

Theory of polarons in multivalley crystals. III. Arbitrary coupling force between the electron and the lattice polarization vibrations

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We consider the interaction of a free electron with longitudinal optical lattice vibrations in a multivalley ionic cubic crystal at arbitrary coupling force. It is shown within the framework of the effective-mass method that the polaron is localized in one of the valleys. The vibrational degrees of freedom are eliminated from the partition function of this system by the method of ordered operators. The resultant nonelementary operator, which depends only on the electron coordinates, can be approximated by some other operator, and this makes it possible to use a variational principle and determine the partition function of the polaron at arbitrary temperatures. The obtained partition function is used to determine the ground-state energy of the polaron and its effective mass. A computer calculation yields the energy of the ground state and the effective mass of the polaron as a function of the coupling constant of the mass anisotropy of the band electron.

In our earlier papers we considered limiting cases of weak^[1] and strong^[2] coupling of an electron with lattice vibrations in crystals with multivalley conduction bands. In most semiconductors, however, an intermediate coupling is realized, wherein neither expansion in powers of the coupling constant (perturbation theory) nor the use of adiabatic approximation is possible.

In this paper we calculate the sum of states of a large-radius polaron in a multivalley semiconductor using a direct variational method without limitation on the coupling force. We have followed the method of^[3], developed for one isotropic valley; in this particular case our results agree with those obtained in^[3], and at zero temperature they coincide also with the results of Feynman and Osaka^[4,5]. At nonzero temperature, our results differ somewhat from those of Osaka^[5]. The case of an anisotropic valley is considered in this paper for the first time.

The Hamiltonian of a system consisting of an electron field with periodic potential $W(\mathbf{r})$, interacting with longitudinal optical phonons, takes in the continual approximation the form

$$H = -\frac{\hbar^2}{2m} \Delta + W(\mathbf{r}) + \sum_{\mathbf{x}} (\hbar\omega a_{\mathbf{x}}^+ a_{\mathbf{x}} + V_{\mathbf{x}} a_{\mathbf{x}} e^{i\mathbf{x}\cdot\mathbf{r}} + V_{\mathbf{x}}^* a_{\mathbf{x}}^+ e^{-i\mathbf{x}\cdot\mathbf{r}}), \quad (1)$$

$$V_{\mathbf{x}} = \frac{e}{|\mathbf{x}|} \left(\frac{2\pi\hbar\omega c}{v} \right)^{1/2}, \quad c = \frac{1}{\hbar^2} - \frac{1}{\epsilon},$$

where m is the mass of the free electron, κ and ω are the wave vector and the frequency of the longitudinal phonon oscillations, ϵ is the static dielectric constant, n is the refractive index of the crystal, v is the volume of the principal cyclicity region, and e is the electron charge.

Having a transition to the effective-mass method in mind, we seek the eigenfunctions of (1) in the form of an expansion in the basis

$$\varphi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \psi_{n\mathbf{K}_j}(\mathbf{r}) \equiv \exp\{i(\mathbf{k} + \mathbf{K}_j)\cdot\mathbf{r}\} u_{n\mathbf{K}_j}(\mathbf{r}), \quad (2)$$

where $\psi_{n\mathbf{K}_j}$ are Bloch functions and \mathbf{K}_j is the position of the energy minimum in the j -th valley. In accordance with the effective-mass method it is assumed for the large-radius polaron that only terms with small \mathbf{k} ($\mathbf{k} \ll d^{-1}$, d is the lattice constant) are retained in the expansion in the functions (2).

