Ground state of a pair of acceptor impurity centers in a cubic semiconductor

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The quadrupole-quadrupole interaction between shallow acceptor impurity centers in a cubic semiconductor is studied. When the distance R between the impurity centers is large, this interaction decreases more slowly with R than the dispersion interaction or the interaction associated with the overlap of the wave functions. The problem of "molecular" terms and of the wave functions of a pair of acceptors is solved exactly for $R \gg a$, where a is the effective Bohr radius. Estimates are obtained for shallow acceptors in germanium.

1. INTRODUCTION

Experimental investigations of the interaction between shallow impurities in semiconductors are currently being made on materials in which the concentration of the main impurity is high, but the degree of compensation K is minimal (see, for example, Ref. 1). In this case at low temperature when the impurities are frozen-out, almost all the impurity centers are neutral, the Coulomb fields are weak, and the interaction between neutral impurity centers can be observed in a fairly pure form. Materials of this kind are of interest also as sensitive extrinsic photodetectors with a relatively long photocarrier lifetime (because of the low concentration of charged impurity centers acting as traps).

We shall consider a cubic semiconductor doped with shallow acceptors and uncompensated. We shall assume that the impurity concentration N is low compared with the concentration N_{sm} corresponding to a semiconductor-metal transition, so that we can ignore the overlap of the wave functions of neighboring impurity centers, but insufficiently low to regard impurity centers as isolated (a semiconductor with such an impurity concentration can be called moderately doped). A special feature of acceptors with the T_d symmetry (substitutional impurities) in cubic semiconductors is that their ground state is quadruply degenerate (Γ_s level) in the absence of deformation and of electric and magnetic fields. The following problem arises: what is the ground state of a system of neutral acceptors for such moderate impurity concentrations N and how do the neighboring acceptors with a complex ground state affect one another. A solution of this problem is required, in particular, to determine the low-temperature thermodynamic properties of a semiconductor doped with acceptor impurities, and to determine the phonon absorption spectrum of such a semiconductor.

Any neutral atoms separated by a sufficiently large distance R from one another experience a dispersion (van der Waals) interaction proportional to R^{-6} and also an interaction which decreases exponentially with R and is due to the overlap of the wave functions of the atoms. A special feature of neutral acceptor atoms in a cubic semiconductor is that there is also a quadrupole-quadrupole interaction between them which decreases on increase in the interatomic distance as R^{-5}, i.e., more slowly than the other two interactions. In fact, although the average (over all four levels of the ground state) quadrupole moment of an atom vanishes like the dipole moment, the quadrupole moments of the individual levels are nonzero because the wave function of an acceptor in each of the four levels of the ground state includes not only a function of the s type ($L = 0$), but also a contribution from a spherical function with $L = 2$ (see Sec. 3).

If we ignore the overlap of the wave functions, we find that at absolute zero a system of impurity centers is in a state corresponding to the minimum of the energy of the quadrupole-quadrupole interaction (QQI) and of the dispersion interaction. In view of the random distribution of impurities, a cubic semiconductor which is doped with shallow acceptors and uncompensated represents a form of quadrupole glass in which the quadrupole moments of the particle are not fixed but are determined by the interaction between the particles.

The main interest lies not in the reduction of the energy of the ground state of a system of impurity centers compared with the energy of isolated impurities, but in the whole structure of levels formed from degenerate levels of the individual impurities under the influence of the impurity-impurity interaction, i.e., the structure of the impurity energy band. It is this structure that determines the thermodynamics of a doped crystal and the absorption of phonons in it. In contrast to the usual case of a compensated semiconductor, for which the width of an impurity energy band is governed by the fields of charged impurities,[2] in the case under discussion the width of the band is governed by the QQI (and also by the dispersion interaction). We shall find the energy spectrum of two acceptor impurity centers formed from the ground states of these centers when they approach each other. This will allow us to determine in particular the scales of the effects which appear in an acceptor-doped semiconductor as a function of the impurity concentration.

