

Hole bound states in the deformation field of screw dislocations in cubic semiconductors

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For the spherically averaged Hamiltonian approximation an accurate nonvariational calculation is reported of the energies of the one-dimensional bands split off from the edge of the valence band by the shear strain fields of screw dislocations in various cubic semiconductors. The calculation gives significantly greater binding energies for holes than previous variational calculations and also a different order of the first two levels when the ratio of light- and heavy-hole masses is less than 0.19. The calculation was performed on the basis of the effective-mass and deformation-potential approximations. This approach is justified because the resulting binding energies are much smaller than the energy gaps. The results may be used for the interpretation of various dislocation-related phenomena such as luminescence, absorption, microwave conductivity, and combined resonance (a kind of electric-dipole spin resonance).

I. INTRODUCTION

Bound states for electrons and holes at dislocations in semiconductors can originate from three main factors: long-range strain and electric fields of the dislocation; dangling bonds and defects in the dislocation core; impurities and intrinsic defects in the vicinity of the dislocation. In principle, different experimental techniques exist to distinguish between the three types of dislocation states,¹ but the results are not always conclusive.

In the present paper we will be interested in dislocation bound states arising from the long-range strain field. These states form a set of one-dimensional (1D) dislocation bands split off from the valence- and conduction-band edges.

This set of 1D-dislocation bands is responsible for a wide range of the dislocation-related phenomena such as dislocation photoluminescence and cathodoluminescence;¹⁻⁶ dislocation light absorption below the intrinsic absorption edge;^{7,8} dislocation conductivity and microwave conductivity.⁹⁻¹¹

Theoretical calculations of the energy positions of the 1D-dislocation bands can be divided in two groups. The first group consist of the quantum chemical calculations, which take into account the discrete atomic structure of the crystal. At present the result of these calculations are contradictory and strongly depend on the approximations made and parameters chosen.¹²⁻¹⁸

The second group consists of the variational calculations made in the continuous media approach,¹⁹⁻²⁷ which is based on empirical effective-mass and deformation-potential approximations. Both these approximations fail in the vicinity of the dislocation core, but the approach seems to be justified for shallow 1D-dislocation bands arising from the dislocation strain field because the characteristic size of the resulting wave functions is larger than dislocation core and therefore core should not affect these states strongly.

Previous theoretical calculations of the structure and

the energy positions of the 1D-dislocation bands in the continuous medium approximation were mainly restricted to the case of electron bound states with few exceptions^{19-21,27} where hole bound states were also considered. This is because of the fact that valence band in cubic semiconductors has a complex structure and consists of subbands of light and heavy holes and thus the variational calculations of hole binding energies becomes very complicated and their accuracy is rather low.

However, the hole 1D-dislocation bands can play an important role in the various dislocation-related optical phenomena and may also be responsible for the dislocation conductivity in *p*-doped crystals.⁹⁻¹¹

In this connection, of special interest is the case of screw dislocations in direct gap semiconductors where the strain field has only shear components and no dislocation bound states exist for electrons in the continuous medium approximation. In this case the 1D-hole dislocation bands should provide the main contribution to the shifts of the dislocation-related optical lines with respect to the band gap and also to the capture cross section of volume excitons into dislocation bound states. It may be noted, for example, that the low-temperature Y_0 cathodoluminescence line in ZnSe has been found in association with screw dislocations.²⁸

In the present paper a highly precise nonvariational method is suggested for calculation of hole binding energies and wave functions at screw dislocations in cubic semiconductors. This method is based on a direct finding with an iteration procedure the four solutions of corresponding Schrödinger equation, which are finite at dislocation line and then making a linear combination of this solution which possesses the correct asymptotic behavior at large distances. Actually this method is a generalization of the method,²⁹ which has been successfully used for highly accurate nonvariational calculations of hole binding energies and wave functions at shallow acceptors.

Using this approach we have found that hole binding energies at screw dislocation are much greater than previ-

ous variational calculation¹⁹⁻²¹ gave and the order of the first two levels is also different when ratio of light- and heavy-hole masses is lower than 0.19.

The calculation was made in the continuous medium approximation assuming that the hole states are rather shallow in comparison with the band gap and possess, typically, binding energies of a few tens of meV.

The spherical approximation was used for description of the deformation field of screw dislocation and hole dispersion law. If necessary the nonspherical terms in the

Hamiltonian can be also taken into account by using perturbation theory.

II. GENERAL HAMILTONIAN

We start by writing down the Hamiltonian for holes in the strain field of the screw dislocation according to the continuous medium approximation.

The hole kinetic energy H_0 can be described by the Luttinger effective-mass Hamiltonian³⁰

$$H_0 = \frac{1}{2m} [(\gamma_1 + \frac{5}{2}\gamma_2)\mathbf{p}^2 I - 2\gamma_2(p_x^2 S_x^2 + p_y^2 S_y^2 + p_z^2 S_z^2) - 4\gamma_3(p_x p_y \{S_x S_y\} + p_x p_z \{S_x S_z\} + p_y p_z \{S_y S_z\})], \quad (1)$$

where $\mathbf{p} = -i\hbar\nabla$; S_i are 4×4 matrices of the hole spin projections, corresponding to hole spin $S = \frac{3}{2}$; $\{S_i S_j\} = (S_i S_j + S_j S_i)/2$ and I is unit matrix; $\gamma_1, \gamma_2, \gamma_3$ are parameters introduced by Luttinger, and m is the free-electron mass.

According to Ref. 31 the potential $V(\mathbf{r})$ for hole interaction with an external strain field has the form

$$V(\mathbf{r}) = -(a + \frac{5}{2}b) \sum_i u_{ii} I + b \sum_i u_{ii} S_i^2 + 2d/\sqrt{3} \sum_{i>j} u_{ij} \{S_i S_j\}, \quad (2)$$

where u_{ij} is a strain tensor which depends on the hole position coordinate \mathbf{r} , a , b , and d are deformation-potential constants. The signs of H_0 and $V(\mathbf{r})$ in (1) and (2) correspond to positive hole energies.