Expanding the periodic function $u_{n\mathbf{K}_j}(\mathbf{r})$ in a Fourier series, we can easily reduce the matrix elements

$$\langle \varphi_{n\mathbf{k}} | e^{i\mathbf{x}\cdot\mathbf{r}} | \varphi_{n'\mathbf{k}'} \rangle$$

to a sum of δ -functions in the form

$$\delta(\mathbf{k}' - \mathbf{k} - \boldsymbol{\kappa} - \mathbf{b}_m + \mathbf{K}_j - \mathbf{K}_j'),$$

where \mathbf{b}_m are the reciprocal-lattice vectors. Inasmuch as $|\mathbf{k}|$, $|\mathbf{k}'|$, $|\boldsymbol{\kappa}| \ll d^{-1}$, and $|\mathbf{K}_j - \mathbf{K}_j'|$ are of the order of d^{-1} but are not equal to the reciprocal-lattice vector, the δ -functions differ from zero only if $j = j'$ and $\mathbf{b}_m = 0$. Thus, the matrix elements with $j \neq j'$ vanish, i.e., the wave function of the electron consists of Bloch functions of only one of the valleys. This reduction of the problem to a single-valley problem takes place also in the limiting cases of weak^[1] and strong^[2] coupling.

With the foregoing taken into account, the use of the effective-mass method is standard^[6,7], and for an anisotropic equal-energy surface the Hamiltonian of the system can be written in the form

$$H = H_0 + H_1,$$

$$H_0 = -\sum_{\mathbf{l}=1}^3 \frac{\hbar^2}{2\mu_{\mathbf{l}}} \frac{\partial^2}{\partial x_{\mathbf{l}}^2}, \quad (3)$$

$$H_1 = \sum_{\mathbf{x}} (\hbar\omega a_{\mathbf{x}}^+ a_{\mathbf{x}} + V_{\mathbf{x}} a_{\mathbf{x}} e^{i\mathbf{x}\cdot\mathbf{r}} + V_{\mathbf{x}}^* a_{\mathbf{x}}^+ e^{-i\mathbf{x}\cdot\mathbf{r}}).$$

The trial Hamiltonian is chosen in the form

$$H' = \sum_{\mathbf{l}=1}^3 H'_{\mathbf{l}},$$

$$H'_{\mathbf{l}} = -\frac{\hbar^2}{2\mu_{\mathbf{l}}} \frac{\partial^2}{\partial x_{\mathbf{l}}^2} + \sum_{\mathbf{i}=1}^3 \left[-\frac{\hbar^2}{2\mu_{\mathbf{i}\mathbf{l}}} \frac{\partial^2}{\partial x_{\mathbf{i}\mathbf{l}}^2} + \frac{C_{\mathbf{i}\mathbf{l}}}{2} (x_{\mathbf{i}} - x_{\mathbf{i}\mathbf{l}})^2 \right], \quad (4)$$

$$C_{\mathbf{i}\mathbf{l}} = \mu_{\mathbf{i}\mathbf{l}} \omega_{\mathbf{i}\mathbf{l}}^2,$$

where the masses $\mu_{\mathbf{l}}$ of the auxiliary particles and the constants $C_{\mathbf{l}}$ of their elastic interaction with the electron are variational parameters determined from the condition that the trial sum of states be a maximum. An attempt is made here to increase the flexibility of the approximation of the Hamiltonian by introducing s auxiliary particles that replace the action exerted by the polarization field on the electron. In^[3-5] and in many subsequent papers, only one isotropic auxiliary particle was used. Two isotropic auxiliary particles

($T = 0$) were used in^[8]. Introduction of the elastic interaction between the auxiliary particles does not improve the approximation, since it can be excluded from the Hamiltonian by a canonical transformation that affects only the coordinates of these particles.

We add to (3) the operator

$$H_a = \sum_{\gamma l} \left(-\frac{\hbar^2}{2\mu_{\gamma l}} \frac{\partial^2}{\partial x_{\gamma l}^2} + \frac{C_{\gamma l}}{2} x_{\gamma l}^2 \right). \quad (5)$$

Since H and H_a commute, the sought sum of states is equal to

$$Z = \text{Sp} e^{-\lambda H} = \frac{\text{Sp} \exp(-\lambda H_t)}{\text{Sp} \exp(-\lambda H_a)} = \frac{Z_t}{Z_a}, \quad (6)$$

where

$$H_t = H + H_a = H' - \sum_{\gamma l} \frac{C_{\gamma l}}{2} (x_{\gamma l}^2 - 2x_{\gamma l} x_{\gamma l}) + H_1. \quad (7)$$