2. HAMILTONIAN OF THE MULTIPOLE INTERACTION BETWEEN TWO NEUTRAL ACCEPTOR IMPURITY CENTERS

We shall consider two acceptors impurity centers which are separated by a fairly large distance $R \gg a$ from one another (a is the effective Bohr radius of an impurity center). We shall use r_1 and r_2 to denote the radius vectors measured from the impurity ions, $x_{1\alpha}$ and $x_{2\alpha}$ to denote their components, and X_α for the components of the vector $\mathbf{R}$ joining the two impurity centers. The energy of the multipole interaction between impurity centers is generally given by (we shall retain only the first two terms of the multipole expansion)

$$H = H_{dd} + H_{QQ}, \tag{1}$$

where

$$H_{dd}=-\frac{e^2}{\varkappa}V_{\alpha\beta}x_{1\alpha}x_{2\beta}, \qquad H_{QQ}=\frac{e^2}{4\varkappa}V_{\alpha\beta\gamma\delta}x_{1\alpha}x_{1\beta}x_{2\gamma}x_{2\delta}, \qquad (2)$$

$$V_{\alpha\beta}=\frac{\partial^2}{\partial X_\alpha\,\partial X_\beta}\frac{1}{R}, \qquad V_{\alpha\beta\gamma\delta}=\frac{\partial^4}{\partial X_\alpha\,\partial X_\beta\,\partial X_\gamma\,\partial X_\delta}\frac{1}{R}. \qquad (2a)$$

Here, H_{dd} and H_{QQ} represent the dipole-dipole and the quadrupole-quadrupole interaction, respectively; $\varkappa$ is the permittivity of the semiconductor.

We shall use $\psi_m(\mathbf{r})$ to denote the wave function of an isolated acceptor corresponding to the mth level of the ground quadruplet. Ignoring the overlap of the wave functions of the acceptors, we shall find the molecular wave functions in the form of a linear combination of products:

$$\Psi_{m_1 m_2}(\mathbf{r}_1,\ \mathbf{r}_2)\equiv|m_1 m_2\rangle=\psi_{m_1}(\mathbf{r}_1)\,\psi_{m_2}(\mathbf{r}_2). \qquad (3)$$

The matrix of the interaction energy derived using the functions described by Eq. (3) includes contributions from the first approximation with respect to H_{QQ} and from the second approximation with respect to H_{dd}:

$$\langle m_1 m_2|H|m_1'm_2'\rangle=\langle m_1 m_2|H_{QQ}|m_1'm_2'\rangle$$
$$+\langle m_1 m_2|H_{dis}|m_1'm_2'\rangle, \qquad (4)$$

$$\langle m_1 m_2|H_{dis}|m_1'm_2'\rangle$$
$$=-\sum_{n_1 n_2}\frac{\langle m_1 m_2|H_{dd}|n_1 n_2\rangle\langle n_1 n_2|H_{dd}|m_1'm_2'\rangle}{E_{n_1}+E_{n_2}-2E_0}. \qquad (4a)$$

The indices n_1 and n_2 are used to label the excited states of the acceptors (including the states in the continuous spectrum) to which dipole optical transitions from the ground level E_0 are allowed; E_n are the energies of these states. The first term on the right-hand side of Eq. (4) is the QQI matrix and the second is the dispersion (the van der Waals) interaction matrix.

3. QUADRUPOLE-QUADRUPOLE INTERACTION MATRIX

Since the Laplacian is $\Delta(1/R)=0$, we can represent the operator H_{QQ} in the form

$$H_{QQ}=\frac{e^2}{4\varkappa}V_{\alpha\beta\gamma\delta}\left(x_{1\alpha}x_{1\beta}-\frac{1}{3}r_1^2\delta_{\alpha\beta}\right)\left(x_{2\gamma}x_{2\delta}-\frac{1}{3}r_2^2\delta_{\gamma\delta}\right). \qquad (5)$$

The parameter $\delta=(\gamma_3-\gamma_2)/\gamma_1$ (the γ_i are the Luttinger parameters of the valence band) describing the correlation of the constant-energy surfaces of holes is small for almost all cubic semiconductors. An important exception to this rule is silicon. We shall therefore consider only the spherical approximation ($\delta=0$) for acceptors. In this approximaton the states of an acceptor are described by the parity, the quantum number F of the total angular momentum, and the quantum number F_z representing the projection of the total momentum. In the ground (even) state we have $F=3/2$ and $m\equiv F_z=\pm1/2,\ \pm3/2$. In the spherical approximation, we have

$$\langle m|x_\alpha x_\beta-\tfrac{1}{3}r^2\delta_{\alpha\beta}|m'\rangle=\tfrac{1}{3}Q(J_{\alpha\beta}^{(2)})_{mm'}, \qquad (6)$$

where

$$J_{\alpha\beta}^{(2)}=\tfrac{1}{2}(J_\alpha J_\beta+J_\beta J_\alpha)-\tfrac{1}{3}J^2\delta_{\alpha\beta},$$

