Topological Interaction of Coulombic Impurity Centers with Dislocations in Semiconductors

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A phenomenon of the topological interaction of impurities with dislocations was studied theoretically. It was found that this interaction reduces the binding energies of carriers to Coulombic impurities for off-center valleys in semiconductors by more than a factor of 2 in the case of an isotropic carrier mass and by a factor of 4 in the case of highly anisotropic valleys.

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In this Letter the theory of gauge-invariant **kp** Hamiltonians for crystals with topological defects [1] is applied to a study of the topological interaction of Coulombic impurity centers with dislocations in semiconductors. It was first observed by Kawamura [2] that the effective mass Hamiltonian for a crystal with a screw dislocation contains additional terms that can produce an Aharonov-Bohm type of scattering of carriers by dislocations. Several more detailed theoretical investigations have been made to find a general form of the effective mass Hamiltonian for crystal with dislocations [3–6]. The most advanced theory [5,6] suggests that, in the presence of a deformation of the crystal lattice, the momentum operator $\mathbf{p}$ changes into a gauge-invariant momentum operator $\mathbf{p} + \mathbf{a}$ and, correspondingly, the band structure energy operator changes from $E(\mathbf{p})$ into $E(\mathbf{p} + \mathbf{a})$, where $\mathbf{a} = \beta^T\mathbf{p}$; $\beta_{ij}(\mathbf{r}) = \partial u_i/\partial r_j$ is distortion tensor and $\mathbf{u}(\mathbf{r})$ is the displacement vector. However, this form of the Hamiltonian leads to confusion since it gives a nonzero gauge potential when applied to an electron embedded in a topologically imperfect lattice with zero crystal potential, i.e., the free electron case.

An investigation of this problem in Ref. [1] has shown that there are two different factors contributing to the gauge potential. One is related to a nonuniform distortion of the crystal lattice around a topological defect, and the other is related to the many-valued character of the mapping of the Bloch-type electron wave function onto a topologically imperfect crystal lattice.

Both factors should be taken into consideration in order to obtain a correct expression for the **kp** Hamiltonian. Having done this, a general form of **kp** Hamiltonian for crystals with dislocations, disclinations, and dispirations can be found [1]. The resulting **kp** Hamiltonian is gauge invariant, and the corresponding gauge group is a non-Abelian group E(3) of proper Euclidean transformations of three-dimensional space. The gauge field is confined within the cores of the topological defects and influences the carriers in the bulk of the crystal only through the gauge potential that extends beyond it. This influence leads to a topological interaction of impurities with dislocations that will be studied in detail below.

For an imperfect crystal that contains only dislocations (as distinct from the case of the crystal with disclinations and dispirations) the gauge group E(3) degenerates into T(3), the Abelian subgroup of translations, and the corresponding gauge potential becomes

$$\hat{\mathbf{A}}(\mathbf{r}) = i\beta^T(\mathbf{r})(\hat{\mathbf{p}}/\hbar - \mathbf{k}), \tag{1}$$

where $\mathbf{k}$ is the electron wave vector related to the point in Brillouin zone for which the **kp** Hamiltonian is written; i.e., the Bloch functions corresponding to the $\mathbf{k}$ point of Brillouin zone are chosen as a basis set for the **kp** Hamiltonian, $\hat{\mathbf{p}}$ is the momentum-operator matrix in the basis of Bloch functions corresponding to the $\mathbf{k}$ point of Brillouin zone, and $\beta^T(\mathbf{r})$ is the transpose of the distortion tensor. In the limit of vanishing crystal potential, the matrix operator $\hat{\mathbf{p}}$ becomes diagonal and equal to the multiplication operator $\hbar\mathbf{k}$, and, therefore, the corresponding gauge potential given in Eq. (1) disappears.

The general **kp** Hamiltonian can be written in the form

$$\hat{H}[\nabla, \mathbf{r}] = \hat{\mathbf{P}}^2/2m + \hat{V}_0 + \delta\hat{V}(\beta) + (i/4m^2c^2)\sum_{s,l,q} e_{slq}\sigma_s\hat{\mathbf{P}}_l[\hat{V}_0 + \delta\hat{V}(\beta)]\hat{\mathbf{P}}_q, \tag{2}$$

where $\hat{\mathbf{P}} = \hat{\mathbf{p}} + i\hbar(\nabla + \mathbf{A})$, $\hat{V}_0$ is the matrix of the crystal potential operator for a perfect crystal in the basis of Bloch functions, $\delta\hat{V}(\beta)$ is a matrix functional of $\beta(\mathbf{r})$ that accounts for the deformation-related changes in crystal potential, and the last term in Eq. (2) describes spin-orbital interaction; σ_s are Pauli matrices, e_{slq} are the components of the Levi-Civita tensor, and m is free electron mass.

