''E_4+(E_2E_6)'+E_4E_4'+2E_2E_2'E_4' +\frac{1}{2!}(E_2)^2E_4'', \qquad (14)$$

where $E_n=E_0^{(n)c}$ and a prime denotes a derivative with respect to $E_0^{(0)}$. All the integrals (10) are evaluated analytically by means of the residue theory[23] without expanding them in powers of P. Then the effective mass of an electron is defined by

$$\frac{1}{2m^*}=\left.\frac{\partial^2E_0}{\partial P^2}\right|_{P=0}. \qquad (15)$$

We 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 polarons.[9]

III. RESULTS

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

$$E_0^{(0)}(P)=\frac{P^2}{2}, \qquad (16)$$

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

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

$$E_0^{(6)}(P)=-\left(5-\frac{63}{8\sqrt{2}}+\frac{1}{16}\sqrt{\frac{4931}{3}-1102\sqrt{2}}\right)\alpha^3 -\frac{P^2}{2}\left(-\frac{15}{4}+\frac{163}{32\sqrt{2}} +\frac{1}{96}\sqrt{\frac{98\,593}{6}-11\,472\sqrt{2}}\right)\alpha^3+o(P^4), \qquad (19)$$

TABLE I. The ground-state energy $E_0(P)$.

α	$-E_0^F$	$-E_0(0)$ from Eq. (21)
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

$$E_0^{(8)}(P) = -\left(\frac{442\,369}{15\,456} - \frac{218\,861}{7728\sqrt{2}} + \frac{151\,925}{2208\sqrt{3}} - \frac{261\,335}{2208\sqrt{6}}\right)\alpha^4 + o(P^2). \quad (20)$$

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 Eqs. (16)–(20) the ground-state energy of a slow-moving polaron is written as

$$E_0(P) = \frac{P^2}{2m^*} - \alpha - 0.060\,660\,17\,\alpha^2 - 0.008\,444\,37\,\alpha^3 - 0.001\,514\,88\,\alpha^4 + o(\alpha^5). \quad (21)$$

The effective mass of the electron is defined by Eq. (15):

$$\begin{aligned} m^* &= 1 + \frac{\alpha}{2} + \frac{5-2\sqrt{2}}{8\sqrt{2}}\alpha^2 + \left(-\frac{33}{8} + \frac{183}{32\sqrt{2}} + \frac{1}{2}\sqrt{\frac{98\,593}{13\,824} - \frac{239}{24\sqrt{2}}}\right)\alpha^3 + o(\alpha^4) \\ &\simeq 1 + 0.5\,\alpha + 0.191\,941\,7\,\alpha^2 + 0.069\,109\,6\,\alpha^3 + o(\alpha^4). \end{aligned} \quad (22)$$

Now let us compare the asymptotic formula obtained for the polaron ground-state energy with the energy obtained in the framework of Feynman polaron theory[17,24] (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%. For $\alpha \gtrsim 5$ Eq. (21) is not correct because 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 Refs. 6 and 14.

TABLE II. First four terms of the sequence $\{R_n\}$.

n	2	4	6	8	∞
R_n	1	4.060207	4.910708	5.068795	R

Let us estimate the radius of convergence of the PT series for $E_0(0)$. The radius of convergence R can be evaluated by the Cauchy-Hadamard criterion[23]

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

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 unevaluated higher-order energy terms conserve the existing 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 this 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 results obtained are compared with the results from Feynman polaron theory. The radius of convergence of the PT series for the one-dimensional polaron is estimated by the Cauchy-Hadamard criterion.

ACKNOWLEDGMENTS

The author wishes to acknowledge L. I. Komarov and I. D. Feranchuk for useful discussions.

*Electronic address: homyakov@phys.bsu.unibel.by

[1] M. H. Degani, Phys. Rev. B **40**, 11 937 (1989).
[2] G. Q. Hai, F. M. Peeters, J. T. Devreese, and L. Wendler, Phys. Rev. B **48**, 12 016 (1993).
[3] H. Akiyama, T. Someya, and H. Sakaki, Phys. Rev. B **57**, 3765 (1998).
[4] Y. Lépine and G. Bruneau, J. Phys.: Condens. Matter **10**, 1495 (1998).
[5] S. Sahoo, J. Phys.: Condens. Matter **10**, 1999 (1998).
[6] G. Ganbold, cond-mat/9910327 (unpublished).
[7] K.-F. Berggren, T. J. Thornton, D. J. Newson, and M. Pepper, Phys. Rev. Lett. **57**, 1769 (1986).
[8] W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. Lett. **42**, 1698 (1980).
[9] O. V. Seljugin and M. A. Smondyrev, Physica A **142**, 555 (1987).
[10] M. A. Smondyrev, Theor. Math. Phys. **68**, 26 (1986).
[11] J. Röseler, Phys. Status Solidi B **25**, 311 (1968).
[12] F. Haga, Prog. Theor. Phys. **11**, 449 (1954).
[13] G. Höhler and A. Müllensiefen, Z. Phys. **157**, 159 (1959).
[14] F. M. Peeters and M. A. Smondyrev, Phys. Rev. B **43**, 4920 (1991).
[15] P. A. Khomyakov, Vesti Nat. Akad. Nauk Belarus: Ser. Fiz.-Mat. **4**, 112 (1999).
[16] T. D. Lee, F. M. Low, and D. Pines, Phys. Rev. **90**, 297 (1953).
[17] R. Feynman, Phys. Rev. **97**, 660 (1955).
[18] F. M. Peeters and J. T. Devreese, Phys. Status Solidi B **112**, 219 (1982).
[19] M. H. Degani and G. A. Farias, Phys. Rev. B **42**, 11 950 (1990).
[20] G. Ganbold and G. V. Efimov, J. Phys.: Condens. Matter **10**, 4845 (1998).
[21] M. A. Smondyrev, Physica A **171**, 191 (1991).
[22] O. V. Selyugin and M. A. Smondyrev, Phys. Status Solidi B **155**, 155 (1989).
[23] P. M. Morse and G. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953).
[24] M. H. Degani, O. Hipólito, R. Lobo, and G. A. Farias, J. Phys. C **19**, 2919 (1986).