J_α are the familiar matrices of the momentum of order $2F+1$, and Q is the quadrupole moment given by

$$Q=-6a^2\left[\frac{2F+1}{(2F-1)(2F+3)F(F+1)}\right]^{1/2}$$

$$\times\Bigg\{(2L+1)\begin{pmatrix}L&2&L\\0&0&0\end{pmatrix}$$

$$\times\begin{Bmatrix}L&F&J\\F&L&2\end{Bmatrix}\int_0^\infty dr\,r^4 R_L^2$$

$$+2[(2L+1)(2L+5)]^{1/2}\begin{pmatrix}L&2&L+2\\0&0&0\end{pmatrix}$$

$$\times\begin{Bmatrix}L&F&J\\F&L+2&2\end{Bmatrix}\int_0^\infty dr\,r^4 R_L R_{L+2}$$

$$+(2L+5)\begin{pmatrix}L+2&2&L+2\\0&0&0\end{pmatrix}$$

$$\times\begin{Bmatrix}L+2&F&J\\F&L+2&2\end{Bmatrix}\int_0^\infty dr\,r^4 R_{L+2}^2\Bigg\}. \qquad (7)$$

Here, $a=\hbar^2\varkappa\gamma_1/m_0 e^2$ is the effective Bohr radius; L is the quantum number of the orbital momentum which is either $F-3/2$ or $F-1/2$, depending on the parity ($L=0$ in the ground state); R_L are the radial functions of an acceptor; the radial variable in the integrand is dimensionless (it is expressed in units of a); the brace contain the $6j$ symbols characterized by $J=3/2$, whereas the parentheses contain the $3j$ symbols.

It follows from Eq. (7) that in the ground state ($F=3/2,\ L=0$), we have

$$Q=\frac{4}{5}a^2\int_0^\infty dr\,r^4 R_0(r)R_2(r), \qquad (8)$$

i.e., a nonzero quadrupole moment of an acceptor appears because the "spin-orbit" term in the Hamiltonian of holes mixes the states $|\gamma L\rangle$ and $|\gamma,L+2\rangle$ (γ is the set of all other quantum numbers).

Using Eq. (8) and the explicit form of the matrices J_α, we can represent the matrix H_{QQ} quite simply using the functions of Eq. (3) (this will be a 16×16 matrix). Let us assume that

$$\hat{B}=\begin{pmatrix}2^{-1/2}B_0&iB_{-1}&-B_{-2}&0\\iB_1&-2^{-1/2}B_0&0&-B_{-2}\\-B_2&0&-2^{-1/2}B_0&-iB_{-1}\\0&-B_2&-iB_1&2^{-1/2}B_0\end{pmatrix}, \qquad (9)$$

where B_q ($q=0,\pm1,\pm2$) are the components of an irreducible second rank tensor (with zero trace) derived in the usual manner[3] from the components of the gradient $\partial/\partial X$. Then, the matrix $\hat{H}_{QQ}$ in Eq. (4) is

$$\hat{H}_{QQ}=^1/_{12}E_a a Q^2(\hat{B}\otimes\hat{B})/R. \qquad (10)$$

Here, $E_a=m_0 e^4/\hbar^2\varkappa^2\gamma_1$ and the symbol $\otimes$ represents the Kronecker multiplication of matrices.

If the direction of the quantization axis is parallel to the radius vector $\mathbf{R}$ joining two impurity centers, then in the case of a tensor $V_{\alpha\beta\gamma\delta}$ symmetric with respect to any pair of indices [see Eq. (2a)] has components which vanish except for those of the $V_{\alpha\alpha\beta\beta}$ type. Then the matrix $\hat{H}_{QQ}$ of Eq.

(10) becomes greatly "rarefied," can be factored, and is easily diagonalized. However, we shall diagonalize directly the total matrix (4) representing the interaction of two acceptors.