Treating ∇ and β-related terms in Eq. (2) as perturbations allows us to obtain an expression for the effective mass Hamiltonian in a crystal with dislocations. It follows from Eq. (2) that this expression can be obtained from the usual expression for the effective mass Hamiltonian of a perfect crystal, based on **kp**-perturbation theory (see, for example, Ref. [7]), by making the substitutions

$$\nabla \to \nabla - i\beta^T(\mathbf{r})\mathbf{k}, \qquad \hat{p}_{mn} \to [1 + \beta^T(\mathbf{r})]\hat{p}_{mn}, \qquad \hat{V}_{mn} \to \hat{V}_{mn} + [\delta\hat{V}(\beta)]_{mn}. \tag{3}$$

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For a band extremum at the $\mathbf{k}$ point of Brillouin zone, the diagonal term $\hat{p}_{mn}$ vanishes and we can interpret the first substitution as a distortion-related effective magnetic potential in the effective mass Hamiltonian. The second and third substitutions are responsible for distortion-related changes in the inverse effective mass tensor and in the crystal potential, respectively.

In a first-order approximation, we can neglect the distortion-related changes in the effective mass tensor and account for changes in the crystal potential by making the deformation-potential approximation. We obtain the effective mass Hamiltonian for simple band extremum

$$H(\nabla, \mathbf{r}) = -(\hbar^2/2)(1/m^*)_{\alpha\beta}[\nabla_\alpha - i\beta_{\gamma\alpha}(\mathbf{r})k_\gamma] \times [\nabla_\beta - i\beta_{\gamma\beta}(\mathbf{r})k_\gamma] + D_{\alpha\beta}\varepsilon_{\alpha\beta}(\mathbf{r}) + V(\mathbf{r}), \tag{4}$$

where $(1/m^*)_{\alpha\beta}$ and $D_{\alpha\beta}$ are the tensors of the inverse effective masses and the deformation-potential constants given by usual $\mathbf{kp}$-perturbation expressions [7], $\varepsilon_{\alpha\beta}(\mathbf{r})$ is the strain tensor, and $V(\mathbf{r})$ is the potential of a macroscopic electric field that may present in the crystal.

For Coulombic impurities, whose interaction with dislocations will be studied in this paper, the macroscopic electrical potential is

$$V(\mathbf{r}) = -Ze^2/\kappa r, \tag{5}$$

where Z is the charge of the center and κ is dielectric constant.

For the case of an extremum with axial symmetry, the tensors of the inverse effective masses and deformation-potential constants can be written in the form

$$(1/m^*)_{\alpha\beta} = (1/m_t)\delta_{\alpha\beta} + (1/m_l - 1/m_t)k_\alpha k_\beta/k^2,$$
$$D_{\alpha\beta} = \Xi_d\delta_{\alpha\beta} + \Xi_u k_\alpha k_\beta/k^2, \tag{6}$$

where m_t and m_l are transverse and longitudinal effective masses and Ξ_d and Ξ_u are deformation potential constants [8].

The Hamiltonian given in Eq. (4) allows us, in principle, to calculate how the dislocation influences the binding energies and wave functions of Coulombic impurities. This influence arises from the deformation-potential and gauge-potential terms in Eq. (4). The former describes the usual deformation-potential interaction, while the latter describes a topological interaction that we will be interested in.

Let us consider the case of a screw dislocation whose axis coincides with the axis of the valley of an indirect-gap semiconductor or an off-center direct-gap semiconductor. In this case, the deformation-potential interaction is symmetry forbidden, and only the topological interaction contributes to changes in the impurity binding states. If m_l is equal to m_t, the Hamiltonian given in Eq. (4) takes the form

$$H(\nabla, \mathbf{r}) = -(\hbar^2/2m_t)[\nabla - i\beta^T(\mathbf{r})\mathbf{k}]^2 - Ze^2/\kappa r, \tag{7}$$

and an exact analytical solution of the corresponding Schrödinger equation exists.

In fact, the Hamiltonian given in Eq. (7) is equivalent to that for a particle bound in a Coulomb potential in the vicinity of an infinite magnetic string. This problem has been studied [8,9] for the case of a general spherical potential, and it was found that noninteger quantization of angular momentum ($[\mathbf{p} + e\mathbf{A}/c] \times \mathbf{r}$) takes place.