In Z_t , the trace over the phonon variables and over $x_{\gamma l}$ is calculated in the same manner as in^[3,4], after which we get

$$\begin{aligned} Z_t &= Z_l \text{Sp} \exp \left\{ \sum_{\kappa} |V_{\kappa}|^2 \int_0^{\lambda} d\lambda_1 \int_0^{\lambda} d\lambda_2 \exp \{ i\kappa (r_{\lambda_1} - r_{\lambda_2}) \right. \\ &\quad \left. - \hbar\omega (\lambda_1 - \lambda_2) \} + \tilde{n} \int_0^{\lambda} d\lambda_1 \int_0^{\lambda} d\lambda_2 \exp \{ i\kappa (r_{\lambda_1} - r_{\lambda_2}) \right. \\ &\quad \left. - \hbar\omega (\lambda_1 - \lambda_2) \} \right\} - \int_0^{\lambda} H_{r\lambda} d\lambda_1 + \sum_{\gamma l} C_{\gamma l} U'_{\gamma l} - \sum_{\gamma l} C_{\gamma l} U'_{\gamma l}, \\ U'_{\gamma l} &= -\frac{1}{2} \int_0^{\lambda} x_{\gamma l}^2 d\lambda_1 + \frac{\hbar\omega_{\gamma l}}{2} \int_0^{\lambda} \int_0^{\lambda} (x_{\gamma l_1}, x_{\gamma l_2}) \exp[\hbar\omega_{\gamma l} (\lambda_2 - \lambda_1)] d\lambda_1 d\lambda_2 \\ &\quad + \frac{\hbar\omega_{\gamma l}}{2[\exp(\lambda\hbar\omega_{\gamma l}) - 1]} \int_0^{\lambda} \int_0^{\lambda} (x_{\gamma l_1}, x_{\gamma l_2}) \exp[\hbar\omega_{\gamma l} (\lambda_2 - \lambda_1)] d\lambda_1 d\lambda_2, \\ Z_l &= \prod_{\kappa} (1 - e^{-\lambda\hbar\omega})^{-1}, \quad \tilde{n} = (e^{\lambda\hbar\omega} - 1)^{-1}. \end{aligned} \quad (8)$$

According to the variational method of^[3], the sum of states (6) should be sought as a maximum of the trial state function $Z_l \leq Z$, where

$$\begin{aligned} Z_l &= \frac{Z_l}{Z_a} \text{Sp} e^{-\lambda H'} e^{\tilde{v}}, \\ O &= \sum_{\gamma l} C_{\gamma l} \left(\frac{\partial}{\partial C_{\gamma l}} \ln \text{Sp} e^{-\lambda H'} \right)_{\omega_{\gamma l} = \text{const}} \\ &\quad + \sum_{\kappa} |V_{\kappa}|^2 \left(\frac{\partial}{\partial |V_{\kappa}|^2} \ln \text{Sp} e^{-\lambda(H'+H_a)} \right)_{|V_{\kappa}|^2=0}. \end{aligned} \quad (9)$$

As seen from (4), the Hamiltonian H'_γ describes one-dimensional motion of a system of $s + 1$ particles that interact elastically in the absence of an external field. Introducing Jacobi coordinates^[9], we can break up H'_γ into two independent conservative parts: the kinetic energy of motion of the center of gravity

$$H'_c = -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial X^2}, \quad M = \mu + \sum_{i=1}^s \mu_i \quad (10)$$

and the Hamiltonian H'_r of the relative motion (the index γ is omitted for the time being for the sake of brevity). Owing to the linearity of the Jacobi transformation the potential energy in H'_r retains the form of a homogeneous quadratic form of the coordinates, making it possible to introduce again normal coordinates q_m by means of a linear transformation. As a result

$$H'_r = \frac{1}{2} \sum_{m=1}^s \hbar\Omega_m \left[q_m^2 - \frac{\partial^2}{\partial q_m^2} \right] = \sum_{m=1}^s \hbar\Omega_m \left(a_m^+ a_m + \frac{1}{2} \right), \quad (11)$$

where Ω_m are the eigenfunctions of the normal oscillations,

and $a_m = q_m + \partial/\partial q_m$ and $a_m^+ = q_m - \partial/\partial q_m$ are the operators of annihilation and creation of the vibrational excitation. The linear connection between the old and new coordinates is

$$x = X + \sum_{m=1}^s Q_m q_m, \quad x_i = X + \sum_{m=1}^s Q_{im} q_m. \quad (12)$$