In the following we will use spherical approximations for the description of the valence band and for the hole-strain field coupling. Performing the spherical averaging of (1) and (2) by the method suggested in Ref. 32 it is easy to obtain a spherically symmetrical effective Hamiltonian

$$H = H_0 + V(\mathbf{r}),$$

$$H_0 = \frac{1}{2m} [(\gamma_1 + \frac{5}{2}\gamma_2)\mathbf{p}^2 I - 2\gamma(\mathbf{p}\mathbf{S})^2], \quad (3)$$

$$V(\mathbf{r}) = -(a + \frac{5}{2}b') \sum_i u_{ii} I + b' \sum_{i,j} u_{ij} \{S_i S_j\},$$

where $\gamma = (2\gamma_2 + 3\gamma_3)/5$ and $b' = (2b + \sqrt{3}d)/5$.

For a screw dislocation which lies along the z axis, the strain tensor for an isotropic continuous medium is well known (e.g., Ref. 33),

$$\begin{aligned} u_{xz}(r) = u_{zx}(r) &= \frac{Br_y}{4\pi r^2}, \\ u_{yz}(r) = u_{zy}(r) &= -\frac{Br_x}{4\pi r^2}, \end{aligned} \quad (4)$$

where $r = \sqrt{r_x^2 + r_y^2}$ is the distance from dislocation axis and B is the modulus of Burgers vector (we use the capital letter in order to distinguish it from deformation potential b).

Using the explicit forms of matrices $\{S_i S_j\}$ given in Ref. 31 we obtain the expression for potential-energy operator,

$$V(r) = \frac{\sqrt{3}Bb'}{4\pi r^2} \begin{vmatrix} 0 & -r_- & 0 & 0 \\ -r_+ & 0 & 0 & 0 \\ 0 & 0 & 0 & r_- \\ 0 & 0 & r_+ & 0 \end{vmatrix}, \quad (5)$$

where $r_{\pm} = r_x \pm ir_y$.

The explicit matrix form of the kinetic-energy operator is

$$H_0 = \frac{1}{2m} \begin{vmatrix} (\gamma_1 - 2\gamma)p_z^2 + (\gamma_1 + \gamma)p_- p_+ & -i2\sqrt{3}\gamma p_z p_- & \sqrt{3}\gamma p_-^2 & 0 \\ i2\sqrt{3}\gamma p_z p_+ & (\gamma_1 + 2\gamma)p_z^2 + (\gamma_1 - \gamma)p_- p_+ & 0 & \sqrt{3}\gamma p_-^2 \\ \sqrt{3}\gamma p_+^2 & 0 & (\gamma_1 + 2\gamma)p_z^2 + (\gamma_1 - \gamma)p_- p_+ & i2\sqrt{3}\gamma p_z p_- \\ 0 & \sqrt{3}\gamma p_+^2 & -i2\sqrt{3}\gamma p_z p_+ & (\gamma_1 - 2\gamma)p_z^2 + (\gamma_1 + \gamma)p_- p_+ \end{vmatrix}, \quad (6)$$

where $p_{\pm} = p_x \pm ip_y$.

The full Hamiltonian, which is the sum of (5) and (6), possesses an axial symmetry and therefore the projection of the total angular momentum \mathbf{J} on the z axis generates $J_z = M$ as a conserving quantum number which can take only half-integer values $\pm\frac{1}{2}, \pm\frac{3}{2}, \pm\frac{5}{2}, \dots$.

The Hamiltonian possesses also a translation symmetry along the z axis and therefore p_z is a conserving quantum number as well.

Thus, the general form of the wave function is

$$\Psi^{M,p_z}(r,z,\phi) = \begin{pmatrix} \exp[i(M-\frac{3}{2})\phi]\chi_{3/2}^{M,p_z}(r) \\ \exp[i(M-\frac{1}{2})\phi]\chi_{1/2}^{M,p_z}(r) \\ \exp[i(M+\frac{1}{2})\phi]\chi_{-1/2}^{M,p_z}(r) \\ \exp[i(M+\frac{3}{2})\phi]\chi_{-3/2}^{M,p_z}(r) \end{pmatrix} e^{ip_z z/\hbar}. \quad (7)$$

The Schrödinger equation for the four-spinor radial part $\chi^{M,p_z}(r)$ of the hole wave function can be found by the unitary transformation, U , of the Hamiltonian (3)

$$H' = U^+ H U, \quad (8)$$

where U and $\chi(r)$ have the forms

$$U = \begin{pmatrix} \exp[i(M-\frac{3}{2})\phi]; 0; 0; 0 \\ 0; \exp[i(M-\frac{1}{2})\phi]; 0; 0 \\ 0; 0; \exp[i(M+\frac{1}{2})\phi]; 0 \\ 0; 0; 0; \exp[i(M+\frac{3}{2})\phi] \end{pmatrix}, \quad (9)$$

$$\chi^{M,p_z}(r) = \begin{pmatrix} \chi_{3/2}^{M,p_z}(r) \\ \chi_{1/2}^{M,p_z}(r) \\ \chi_{-1/2}^{M,p_z}(r) \\ \chi_{-3/2}^{M,p_z}(r) \end{pmatrix},$$

and $\chi^{M,p_z}(r)$ satisfies the equation

$$H' \chi^{M,p_z}(r) = E \chi^{M,p_z}(r). \quad (10)$$

Using the relations

$$\begin{aligned} p_+ \exp[ia\phi] f(r) &= \exp[i(a+1)\phi] \left[p_r + \frac{ia\hbar}{r} \right] f(r), \\ p_- \exp[ia\phi] f(r) &= \exp[i(a-1)\phi] \left[p_r - \frac{ia\hbar}{r} \right] f(r), \end{aligned} \quad (11)$$

where $p_r = -i\hbar\partial/\partial r$, we can easily find, from (6) to (10), the unitary transformed form of H as

$$H' = \frac{1}{2m} \left[p_r^2 A - \frac{i\hbar}{r} p_r B + \frac{\hbar^2}{r^2} C + p_z^2 D + ip_z p_r F + p_z \frac{\hbar}{r} G \right] + \frac{q^2}{r} Q, \quad (12)$$