4. DISPERSION INTERACTION

In the spherical approximation the numerator of Eq. (4a) can be represented in the form of a product of two sums over F_z and F'_z:

$$V_{\alpha\beta}V_{\gamma\delta}\frac{e^2}{\varkappa}\sum_{F_z}\langle m_1|x_\alpha|n_1F_1F_z\rangle\langle n_1F_1F_z|x_\gamma|m_1'\rangle$$

$$\times\frac{e^2}{\varkappa}\sum_{F_z'}\langle m_2|x_\beta|n_2F_2F_z'\rangle\langle n_2F_2F_z'|x_\delta|m_2'\rangle. \quad (11)$$

Here, n labels the energy levels of the states with F, the indices n_0F_0 of the ground state are omitted for the sake of simplicity, and the values of L are not given because they are determined uniquely by the parity selection rule and by the magnitude of F for a given state.

We can show that the sum over F_z in Eq. (11) is

$$\frac{e^2}{\varkappa}\sum_{F_z}\langle m|x_\alpha|nFF_z\rangle\langle nFF_z|x_\gamma|m'\rangle$$

$$=\frac{1}{2}a^3E_a\frac{f(nF)}{E_{nF}-E_0}\{\delta_{mm'}\delta_{\alpha\gamma}+\lambda(F)(J_{\alpha\gamma}^{(2)})_{mm'}\}. \quad (12)$$

Here, $f(nF)$ is the oscillator strength of a dipole optical transition from the groun state to a state nF. In the spherical approximation these transitions are allowed only to the states with $F = 1/2, 3/2$, and $5/2$. The coefficients $\lambda(F)$ for such values F are $-1, 4/5$, and $-1/5$, respectively.

We shall define a matrix B^F with the following elements:

$$B_{11}^F=B_{44}^F=[1-{}^1\!/_2\lambda(F)](V_{x,x}+V_{y,y})+[1+\lambda(F)]V_{z,z},$$
$$B_{22}^F=B_{33}^F=[1+{}^1\!/_2\lambda(F)](V_{x,x}+V_{y,y})+[1-\lambda(F)]V_{z,z},$$

$$B_{12}^F=B_{21}^{F\bullet}=-B_{34}^F=-B_{43}^{F\bullet}$$
$$=\frac{\sqrt{3}}{2}\lambda(F)(V_{y,z}+V_{z,y}+iV_{x,z}+iV_{z,x}), \quad (13)$$

$$B_{13}^F=B_{31}^{F\bullet}=B_{24}^F=B_{42}^{F\bullet}=\frac{\sqrt{3}}{2}\lambda(F)(-V_{x,x}+V_{y,y}+iV_{x,y}+iV_{y,x}),$$

$$B_{14}^F=B_{23}^F=B_{32}^F=B_{41}^F=0.$$

The quantities $V_{\alpha,\beta}$ introduced here obey the following multiplication rule: $V_{\alpha,\gamma}V_{\beta,\delta}=V_{\alpha\beta}V_{\gamma\delta}$.

It follows from Eq. (2), (4a), and (12) that

$$\hat{H}_{dis}=-E_a\sum_{n_1F_1n_2F_2}A(n_1F_1n_2F_2)\hat{B}^{F_1}\otimes\hat{B}^{F_2}, \quad (14)$$

where

$$A=\frac{1}{4}\frac{f(n_1F_1)}{E_{n_1F_1}-E}\frac{f(n_2F_2)}{E_{n_2F_2}+E_0}\frac{1}{E_{n_1F_1}+E_{n_2F_2}-2E_0}. \quad (15)$$

In the expression for A the energies are measured in units of E_a.

If the quantization axis is parallel to the vector joining the impurity atoms, then the only nonzero diagonal elements are $V_{\alpha\beta}$, where $V_{xx}=V_{yy}=R^{-3}$ and $V_{zz}=-2R^{-3}$. In

the case of the matrix $\hat{H}_{dis}$ of Eq. (14) the nonzero elements are the same as those of the matrix $\hat{H}_{QQ}$ of Eq. (10). They can be expressed in terms of linear combinations of three dimensionless constants:

$$C_1=12\sum_{n_1F_1n_2F_2}A(n_1F_1n_2F_2), \quad C_2=12\sum_{n_1F_1n_2F_2}\lambda(F_1)A(n_1F_1n_2F_2),$$