The coefficients Q are determined from the condition that the operator (4) be equal to the sum of the operators (10) and (11).

Restoring again the index γ and taking H' to mean the first of the formulas in (4), we obtain ultimately

$$Z' = \text{Sp} e^{-\lambda H'} = \prod_{\gamma=1}^s \left(\frac{M_\gamma}{2\pi\hbar^2\lambda} \right)^{1/2} \prod_{m=1}^s \left[2 \text{sh} \left(\frac{\lambda}{2} \hbar\Omega_{\gamma m} \right) \right]^{-1}. \quad (13)$$

To calculate in (9) the derivative with respect to $|V_{\kappa}|^2$ at the point $|V_{\kappa}|^2 = 0$, it is necessary to separate in the operator H_1 of (3) the term with one fixed $\kappa - H_{\kappa}$, and calculate in second order in V_{κ} the quantity

$$Z_{\kappa} = \text{Sp} \exp \{ -\lambda (H' + H_{\kappa}) \}, \quad (14)$$

by using the Schwinger formula^[10] and the auxiliary relation

$$\begin{aligned} &\text{Sp} e^{-\lambda(1-u)\alpha^+ \alpha} e^{-ik(\alpha+\alpha^+)} e^{-\lambda u \alpha^+ \alpha} e^{ik(\alpha+\alpha^+)} \\ &= \frac{1}{1-e^{-\lambda}} \exp \left\{ -\frac{2k^2}{\text{cth}(\lambda u/2) + \text{cth}(\lambda(1-u)/2)} \right\}. \end{aligned} \quad (15)$$

As a result of the calculation we obtain ultimately

$$\begin{aligned} Z_l &= Z^0 \prod_{\gamma} \left(\frac{M_\gamma}{\mu_\gamma} \right)^{1/2} \prod_i \frac{\text{sh}(\lambda\hbar\omega_{\gamma i}/2)}{\text{sh}(\lambda\hbar\Omega_{\gamma i}/2)} \exp \left\{ \frac{\lambda}{2} \sum_{\gamma l} \text{cth} \left(\frac{\lambda\hbar}{2} \Omega_{\gamma l} \right) C_{\gamma l} \frac{\partial \hbar\Omega_{\gamma l}}{\partial C_{\gamma l}} \right. \\ &\quad \left. - \frac{1}{2} \sum_{\gamma l} \frac{\mu_{\gamma l}}{M_\gamma} + U_\alpha \right\}, \quad Z^0 = v Z_l \prod_{\gamma} \left(\frac{\mu_\gamma}{2\pi\hbar^2\lambda} \right)^{1/2}, \\ U_\alpha &= \frac{\lambda^2}{2} \sum_{\kappa} |V_{\kappa}|^2 \int_0^{\lambda} dv \frac{\text{ch}(\lambda\hbar\omega v/2)}{\text{sh}(\lambda\hbar\omega/2)} \exp \left\{ -\frac{\lambda\hbar^2}{8} (1-v^2) \sum_{\gamma} \frac{\kappa_\gamma^2}{M_\gamma} \right. \\ &\quad \left. - \frac{1}{4} \sum_{\gamma l} \kappa_\gamma^2 Q_{\gamma l}^2 \left[\text{cth} \frac{\lambda\hbar\Omega_{\gamma l}}{2} - \frac{\text{ch}(\lambda\hbar\Omega_{\gamma l} v/2)}{\text{sh}(\lambda\hbar\Omega_{\gamma l}/2)} \right] \right\}. \end{aligned} \quad (16)$$