where $q = (\sqrt{3}Bb'/4\pi)^{1/2}$ is an "effective charge" and the explicit forms of the 4×4 matrix A, B, C, D, F, G, Q are

$$\begin{aligned} A &= \begin{pmatrix} \gamma_1 + \gamma & 0 & \sqrt{3}\gamma & 0 \\ 0 & \gamma_1 - \gamma & 0 & \sqrt{3}\gamma \\ \sqrt{3}\gamma & 0 & \gamma_1 - \gamma & 0 \\ 0 & \sqrt{3}\gamma & 0 & \gamma_1 + \gamma \end{pmatrix}, \quad B = \begin{pmatrix} \gamma_1 + \gamma & 0 & 2\sqrt{3}\gamma M & 0 \\ 0 & \gamma_1 - \gamma & 0 & 2\sqrt{3}\gamma(M+1) \\ -2\sqrt{3}\gamma(M-1) & 0 & \gamma_1 - \gamma & 0 \\ 0 & -2\sqrt{3}\gamma M & 0 & \gamma_1 + \gamma \end{pmatrix}, \\ C &= \begin{pmatrix} (\gamma_1 + \gamma)(M - \frac{3}{2}) & 0 & -\sqrt{3}\gamma(M + \frac{1}{2})(M - \frac{3}{2}) & 0 \\ 0 & (\gamma_1 - \gamma)(M - \frac{1}{2})^2 & 0 & -\sqrt{3}\gamma(M + \frac{1}{2})(M - \frac{3}{2}) \\ -\sqrt{3}\gamma(M + \frac{1}{2})(M - \frac{3}{2}) & 0 & (\gamma_1 - \gamma)(M + \frac{1}{2})^2 & 0 \\ 0 & -\sqrt{3}\gamma(M + \frac{1}{2})(M - \frac{3}{2}) & 0 & (\gamma_1 + \gamma)(M + \frac{3}{2})^2 \end{pmatrix}, \quad (13) \\ D &= \begin{pmatrix} (\gamma_1 - 2\gamma) & 0 & 0 & 0 \\ 0 & (\gamma_1 + 2\gamma) & 0 & 0 \\ 0 & 0 & (\gamma_1 + 2\gamma) & 0 \\ 0 & 0 & 0 & (\gamma_1 - 2\gamma) \end{pmatrix}, \quad F = \begin{pmatrix} 0 & -2\sqrt{3}\gamma & 0 & 0 \\ 2\sqrt{3}\gamma & 0 & 0 & 0 \\ 0 & 0 & 0 & 2\sqrt{3}\gamma \\ 0 & 0 & -2\sqrt{3}\gamma & 0 \end{pmatrix}, \\ G &= \begin{pmatrix} 0 & -2\sqrt{3}\gamma(M - \frac{1}{2}) & 0 & 0 \\ -2\sqrt{3}\gamma(M - \frac{3}{2}) & 0 & 0 & 0 \\ 0 & 0 & 0 & 2\sqrt{3}\gamma(M + \frac{3}{2}) \\ 0 & 0 & 2\sqrt{3}\gamma(M + \frac{1}{2}) & 0 \end{pmatrix}, \quad Q = \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \end{aligned}$$

Because of time-reversal symmetry of the Hamiltonian (12) the solutions of (10) with $M < 0$ can be found from those with $M > 0$ by application of the time-reversal operator

$$\chi^{-M, p_z}(r) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \left[\chi^{M, -p_z}(r) \right]^* . \quad (14)$$

Thus, in the following, we will restrict ourselves to considering only states with $M > 0$.

Because the heavy-hole subband provides the main contribution in the hole binding energies at screw dislocation, it is convenient to use the corresponding effective atomic units of distance r_0 , momentum p_0 , and energy Ry^* (the effective Rydberg), which are given by the formulas

$$r_0 = \frac{\hbar^2}{m_h q^2}, \quad p_0 = \frac{\hbar}{r_0}, \quad Ry^* = \frac{m_h q^2}{2\hbar^2}, \quad (15)$$

where $m_h = m / (\gamma_1 - 2\gamma)$ is the mass of the heavy hole.

In these units the Schrödinger equation (10) for four-spinor radial part of wave function $\chi^{M, p_z}(r)$ takes the form

$$(H'' + \varepsilon)\chi^{M, p_z}(x) = 0, \quad (16)$$

where $x = r/r_0$ is the distance in effective Bohr radii and $\varepsilon = -E/Ry^*$ is hole binding energy measured in effective Rydbergs.

$$\begin{aligned} T(M, n)f_n^{(1)} &= (\gamma_1 - 2\gamma)(\varepsilon f_{n-2}^{(1)} - 2Qf_{n-1}^{(1)}) - [(2n-1)A + B]f_n^{(2)} - 2Af_n^{(3)}, \\ T(M, n)f_n^{(2)} &= (\gamma_1 - 2\gamma)(\varepsilon f_{n-2}^{(2)} - 2Qf_{n-1}^{(2)}) - 2[(2n-1)A + B]f_n^{(3)} - 6Af_n^{(4)}, \\ T(M, n)f_n^{(3)} &= (\gamma_1 - 2\gamma)(\varepsilon f_{n-2}^{(3)} - 2Qf_{n-1}^{(3)}) - 3[(2n-1)A + B]f_n^{(4)}, \\ T(M, n)f_n^{(4)} &= (\gamma_1 - 2\gamma)(\varepsilon f_{n-2}^{(4)} - 2Qf_{n-1}^{(4)}), \end{aligned} \quad (20)$$

where $T(M, n) = n(n-1)A + nB + C$.