$$C_3=3\sum_{n_1F_1n_2F_2}\lambda(F_1)\lambda(F_2)A(n_1F_1n_2F_2). \quad (16)$$

5. MOLECULAR TERMS AND WAVE FUNCTIONS OF AN ACCEPTOR PAIR

The matrix (4) of the interaction between acceptor impurity centers deduced using Eqs. (10) and (14), can be factored and is easily diagonalized. We shall classify the resultant "molecular" terms on the basis of a general theory of terms of diatomic molecules.[4] Since we are assuming that the distances between the atoms are large, the interaction between them is weak compared with the spin-orbit interaction in each of the atoms and the system then represents the case of Hund c-coupling.[4] Since the system consists of identical atoms located at identical distances, the molecular terms can be described by the absolute value $|\Omega|$ of the projection of the total angular momentum of a molecule along the axis joining the atoms, by the parity of the relative change of the signs of the coordinates of holes (indices g or u), and if $\Omega = 0$-also by the $+$ and $-$ sign corresponding to whether the sign of the wave function does not change or changes as a result of reflection in a plane containing the axis of the molecule. There is a total of $(2F+1)\times(F+1)=10$ terms: one of the $3_u, 2_u, 2_g, 1_g$ each and two terms of the $1_u, 0_g^+$, and 0_u^- types. All the terms with $\Omega\neq 0$ are doubly degenerate, whereas those with $\Omega = 0$ are nondegenerate.

We shall now define the following characteristic quantities with the dimensions of energy

$$E_{QQ}=\frac{1}{2}E_a\left(\frac{Q^2}{a^4}\frac{a}{R}\right)^5, \quad E_{dis}=\frac{1}{2}E_a\left(\frac{a}{R}\right)^6. \quad (17)$$

Then, the molecular terms of an acceptor pair originating from the ground states of the acceptors are (in the order of increasing energy of the QQI):

$$E_1(2_u)=-7E_{QQ}-(C_1-7C_3)E_{dis},$$
$$E_2(1_g)=-4E_{QQ}-(C_1-5C_3)E_{dis},$$
$$E_3(1_u)=-2E_{QQ}-(C_1-C_3)E_{dis},$$
$$E_4(0_u^-)=3E_{QQ}-(C_1+3C_3)E_{dis}$$
$$-[C_2^2E_{dis}^2+(5E_{QQ}-6C_3E_{dis})^2]^{1/2},$$
$$E_5(0_g^+)=3E_{QQ}-(C_1+3C_3)E_{dis}$$
$$-[C_2^2E_{dis}^2+(3E_{QQ}-2C_3E_{dis})^2]^{1/2},$$
$$E_6(2_g)=E_{QQ}-(C_1+C_3)E_{dis}, \quad (18)$$
$$E_7(1_u)=3E_{QQ}-(C_1-C_2+3C_3)E_{dis},$$
$$E_8(3_u)=3E_{QQ}-(C_1+C_2+3C_3)E_{dis},$$
$$E_9(0_g^+)=3E_{QQ}-(C_1+3C_3)E_{dis}$$
$$+[C_2^2E_{dis}^2+(3E_{QQ}-2C_3E_{dis})^2]^{1/2},$$
$$E_{10}(0_u^-)=3E_{QQ}-(C_1+3C_3)E_{dis}$$
$$+[C_2^2E_{dis}^2+(5E_{QQ}-6C_3E_{dis})^2]^{1/2}.$$

We shall see from the estimates given below that for the

Sh. M. Kogan and A. F. Polupanov   171

distances between the impurity centers under consideration the order of the terms given by Eq. (18) is retained when we allow not only for the QQI, but also for the dispersion interaction.

In view of the complexity of the expressions (in particular, in the expression for the wave functions the coefficients of the 0_g^+ and 0_u^- terms at dependent R), we shall give only the wave functions of two orders of the ground state (because we either take all the upper signs or all the lower signs):

$$\psi_1(2_u) = 2^{-1/2}\{|\pm^3/_2\rangle_1|\pm^1/_2\rangle_2 + |\pm^1/_2\rangle_1|\pm^3/_2\rangle_2\}, \quad (19)$$

and also the wave functions of the terms $E_3(1_u)$ and $E_7(1_u)$:

$$\psi_3(1_u) = 2^{-1/2}\{|\pm^3/_2\rangle_1|\mp^1/_2\rangle_2 + |\mp^1/_2\rangle_1|\pm^3/_2\rangle_2\},$$
$$\psi_7(1_u) = |\pm^1/_2\rangle_1|\pm^1/_2\rangle_2.$$