For the ordinary polaron, V_{κ} is determined by formula (1). In this case, replacing in (16) the summation over κ by integration, we obtain

$$\begin{aligned} U_\alpha &= \frac{e^2 \hbar \omega c}{2\hbar} \left(\frac{\lambda}{2\pi} \right)^{3/2} \frac{1}{\text{sh}(\lambda\hbar\omega/2)} \int_0^{\lambda} \int_0^{\lambda} \left(\sum_{\gamma} \left\{ (1-v^2) \frac{1}{M_\gamma} + \frac{2}{\lambda\hbar^2} \sum_l Q_{\gamma l}^2 \right. \right. \\ &\quad \left. \left. \times \left[\text{cth} \frac{\lambda\hbar\Omega_{\gamma l}}{2} - \frac{\text{ch}(\lambda\hbar\Omega_{\gamma l} v/2)}{\text{sh}(\lambda\hbar\Omega_{\gamma l}/2)} \right] \right\} s_\gamma^2 \right)^{-1/2} \text{ch} \frac{\lambda\hbar\omega v}{2} d\Omega dv. \end{aligned} \quad (17)$$

Here $d\Omega$ is a solid-angle element, and s_γ is the projection of the unit vector \mathbf{s} lying inside $d\Omega$; M_γ and $Q_{\gamma l}$ are determined by formulas (10) and (12). For example, in the case of the two auxiliary particles ($s = 2$), the eigenfrequencies $\Omega_{\gamma l}$ are determined from the following secular equation:

$$\Omega_{\gamma 1}^4 - \Omega_{\gamma 2}^2 \left[\omega_{\gamma 1}^2 \left(1 + \frac{\mu_{\gamma 1}}{\mu_\gamma} \right) + \omega_{\gamma 2}^2 \left(1 + \frac{\mu_{\gamma 2}}{\mu_\gamma} \right) \right] + \omega_{\gamma 1}^2 \omega_{\gamma 2}^2 \left(1 + \frac{\mu_{\gamma 1} + \mu_{\gamma 2}}{\mu_\gamma} \right) = 0, \quad (18)$$

$$Q_{\gamma l}^2 = \frac{2\hbar}{\omega} \frac{\mu_{\gamma 1} + \mu_{\gamma 2}}{M_\gamma} \left| \frac{1}{\Omega_{\gamma 1}^2 - \Omega_{\gamma 2}^2} \left[\Omega_{\gamma 1}^2 - \frac{\omega_{\gamma 1}^2 \mu_{\gamma 2} + \omega_{\gamma 2}^2 \mu_{\gamma 1}}{(\mu_{\gamma 1} + \mu_{\gamma 2}) \Omega_{\gamma l}} \right] \right| \quad (19)$$

If we put in these formulas $\mu_{\gamma 2} = 0$, then we arrive at the case of one auxiliary particle ($s = 1$). Then $\Omega_{\gamma 2} = \omega_{\gamma 2}$ and $Q_{\gamma 2} = 0$.

To determine the energy of the ground state of the polaron and its effective mass, we consider henceforth only the limiting case of low temperatures, i.e., large λ . We expand the logarithm of the trial function of the states in powers of λ^{-1}

$$\ln Z_1 = \ln Z^0 + \frac{\lambda \hbar \omega}{2} f_0 + f_1 + O\left(\frac{1}{\lambda}\right); \quad (20)$$

here

$$f_0 = \frac{1}{\omega} \sum_{\gamma} \left(\omega_{\gamma} - \Omega_{\gamma} + \sum_{\nu} C_{\nu\gamma} \frac{\partial \Omega_{\nu\gamma}}{\partial C_{\nu\gamma}} \right) + \frac{e^2 c}{2\pi \hbar (2\pi \hbar \omega)^{1/2}} \int_0^{\infty} \mathcal{L} e^{-x} d\Omega dx,$$