In order for the spinor coefficients $f_n^{(i)}$ to become zero when $n < N$, it is necessary that $\det\{T(M, N)\} = 0$. The direct calculation with the use of (13) gives

$$\det\{T(M, n)\} = D_1 D_2, \quad (21)$$

where

$$\begin{aligned} D_1 &= (\gamma_1^2 - 4\gamma^2)[n^2 - (M - \frac{3}{2})^2][n^2 - (M + \frac{1}{2})^2], \\ D_2 &= (\gamma_1^2 - 4\gamma^2)[n^2 - (M - \frac{1}{2})^2][n^2 - (M + \frac{3}{2})^2]. \end{aligned} \quad (22)$$

Thus the determinant is equal to zero when $n = M - \frac{3}{2}$, $M - \frac{1}{2}$, $M + \frac{1}{2}$, $M + \frac{3}{2}$ for $M \geq \frac{3}{2}$.

A special case is that of $M = \frac{1}{2}$ when $\det\{T(\frac{1}{2}, n)\}$ has two single roots when $n = 0$, $n = 2$ and one double root when $n = 1$.

Let us start with this special case.

Because $\det\{T(\frac{1}{2}, n)\} = 0$ when $n = 0, 2$ and has a double root when $n = 1$ we can find four four-spinors $e_0, e_1, \tilde{e}_1, e_2$ such that

The corresponding Hamiltonian H'' is

$$H'' = \frac{1}{\gamma_1 - 2\gamma} \left[-A \frac{\partial^2}{\partial x^2} - \frac{B}{x} \frac{\partial}{\partial x} - \frac{C}{x^2} + D \left(\frac{p_z}{p_0} \right)^2 + F \left(\frac{p_z}{p_0} \right) \frac{\partial}{\partial x} + \frac{Gp_z}{x} \right] + \frac{2Q}{x}, \quad (17)$$

III. WAVE FUNCTIONS AND BINDING ENERGIES

In the present paper we will be interested in the hole binding energies at the centers of 1D-dislocation bands and thus will put $p_z = 0$ in (17), but the method to be considered for solving (16) at $p_z = 0$ is also applicable for $p_z \neq 0$.

First we would like to note that the four solutions of (16) which are finite at $x = 0$ can be found in the form

$$\chi^{M, p_z}(x) = \phi_1(x) + \phi_2(x)\ln(x) + \phi_3(x)\ln^2(x) + \phi_4(x)\ln^3(x), \quad (18)$$

where the four-spinor functions $\phi_i(x)$ are analytical at $x = 0$ and can be expanded in series of powers of x

$$\phi_i(x) = \sum_{n=0}^{\infty} f_n^{(i)} x^n. \quad (19)$$

The substitution of (18), (19) in (16), (17) at $p_z = 0$ leads to the following recurrence relations between four-spinor coefficients $f_n^{(i)}$:

$$\begin{aligned} T(\frac{1}{2}, 0)e_0 &= 0, \quad T(\frac{1}{2}, 1)e_1 = 0, \\ T(\frac{1}{2}, 1)\tilde{e}_1 &= 0, \quad T(\frac{1}{2}, 2)e_2 = 0, \end{aligned} \quad (23)$$

and also four four-spinors $g_0, g_1, \tilde{g}_1, g_2$ such as that

$$\begin{aligned} g_0 T(\frac{1}{2}, 0) &= 0, \quad g_1 T(\frac{1}{2}, 1) = 0, \\ \tilde{g}_1 T(\frac{1}{2}, 1) &= 0, \quad g_2 T(\frac{1}{2}, 2) = 0. \end{aligned} \quad (24)$$

TABLE I. Spinor coefficients $f_n^{(i)}$ of four solutions of Eq. (16) for radial part of hole wave function. $\chi^{M, p_z}(x) = \sum_{n=0}^{\infty} x^n \{f_n^{(1)} + f_n^{(2)}\ln(x) + f_n^{(3)}\ln^2(x) + f_n^{(4)}\ln^3(x)\}$, for the case $M = \frac{1}{2}$, $p_z = 0$. [Coefficients a_n, b_n, c_n, d_n and factors k_1, k_2, k_3, k_4 should be found from recurrence relations (20).]

	Solution 1	Solution 2	Solution 3	Solution 4
$f_n^{(1)}$	a_n	b_n	c_n	d_n
$f_n^{(2)}$	0	0	$k_1 a_n$	$k_4 a_n + k_3 b_n + k_2 c_n$
$f_n^{(3)}$	0	0	0	$k_1 k_2 a_n / 2$
$f_n^{(4)}$	0	0	0	0

The explicit forms of these spinors are

$$\begin{aligned}
 e_0 &= \begin{vmatrix} 0 \\ 1 \\ 0 \\ 0 \end{vmatrix}, \quad e_1 = \begin{vmatrix} 1 \\ 0 \\ 0 \\ 0 \end{vmatrix}, \quad \bar{e}_1 = \begin{vmatrix} 0 \\ 0 \\ 1 \\ 0 \end{vmatrix}, \quad e_2 = \begin{vmatrix} 0 \\ 2\sqrt{3}\gamma \\ 0 \\ \gamma - \gamma_1 \end{vmatrix}, \\
 g_0 &= \begin{vmatrix} 0 \\ 1 \\ 0 \\ 0 \end{vmatrix}, \quad g_1 = \begin{vmatrix} 1 \\ 0 \\ 0 \\ 0 \end{vmatrix}, \quad \bar{g}_1 = \begin{vmatrix} 0 \\ 0 \\ 1 \\ 0 \end{vmatrix}, \quad g_2 = \begin{vmatrix} 0 \\ 0 \\ 0 \\ 1 \end{vmatrix}.
 \end{aligned}
 \tag{25}$$

$$T^{-1}(\frac{1}{2}, 1) = \begin{vmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{T_{44}(\frac{1}{2}, 1)}{D_2} & 0 & -\frac{T_{24}(\frac{1}{2}, 1)}{D_2} \\ 0 & 0 & 0 & 0 \\ 0 & -\frac{T_{42}(\frac{1}{2}, 1)}{D_2} & 0 & \frac{T_{22}(\frac{1}{2}, 1)}{D_2} \end{vmatrix}, \tag{26}$$

$$T^{-1}(\frac{1}{2}, 2) = \begin{vmatrix} \frac{T_{33}(\frac{1}{2}, 2)}{D_1} & 0 & -\frac{T_{13}(\frac{1}{2}, 2)}{D_1} & 0 \\ 0 & \frac{1}{T_{22}(\frac{1}{2}, 2)} & 0 & 0 \\ -\frac{T_{31}(\frac{1}{2}, 2)}{D_1} & 0 & \frac{T_{11}(\frac{1}{2}, 2)}{D_1} & 0 \\ 0 & 0 & 0 & 0 \end{vmatrix}. \tag{27}$$

To solve (16) we also will need the matrices $T^{-1}(\frac{1}{2}, n)$ in order to use (20) for recursion finding $f_n^{(i)}$. These matrices are well defined for $n > 2$ when $\det\{T(\frac{1}{2}, n)\} \neq 0$ but for $n = 1, 2$ we need to introduce an additional definition of $T^{-1}(\frac{1}{2}, n)$ because the usual inverse matrices do not exist in these cases.