6. ESTIMATE OF THE SPLITTING OF THE MOLECULAR TERMS OF A PAIR OF ACCEPTORS IN Ge

We shall estimate the energies of Eq. (18) in the case of acceptors in Ge, because the spherical approximation for shallow acceptors is satisfactory for Ge and, moreover, in the case of acceptors in Ge we know quite well both the spectrum, including the oscillator strengths and the photoeffect cross sections[5] and the quadrupole moments and the polarizability.[6] We shall obtain estimates for the minimum distance $R = R_0$ at which these approximations are still valid. In accordance with a criterion used in molecular spectroscopy,[7] we can represent the energy of the interaction between two atoms A and B in the form of a sum of the first terms of the multipole expansion for $R > 2[\langle r_A^2 \rangle^{1/2} + \langle r_B^2 \rangle^{1/2}]$, where $\langle r_A^2 \rangle$ is the mean-square value of the distance of an electron from a nucleus in the atom A. A calculation carried out using the wave functions obtained earlier[5] gives $R_0 = 4\langle r^2 \rangle^{1/2} = 350$ Å for Ge. Substituting the known value of the quadrupole moment,[6] we find that $E_{QQ}(R_0) \approx 0.8$ μeV. If $R = R_0$, then $E_{dis} = 3.9$ μeV.

In calculating the coefficients C_i one would need to determine multiple sums over the states in a discrete spectrum and integrate the continuous spectrum, which is a difficult task. One can use the London approximation to estimate the dispersion interaction[8] by approximating each sum in Eq. (16) by just one term. Such an estimate is valid because the polarizability of shallow acceptors in Ge considered in the spherical approximation is governed largely by one contribution from the strongest dipole transition to the level with $F = 5/2$ (Ref. 6). We then have

$$C_1 = \frac{3}{2}\left(\frac{\alpha}{\alpha_0}\right)^2 |E|, \quad C_2 = \frac{3}{2}\frac{\alpha\alpha_1}{\alpha_0^2} |E|,$$
$$C_3 = \frac{3}{8}\left(\frac{\alpha_1}{\alpha_0}\right)^2 |E|. \quad (20)$$

The polarizabilities are now given by

$$\alpha = \alpha_0 \sum_{nF} \frac{f(nF)}{(E_{nF}-E_0)^2}, \quad \alpha_1 = \alpha_0 \sum_{nF} \lambda(F) \frac{f(nF)}{(E_{nF}-E_0)^2},$$
$$\alpha_0 = \varkappa a^3, \quad (21)$$

where $|E|$ is the characteristic energy usually assumed to be equal to the ionization energy of an atom. In the case of shallow acceptors in Ge, we have $|E| \approx 1.25$ and the polarizabilities α and α_1 have been calculated earlier[6]: $\alpha/\alpha_0 = 0.36$, $\alpha_1/\alpha_0 = -0.092$.

Substituting the above values of the parameters in Eq. (18), we can find the energies of the molecular terms originating from the ground levels of shallow acceptors in Ge when they approach each other to a distance of $R_0 = 350$ Å (these energeis are in μeV): -6.4, -4.1; -2.51; -2.49; -0.96; -0.14; 1.2; 1.7; 3.8; 5.3. We can demonstrate that the depth of the ground state and the width of the whole impurity band are determined primarily by the QQI and are of the order of $10\,\mu$eV. The dispersion interaction is important only for the terms 5 and 6; it slightly splits the terms 3 and 4, and 7 and 8. The difference between the energies of these terms is $\sim 1\,\mu$eV. It follows from these estimates that at the acceptor concentrations such that the influence of the overlap of the wave functions of the ground states can be ignored, compared with the multipole interaction, this interaction may be manifested in the thermodynamics of acceptor-doped Ge crsytals only at temperatures below 1 K. One would expect the absorption of sound to manifest the molecular splitting of terms due to the QQI and the dispersion interaction also at higher temperatures.

We shall conclude by noting the relationships analogous to Eqs. (6) and (12) (see Ref. 6) and, therefore, the method of constructing the perturbation matrices $\hat{H}_{QQ}$ of Eq. (10) and $\hat{H}_{dis}$ of Eq. (14) can be generalized to the case when the spherical approximation is invalid and the quantization axis is linked to the cubic axes.

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