$$f_1 = \frac{1}{2} \sum_{\gamma} \ln \frac{M_{\gamma}}{\mu_{\gamma}} - \frac{1}{2} \sum_{\gamma} \frac{\mu_{\nu\gamma}}{M_{\gamma}} + \frac{e^2 c}{8\pi \hbar (2\pi \hbar \omega)^{1/2}} \int_0^{\infty} \mathcal{L}^2 \sum_{\gamma} \frac{s_{\gamma}^2}{M_{\gamma}} x^2 e^{-x} d\Omega dx, \quad (21)$$

$$\mathcal{L} = \left(\sum_{\gamma} \left\{ \frac{x}{M_{\gamma}} + \sum_{\nu} \frac{\omega}{2\hbar} Q_{\nu\gamma} \left[1 - \exp\left(-\frac{\Omega_{\nu\gamma} x}{\omega}\right) \right] \right\} s_{\gamma}^2 \right)^{-1/2}.$$

In the case $s = 2$ we have

$$f_0 = \frac{1}{\omega} \sum_{\gamma} \left\{ \omega_{\gamma 1} + \omega_{\gamma 2} - \Omega_{\gamma 1} - \Omega_{\gamma 2} + \frac{\omega_{\gamma 1} \omega_{\gamma 2}}{2(\Omega_{\gamma 1} + \Omega_{\gamma 2}) \mu_{\gamma}} \left[\frac{\mu_{\gamma 1} + \mu_{\gamma 2}}{\sqrt{M_{\gamma} \mu_{\gamma}}} + \mu_{\gamma 1} \frac{\omega_{\gamma 1}}{\omega_{\gamma 2}} + \mu_{\gamma 2} \frac{\omega_{\gamma 2}}{\omega_{\gamma 1}} \right] \right\} + \frac{e^2 c}{2\pi \hbar (2\pi \hbar \omega)^{1/2}} \int_0^{\infty} \mathcal{L} e^{-x} d\Omega dx. \quad (22)$$

The average energy of the system is

$$\bar{E} = -\frac{d}{d\lambda} \ln Z, \quad (23)$$

and the limit of this expression as $\lambda \rightarrow \infty$ yields the energy E_0 of the polaron ground state.

Let T_n be the operator of the translation of the electron and polarization of the crystal through a whole-number lattice vector n . The Hamiltonian (1) is an invariant of this translation and commutes with T_n . Therefore the state of the polaron is an eigenfunction of T_n with eigenvalue $\exp(i\mathbf{K} \cdot \mathbf{n})$. Thus, \mathbf{K} is a continuous quantum number (the quasimomentum of the polaron) and the polaron energy depends on \mathbf{K} . The dispersion law near the energy minimum in the polaron band is assumed to be of the form

$$E(\mathbf{K}) = E_0 + \sum_{\gamma} \frac{\hbar^2}{2\mathfrak{M}_{\gamma}} (K_{\gamma} - K_{\gamma \min})^2, \quad (24)$$

where \mathfrak{M}_{γ} are the effective masses of the polaron. Calculating on the basis of (24) the sum of states at low temperatures and comparing it with (20), we obtain for the dimensionless average polaron mass

$$\mathfrak{M}_0 = \left(\prod_{\gamma} \frac{\mathfrak{M}_{\gamma}}{\mu_{\gamma}} \right)^{1/3} = e^{2/3}. \quad (25)$$

We obtained the maximum of the trial sum of states Z_1 with respect to the parameters μ_{γ} and $C_{\nu\gamma}$ with the aid of a computer, for cases when the equal-energy surface has axial symmetry. We calculated the polaron ground-state energy E_0 and \mathfrak{M}_0 as functions of the dimensionless coupling constant α and of the anisotropy parameter χ of the band effective masses:

$$\alpha = \frac{ce^2}{2\hbar} \left(\frac{2\mu_{\perp}}{\hbar\omega} \right)^{1/2}, \quad \chi = \frac{\mu_{\parallel}}{\mu_{\perp}}, \quad (26)$$