We like to define the $T^{-1}(\frac{1}{2}, n)$ in these cases in the following way:

$$\begin{aligned}
 a_0 &= 0, \quad a_1 = 0, \quad a_2 = e_2, \\
 a_n &= T^{-1}(\frac{1}{2}, n)[(\gamma_1 - 2\gamma)(\epsilon a_{n-2} + 2Qa_{n-1})] \quad \text{for } n > 2; \\
 b_0 &= 0, \quad b_1 = e_1, \\
 b_n &= T^{-1}(\frac{1}{2}, n)[(\gamma_1 - 2\gamma)(\epsilon b_{n-2} + 2Qb_{n-1})] \quad \text{for } n > 1; \\
 c_0 &= 0, \quad c_1 = \bar{e}_1, \\
 c_n &= T^{-1}(\frac{1}{2}, n)\{(\gamma_1 - 2\gamma)(\epsilon c_{n-2} + 2Qc_{n-1}) - [2(n-1)A + B]k_1 a_n\} \quad \text{for } n > 1; \\
 d_0 &= e_2, \quad d_n = T^{-1}(\frac{1}{2}, n)\{(\gamma_1 - 2\gamma)(\epsilon c_{n-2} + 2Qc_{n-1}) - [2(n-1)A + B](k_4 a_n + k_3 b_n + k_2 c_n) - Ak_1 k_2 a_n\} \quad \text{for } n > 0,
 \end{aligned}
 \tag{28}$$

and the factors k_1, k_2, k_3, k_4 should be found from conditions

$$\begin{aligned}
 \langle g_2 | (\gamma_1 - 2\gamma)(\epsilon c_{n-2} + 2Qc_{n-1}) - [2(n-1)A + B]k_1 a_n \rangle &= 0 \quad \text{for } n = 2, \\
 \langle g_n | (\gamma_1 - 2\gamma)(\epsilon c_{n-2} + 2Qc_{n-1}) - [2(n-1)A + B](k_4 a_n + k_3 b_n + k_2 c_n) - Ak_1 k_2 a_n \rangle &= 0 \quad \text{for } n = 1, 2, \\
 \langle \bar{g}_n | (\gamma_1 - 2\gamma)(\epsilon c_{n-2} + 2Qc_{n-1}) - [2(n-1)A + B](k_4 a_n + k_3 b_n + k_2 c_n) - Ak_1 k_2 a_n \rangle &= 0 \quad \text{for } n = 1.
 \end{aligned}
 \tag{29}$$

Thus, for case $M = \frac{1}{2}, p_z = 0$ we have built all four solutions $\chi^{M, p_z, i}(x)$, where $i = 1, 2, 3, 4$ is the solution number, of the Schrödinger equation (16), which are finite at $x = 0$.

Now let us consider the case of $M \geq \frac{3}{2}$.

In this case $\det\{T(M, n)\}$ has a single root when $n = M - \frac{3}{2}, M - \frac{1}{2}, M + \frac{1}{2}, M + \frac{3}{2}$, and corresponding eight four-spinors $e_n^{(M)}, g_n^{(M)}$ which met the conditions

$$T(M, n)e_n^{(M)} = 0, \quad g_n^{(M)}T(M, n) = 0 \tag{30}$$

are

$$\begin{aligned}
 e_{M-3/2}^{(M)} &= \begin{vmatrix} 1 \\ 0 \\ 0 \\ 0 \end{vmatrix}, \quad e_{M-1/2}^{(M)} = \begin{vmatrix} 0 \\ 1 \\ 0 \\ 0 \end{vmatrix}, \quad e_{M+1/2}^{(M)} = \begin{vmatrix} \sqrt{3}\gamma(4M^2-1) \\ 0 \\ -2(\gamma_1+\gamma)(2M-1) \\ 0 \end{vmatrix}, \\
 e_{M+3/2}^{(M)} &= \begin{vmatrix} 0 \\ \sqrt{3}\gamma[4(M+1)^2-1] \\ 0 \\ -2(\gamma_1-\gamma)(2M+1) \end{vmatrix}, \quad g_{M-3/2}^{(M)} = \begin{vmatrix} (\gamma_1-\gamma)[(M-\frac{3}{2})^2-(M-\frac{1}{2})^2] \\ 0 \\ \sqrt{3}\gamma[4(M+1)^2-1] \\ 0 \end{vmatrix}, \\
 g_{M-1/2}^{(M)} &= \begin{vmatrix} 0 \\ (\gamma_1-\gamma)[(M-\frac{1}{2})^2-(M+\frac{3}{2})^2] \\ 0 \\ -\sqrt{3}\gamma(4M^2-1)^2 \end{vmatrix}, \quad g_{M+1/2}^{(M)} = \begin{vmatrix} 0 \\ 0 \\ 1 \\ 0 \end{vmatrix}, \quad g_{M+1/2}^{(M)} = \begin{vmatrix} 0 \\ 0 \\ 0 \\ 1 \end{vmatrix}.
 \end{aligned} \tag{31}$$

In order to find the solutions of (16) we will also need matrices $T^{-1}(M, n)$, which are well defined for $n > M + \frac{3}{2}$ but additional definitions should be made for $n = M + \frac{3}{2}, M + \frac{1}{2}, M - \frac{1}{2}$.

We like to define $T^{-1}(M, n)$ in these cases in the following way.

For $n = M + \frac{3}{2}$,

$$T^{-1}(M, n) = \begin{vmatrix} \frac{T_{33}(M, n)}{D_1} & 0 & -\frac{T_{13}(M, n)}{D_1} & 0 \\ 0 & \frac{1}{T_{22}(M, n)} & 0 & 0 \\ -\frac{T_{31}(M, n)}{D_1} & 0 & \frac{T_{11}(M, n)}{D_1} & 0 \\ 0 & 0 & 0 & 0 \end{vmatrix}. \tag{32}$$

For $n = M + \frac{1}{2}$,

$$T^{-1}(M, n) = \begin{vmatrix} \frac{1}{T_{11}(M, n)} & 0 & 0 & 0 \\ 0 & \frac{T_{44}(M, n)}{D_2} & 0 & -\frac{T_{24}(M, n)}{D_2} \\ 0 & 0 & 0 & 0 \\ 0 & -\frac{T_{42}(M, n)}{D_2} & 0 & \frac{T_{22}(M, n)}{D_2} \end{vmatrix}. \tag{33}$$

For $n = M - \frac{1}{2}$,

$$T^{-1}(M, n) = \begin{vmatrix} \frac{T_{33}(M, n)}{D_1} & 0 & -\frac{T_{13}(M, n)}{D_1} & 0 \\ 0 & 0 & 0 & 0 \\ -\frac{T_{31}(M, n)}{D_1} & 0 & \frac{T_{11}(M, n)}{D_1} & 0 \\ 0 & 0 & 0 & \frac{1}{T_{44}(M, n)} \end{vmatrix}. \tag{34}$$

The four solutions of (16) for the case of $M \geq \frac{3}{2}$ can be taken in the forms (18), (19) with $f_n^{(i)}$ shown in Table II, where four-spinor coefficients a_n, b_n, c_n, d_n , found from recurrence relations (20), are

TABLE II. Spinor coefficients $f_n^{(i)}$ of four solutions of Eq. (16) for the radial part of the hole wave function. $\chi^{M,p_z}(x) = \sum_{n=0}^{\infty} x^n \{f_n^{(1)} + f_n^{(2)} \ln(x) + f_n^{(3)} \ln^2(x) + f_n^{(4)} \ln^3(x)\}$, for the case $M \geq \frac{3}{2}$, $p_z = 0$. [Coefficients a_n, b_n, c_n, d_n and factors k_1, k_2, k_3, k_4 should be found from recurrence relations (20).]

	Solution 1	Solution 2	Solution 3	Solution 4
$f_n^{(1)}$	a_n^M	b_n^M	c_n^M	d_n^M
$f_n^{(2)}$	0	$k_1^M a_n^M$	$k_3^M a_n^M + k_2^M b_n^M$	$k_6^M a_n^M + k_5^M b_n^M + k_4^M c_n^M$
$f_n^{(3)}$	0	0	$k_1^M k_2^M a_n^M / 2$	$(k_1^M k_5^M + k_3^M k_4^M) a_n^M / 2 + k_2^M k_4^M b_n^M / 2$
$f_n^{(4)}$	0	0	0	$k_1^M k_2^M k_4^M a_n^M / 6$

$$\begin{aligned}
a_n^{(M)} &= 0 \text{ for } n < M + \frac{3}{2}, \quad a_{M+3/2}^{(M)} = e_{M+3/2}^{(M)}, \\
a_n^M &= T^{-1}(M, n) [(\gamma_1 - 2\gamma)(\epsilon a_{n-2}^M + 2Qa_{n-1}^M)] \text{ for } n > M + \frac{3}{2}; \\
b_n^M &= 0 \text{ for } n < M + \frac{1}{2}, \quad b_{M+1/2}^{(M)} = e_{M+1/2}^{(M)}, \\
b_n^M &= T^{-1}(M, n) \{(\gamma_1 - 2\gamma)(\epsilon b_{n-2}^M + 2Qb_{n-1}^M) - [2(n-1)A + B]k_1^M a_n^M\} \text{ for } n > M + \frac{1}{2}; \\
c_n^M &= 0 \text{ for } n < M - \frac{1}{2}, \quad c_{M-1/2}^{(M)} = e_{M-1/2}^{(M)}, \\
c_n^M &= T^{-1}(M, n) \{(\gamma_1 - 2\gamma)(\epsilon c_{n-2}^M + 2Qc_{n-1}^M) - [2(n-1)A + B](k_3^M a_n^M + k_2^M b_n^M) - Ak_1^M k_2^M a_n^M\} \text{ for } n > M - \frac{1}{2}; \\
d_n^M &= 0 \text{ for } n < M - \frac{3}{2}, \quad d_{M-3/2}^{(M)} = e_{M-3/2}^{(M)}, \\
d_n^M &= T^{-1}(M, n) \{(\gamma_1 - 2\gamma)(\epsilon d_{n-2}^M + 2Qd_{n-1}^M) \\
&\quad + [2(n-1)A + B](k_6^M a_n^M + k_5^M b_n^M + k_4^M c_n^M) - A[(k_1^M k_5^M + k_3^M k_4^M) a_n^M / 2 + k_2^M k_4^M b_n^M]\} \text{ for } n > M - \frac{3}{2};
\end{aligned} \tag{35}$$

and the factors $k_1^M, k_2^M, k_3^M, k_4^M, k_5^M, k_6^M$ should be found from the conditions

$$\begin{aligned}
\langle g_n^{(M)} | (\gamma_1 - 2\gamma)(\epsilon b_{n-2}^M + 2Qb_{n-1}^M) - [2(n-1)A + B]k_1^M a_n^M \rangle &= 0 \text{ for } n = M + \frac{3}{2}; \\
\langle g_n^{(M)} | (\gamma_1 - 2\gamma)(\epsilon c_{n-2}^M + 2Qc_{n-1}^M) - [2(n-1)A + B](k_3^M a_n^M + k_2^M b_n^M) - Ak_1^M k_2^M a_n^M \rangle &= 0 \text{ for } n = M + \frac{1}{2}, M + \frac{3}{2}; \\
\langle g_n^{(M)} | (\gamma_1 - 2\gamma)(\epsilon d_{n-2}^M + 2Qd_{n-1}^M) - [2(n-1)A + B](k_6^M a_n^M + k_5^M b_n^M + k_4^M c_n^M) \\
&\quad \times A[(k_1^M k_5^M + k_3^M k_4^M) a_n^M / 2 + k_2^M k_4^M b_n^M] \rangle = 0 \text{ for } n = M - \frac{1}{2}, M + \frac{1}{2}, M + \frac{3}{2}.
\end{aligned} \tag{36}$$