where $\mu_{\perp} = \mu_1 = \mu_2$, $\mu_{\parallel} = \mu_3$. In the isotropic case, i.e., at $\chi = 1$ and when one auxiliary particle is used, our results (23) and (25) go over exactly into the corresponding formulas of [9]. In the case of two auxiliary particles and $\chi = 1$, the only published calculation of E_0 and \mathfrak{M}_0 is for $\alpha = 3$ [8]. Our results agree in this case with [8]. As seen from the tables, the introduction of the second auxiliary particle changes E_0 and \mathfrak{M}_0 by fractions of one percent in comparison with the case of one auxiliary particle. Therefore the anisotropic cases were calculated only with one auxiliary particle. In this case

$$f_0 = -\frac{\omega_1(\nu_1-1)^2}{\omega \nu_1} - \frac{\omega_3(\nu_3-1)^2}{\omega 2\nu_3} + 2\alpha \nu_3 \sqrt{\frac{\chi}{\pi}} \int_0^{\infty} \frac{e^{-x} f(y-1)}{X_3^{1/2}} dx, \quad (27)$$

$$f_1 = 2 \ln \nu_1 + \ln \nu_3 - \frac{3}{2} + \frac{1}{\nu_1^2} + \frac{1}{2\nu_3^2} \quad (28)$$

$$+ \frac{\alpha \nu_3}{2} \sqrt{\frac{\chi}{\pi}} \int_0^{\infty} \left[f(y-1) - 2f'(y-1) \left(\chi \frac{\nu_3^2}{\nu_1^2} - y \right) \right] \frac{x^2 e^{-x}}{X_3^{1/2}} dx,$$

where

$$X_i = x + \frac{\omega}{\omega_i} \left(\nu_i - \frac{1}{\nu_i} \right) \left[1 - \exp\left(-\frac{\omega_i}{\omega} \nu_i x\right) \right], \quad i=1, 3, \quad (29)$$

$$y = \chi \left(\frac{\nu_3}{\nu_1} \right)^2 \frac{X_1}{X_3}, \quad (30)$$

$$f(y) = \begin{cases} y^{-1/2} \operatorname{arctg} y^{1/2}, & y \geq 0 \\ 1/2 (-y)^{-1/2} \ln \left[(1+(-y)^{1/2}) / (1-(-y)^{1/2}) \right], & y < 0 \end{cases}$$

and $\omega_1, \omega_3, \nu_1 = (1 + \mu_{11}/\mu_{\perp})^{1/2}$, $\nu_3 = (1 + \mu_{31}/\mu_{\parallel})$ are variational parameters.

In the limiting case of weak coupling, formulas (27) and (28) yield results that coincide with [1]. Even at $\alpha = 2$, the value of E_0 obtained in the present paper is only 3–4% lower than in [1]. In the limiting case of strong coupling, Eq. (27) goes over into the correspond-

TABLE I. Dependence of the negative dimensionless polaron energy $-E_0/\hbar\omega$ on the coupling constant α and on the anisotropy parameter χ