Thus we have found a recursion procedure which allows us to obtain for case $p_z = 0$ all four solutions $\chi^{M,p_z,i}(x)$ of the Schrödinger equation (16) which are finite at $x = 0$ ($i = 1, 2, 3, 4$ is the solution number).

In order to get the eigenfunctions of (16) and corresponding energies of bound states we need to make a linear combination of $\chi^{M,p_z,i}(x)$ which decreases at $x = \infty$.

The four asymptotic solutions $\chi^{M,p_z,i(as)}(x)$ which decreases at $x = \infty$ can be obtained directly from (16) in the form

$$\chi^{M,p_z,i(as)}(x) = x^{-1/2} e^{-\eta_i x} s_i, \tag{37}$$

where $\eta_1 = \eta_2 = \sqrt{\epsilon}$, $\eta_3 = \eta_4 = \sqrt{\epsilon(\gamma_1 - 2\gamma)/(\gamma_1 + 2\gamma)}$, and four four-spinors s_i are

$$s_1 = \begin{pmatrix} 1 \\ 0 \\ -\sqrt{3} \\ 0 \end{pmatrix}, \quad s_2 = \begin{pmatrix} 0 \\ -\sqrt{3} \\ 0 \\ 1 \end{pmatrix}, \quad s_3 = \begin{pmatrix} \sqrt{3} \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad s_4 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \sqrt{3} \end{pmatrix}. \tag{38}$$

The linear combination of $\chi^{M,p_z,i}(x)$ decreasing at $x = \infty$ exists only for such energies ϵ when eight eight-spinors $V^k(x)$, $k = 1, \dots, 8$, which are determined as

$$V^i(x) = \begin{vmatrix} \chi^{M,p_z,i}(x) \\ \frac{\partial}{\partial x} \chi^{M,p_z,i}(x) \end{vmatrix}, \quad V^{i+4}(x) = \begin{vmatrix} \chi^{M,p_z,i(as)}(x) \\ \frac{\partial}{\partial x} \chi^{M,p_z,i(as)}(x) \end{vmatrix}, \tag{39}$$

$i = 1, \dots, 4,$

become linear dependent at $x = \infty$.

This condition can be written in the form

$$\det W(x) = 0 \text{ when } x = \infty, \tag{40}$$

where $W(x)$ is an 8×8 matrix $W_{sk}(x) = V_s^k(x)$, and s is a spinor index of $V^k(x)$.

Actually (40) is the quantization condition which allows to calculate the hole binding energies and wave functions with high accuracy using the recursion procedure described above.

Applying this approach we have calculated the binding energies of the six deepest hole levels at screw dislocation whose quantum numbers are $M = \frac{1}{2}$, $n = 0, 1, 2$; $M = \frac{3}{2}$,

$n=0, 1$; $M=\frac{5}{2}$, $n=0$, where n is a radial quantum number.

In this calculation we have approximated the infinite sum in (19) by the finite sum of 70 first terms and the $x \rightarrow \infty$ in quantization condition (57) was approximated by $x = 10/\sqrt{\epsilon}$. These approximations provide the accuracy of the binding energies of about 1%.

The results of this calculation for various ratios m_l/m_h of the light m_l and the heavy m_h hole masses are shown in Figs. 1 and 2. A comparison of the results with the previous variational calculation¹⁹ shows that for case $m_l=m_h$ our calculation gives for the main states corresponding to $M=\frac{3}{2}$, $n=0$ and $M=\frac{1}{2}$, $n=0$ binding energies only greater by a factor of 1.07. But for the case $m_l/m_h=0.1$ the hole energy levels have been found to be significantly deeper than those given in Ref. 19. For the state with $M=\frac{3}{2}$, $n=0$ the binding energy is 1.58 times greater, and for the state with $M=\frac{1}{2}$, $n=0$, 2.43 times greater.

We also have found that for $m_l/m_h < 0.19$ the order of the two deepest levels with $M=\frac{3}{2}$, $n=0$ and $M=\frac{1}{2}$, $n=0$ changes and the level with $M=\frac{1}{2}$, $n=0$ becomes the main bound state.

The results of the calculation of binding energies for various cubic semiconductors are shown in Table III and the parameters used in the calculation of the effective Rydbergs value are shown in Table IV.

It can be seen from Table III that the hold bound states in all cases are rather shallow and, therefore, the continuous medium approximation, used in this paper, was justified.

We have also used the spherical approximation to the hole dispersion law and an isotropic dislocation strain field. Further improvement of the precision of our calculation of the binding energies could be achieved by taking into account the anisotropic terms in the Hamiltonian (1), (2) by use of perturbation theory.

The anisotropic part of the Hamiltonian (1), (2) has only nondiagonal matrix elements between eigenfunctions of the spherically averaged Hamiltonian (3) being

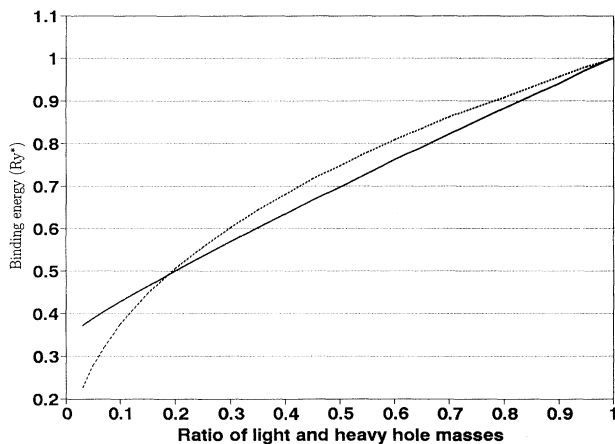


FIG. 1. Hole binding energies at the screw dislocation: $M=\frac{1}{2}$, $n=0$ (—); $M=\frac{3}{2}$, $n=0$ (---).

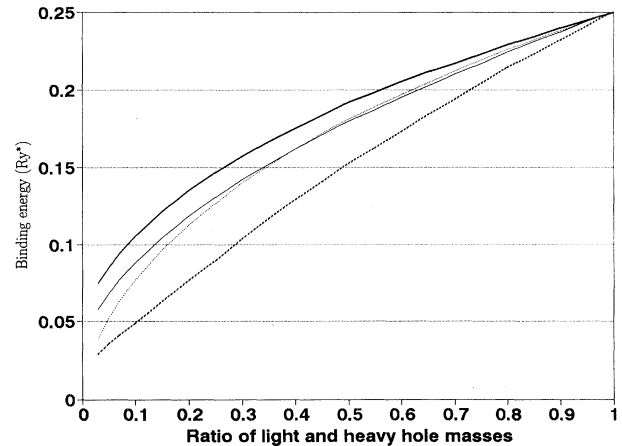


FIG. 2. Hole binding energies at the screw dislocation: $M=\frac{1}{2}$, $n=1$ (—); $M=\frac{3}{2}$, $n=1$ (---); $M=\frac{5}{2}$, $n=0$ (· · ·); $M=\frac{1}{2}$, $n=2$ (- · - ·).

nonzero and thus the perturbation should lead to an additional increase in the hole binding energy for the main bound state.

A comparison of the hole binding energies for Si and Ge given in Table III with the results of previous variational calculations^{20,21} (26 meV for Si and 8 and 12 meV for Ge) shows a significant increase in the corresponding energies due to a more precise solution of the Schrödinger equation with the spherically averaged continuous-medium-approximated Hamiltonian (3) in this paper.

Experimental binding energies for holes at screw dislocations found from measurements of the dislocation-related Hall effect for Ge (Refs. 34–36) and the dislocation-related microwave conductivity for Si (Refs. 10 and 11) are 35 and 80 meV, respectively.

For ZnSe the hole binding energy 163 meV can be obtained from the energy of the screw dislocation-related photoluminescence line (2.60 eV) and the screw

TABLE III. Hole binding energies for two deepest bound states $E(M=\frac{1}{2}, n=0)$ and $E(M=\frac{3}{2}, n=0)$ at the screw dislocation in various semiconductors.

Compound	$E(M=\frac{1}{2}, n=0)$ (meV)	$E(M=\frac{3}{2}, n=0)$ (meV)
Si	37	39
Ge	20	19
AlSb	62	53
GaP	33	34
GaAs	36	34
GaSb	24	21
InP	46	42
InAs	18	13
InSb	27	17
ZnS	32	30
ZnSe	53	50
ZnTe	63	58
CdTe	72	62

TABLE IV. Parameters used for calculating the effective Rydberg values Ry^* for various semiconductors. The experimental values for deformation-potential constants were taken from the review article (Ref. 40) and the Luttinger constants were taken from Ref. 41.

Compound	B (Å)	b (eV)	d (eV)	b' (eV)	γ_1	γ_2	γ_3	γ	m_l/m_h	Ry^* (meV)
Si	3.84	-2.2	-5.1	-2.65	4.22	0.39	1.44	1.02	0.35	60
Ge	4.00	-2.3	-5.0	-2.65	13.4	4.25	5.69	5.11	0.135	44
AlSb	4.34	-1.4	-4.3	-2.05	4.15	4.15	1.01	1.75	0.085	152
GaP	3.85	-1.8	-4.5	-2.28	4.20	0.98	1.66	1.39	0.204	67
GaAs	4.00	-2.0	-5.4	-2.67	7.65	2.41	3.28	2.93	0.132	80
GaSb	4.31	-1.8	-4.6	-2.31	11.8	4.03	5.26	4.77	0.107	55
InP	4.14	-2.0	-5.0	-2.53	6.28	2.08	2.76	2.49	0.114	106
InAs	4.28	-1.8	-3.6	-1.97	19.7	8.37	9.23	8.89	0.052	46
InSb	4.57	-2.0	-5.0	-2.53	35.1	15.6	16.9	16.4	0.035	72
ZnS	3.82	-0.7	-3.7	-1.56	2.54	0.75	1.09	0.95	0.144	69
ZnSe	4.00	-1.2	-4.9	-2.18	3.77	1.24	1.67	1.50	0.115	124
ZnTe	4.31	-1.8	-4.6	-2.31	3.74	1.07	1.64	1.41	0.140	135
CdTe	4.58	-1.2	-5.4	-2.35	5.29	1.89	2.46	2.23	0.085	174

dislocation-related exciton activation energy (57 meV), suggesting that the electron binding energy at screw dislocation is negligible.²⁸

It can be seen from Table III that the present calculations significantly improve the agreement between theory and experiment but a discrepancy still exists. The disagreement may arise from neglecting the anisotropy and dislocation-core-related effects in present calculations as well as from the impurity and point defect contributions to experimental binding energies.

IV. CONCLUSIONS

In this paper, accurate nonvariational calculations for the spherically averaged continuous-medium-approximated Hamiltonian have been made of hole states bound in the shear strain field of screw dislocations. The

corresponding binding energies were found to be rather small and comparable with the binding energies typical of shallow acceptors.

low-temperature dislocation-luminescence phenomena in pure semiconductors because of the very large capture cross section for carriers in dislocation strain fields^{4,5} as well as in various one-dimensional electronic-transport-related phenomena such as dislocation conductivity and microwave conductivity⁹⁻¹¹ and dislocation combined resonance (a kind of electric-dipole spin resonance).³⁷⁻³⁹

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