χ	$\log_{10} \chi$	α								
		1	2	3	4	5	6	7	8	9
$s = 1$										
0.107	-10	0.623	1.259	1.908	2.574	3.258	3.964	4.696	5.460	—
0.134	-9	0.661	1.335	2.024	2.731	3.459	4.212	4.995	5.817	6.686
0.165	-8	0.699	1.412	2.143	2.833	3.666	4.468	5.305	6.187	7.128
0.210	-7	0.737	1.491	2.263	3.038	3.878	4.731	5.624	6.572	7.591
0.262	-6	0.777	1.571	2.383	3.225	4.094	4.999	5.953	6.971	8.077
0.328	-5	0.816	1.652	2.510	3.335	4.313	5.274	6.291	7.386	8.586
0.410	-4	0.856	1.733	2.635	3.567	4.536	5.553	6.637	7.815	9.119
0.512	-3	0.896	1.814	2.760	3.733	4.760	5.837	6.993	8.261	9.676
0.64	-2	0.935	1.896	2.886	3.912	4.986	6.125	7.357	8.723	10.26
0.8	-1	0.974	1.976	3.010	4.085	5.213	6.416	7.730	9.202	10.86
$s = 2$										
1	0	1.013	2.056	3.136	4.262	5.448	6.722	8.126	9.740	11.50
$s = 1$										
1	0	1.013	2.055	3.133	4.256	5.440	6.711	8.113	9.696	11.48
1.25	1	1.051	2.133	3.255	4.427	5.667	7.008	8.504	10.20	12.13
1.562	2	1.088	2.210	3.374	4.599	5.893	7.309	8.903	10.72	12.79
1.953	3	1.123	2.284	3.492	4.761	6.118	7.612	9.309	11.26	13.47
2.441	4	1.158	2.356	3.606	4.924	6.342	7.917	9.722	11.80	14.16
3.052	5	1.191	2.426	3.717	5.083	6.564	8.224	10.14	12.35	14.85
3.815	6	1.223	2.493	3.824	5.239	6.783	8.532	10.56	12.90	15.56
4.768	7	1.253	2.557	3.928	5.391	7.001	8.840	10.98	13.46	16.26
5.960	8	1.282	2.619	4.027	5.540	7.216	9.147	11.41	14.01	16.96
7.450	9	1.310	2.677	4.123	5.684	7.427	9.454	11.83	14.57	17.67
9.313	10	1.335	2.732	4.214	5.823	7.636	9.758	12.25	15.12	18.36

TABLE II. Dependence of the average polaron effective mass \mathfrak{M}_0 on α and χ

χ	$\log_{10} \chi$	α								
		1	2	3	4	5	6	7	8	9
$s = 1$										
0.107	-10	1.114	1.256	1.437	1.677	1.997	2.452	3.135	4.211	—
0.134	-9	1.122	1.275	1.473	1.735	2.103	2.637	3.463	4.818	7.227
0.168	-8	1.129	1.294	1.510	1.805	2.219	2.845	3.858	5.615	8.891
0.210	-7	1.137	1.314	1.549	1.874	2.350	3.031	4.348	6.677	11.23
0.262	-6	1.145	1.334	1.590	1.951	2.495	3.382	4.959	8.065	14.32
0.328	-5	1.153	1.356	1.634	2.037	2.660	3.726	5.728	9.897	18.65
0.410	-4	1.162	1.378	1.681	2.133	2.853	4.129	6.725	12.42	24.19
0.512	-3	1.170	1.401	1.729	2.229	3.063	4.617	7.991	15.70	31.13
0.64	-2	1.179	1.424	1.781	2.338	3.323	5.227	9.589	19.97	39.96
0.8	-1	1.187	1.448	1.834	2.456	3.578	5.955	11.79	25.04	50.96
$s = 2$										
1	0	1.196	1.474	1.896	2.597	3.922	6.894	14.42	31.54	62.79
$s = 1$										
1	0	1.196	1.473	1.892	2.587	3.910	6.880	14.32	31.49	62.60
1.25	1	1.204	1.498	1.952	2.729	4.275	7.998	17.74	39.39	77.22
1.562	2	1.213	1.524	2.015	2.887	4.704	9.361	21.98	48.29	92.59
1.953	3	1.221	1.549	2.082	3.054	5.228	11.07	26.59	58.62	110.1
2.441	4	1.229	1.576	2.152	3.245	5.835	13.08	32.14	69.61	128.6
3.052	5	1.237	1.602	2.225	3.465	6.518	15.40	37.88	80.96	149.0
3.815	6	1.245	1.629	2.302	3.698	7.351	18.21	44.46	93.52	169.8
4.768	7	1.253	1.656	2.383	3.957	8.287	21.14	51.78	106.6	193.4
5.960	8	1.260	1.683	2.469	4.242	9.402	24.55	59.38	121.3	217.4
7.450	9	1.268	1.710	2.557	4.562	10.54	28.28	67.20	135.0	240.6
9.313	10	1.275	1.737	2.650	4.910	11.88	32.28	75.26	149.3	263.6

ing formula of^[2], if we confine ourselves in^[2] to approximation of the electron wave function by a Gaussian curve.

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