Using a spherical coordinate system with its origin on the dislocation line and applying a gauge transformation [10]

$$\Psi \to \Psi \exp\{i[\mathbf{ku}(\mathbf{r}) - \mathbf{kb}\varphi(\mathbf{r})/2\pi]\},$$
$$\nabla \to \nabla + i\beta^T(\mathbf{r})\mathbf{k} - (\mathbf{kb})\nabla\varphi(\mathbf{r})/2\pi, \tag{8}$$

where $\mathbf{u}(\mathbf{r})$ is the multivalued displacement field and $\varphi(\mathbf{r})$ is the azimuthal angle, we obtain the following Hamiltonian for a Coulombic impurity at dislocation line:

$$H = -(\hbar^2/2m_t)[\partial^2/\partial r^2 + (2/r)\partial/\partial r - \Lambda^2/r^2] - Ze^2/\kappa r. \tag{9}$$

Λ^2 is the operator of the total angular momentum, given by

$$\Lambda^2 = -(1/\sin\vartheta)\partial/\partial\theta(\sin\theta\,\partial/\partial\vartheta) - (1/\sin^2\vartheta) \times [i\partial/\partial\varphi + (\mathbf{kb})/2\pi]. \tag{10}$$

An exact analytical solution of the Schrödinger equation with the Hamiltonian given in Eq. (9) can be found in the same way as for the hydrogen atom, but taking into account the noninteger angular-momentum quantization. The corresponding wave functions and energies are

$$\Psi_{m,n_1,n_2}(r, \vartheta, \varphi) = Ae^{im\varphi}(\sin\vartheta)^{|m-\Phi|}C_{n_1}^{|m-\Phi|+1/2} \times (\cos\vartheta)e^{-r/2r_0}(r/r_0)^{|m-\Phi|+n_1} \times L_{n_2}^{2|m-\Phi|+2n_1+1}(r/r_0), \tag{11}$$

where quantum numbers m, n_1, n_2 take values $0, 1, 2, \ldots$; A is a normalizing constant, $\Phi = (\mathbf{kb})/2\pi$ is the flux of the effective magnetic field confined inside the dislocation line expressed in the units of the flux quantum, $r_0 = 2\hbar^2\kappa(n_1 + n_2 + |m - \Phi| + 1)/Ze^2m_t$, and $C_n^\mu(x)$ and $L_n^\mu(x)$ are Gegenbauer and generalized Laguerre polynomials given by

$$C_n^\mu(x) = \sum_{k=0}^{[n/2]} \frac{(-1)^k\Gamma(\mu + n - k)}{k!(n - 2k)!\,\Gamma(\mu)}(2x)^{n-2k},$$

$$L_n^\mu(x) = \sum_{k=0}^{n} \frac{(-1)^k\Gamma(\mu + n + 1)}{k!(n - k)!\,\Gamma(\mu + k + 1)}x^k, \tag{12}$$

where the symbol $[n/2]$ means taking integer part of $n/2$.

The normalization constant A in Eq. (11) is

$$A = 2^{|m-\Phi|-1}\Gamma(|m-\Phi|+1/2)\{n_1!\,n_2!\,(|m-\Phi|+n_1+1/2)\}^{1/2} \times \{\pi^2 r_0^3(|m-\Phi|+n_1+n_2+1)\Gamma(2|m-\Phi|+n_1+1)\Gamma(2|m-\Phi|+2n_1+n_2+2)\}^{-1/2}. \quad (13)$$

The corresponding binding energies are given by a Bohr-type formula

$$E_{m,n_1,n_2} = -\mathrm{Ry}^*/(n_1+n_2+|m-\Phi|+1)^2, \quad (14)$$

where $\mathrm{Ry}^* = m_t Z^2 e^4/2\hbar^2\kappa^2$ is an effective Rydberg.

For a band extremum at the edge of Brillouin zone and a Burgers vector equal to the shortest repeat distance in the crystal lattice, the flux Φ takes values 0 or $\pm 1/2$. The case $\Phi = 0$ is trivial and corresponds to complete absence of the topological interaction. In the case $\Phi = \pm 1/2$, the main state is doubly degenerate and the corresponding wave functions and binding energy are

$$\Psi_{0,0,0}(r,\vartheta,\varphi) = (r\sin\vartheta)^{1/2} e^{-r/2r_0}/\sqrt{6\pi r_0^2},$$
$$\Psi_{\pm 1,0,0}(r,\vartheta,\varphi) = e^{+i\varphi}(r\sin\vartheta)^{1/2} e^{-r/2r_0}/\sqrt{6\pi r_0^2}, \quad (15)$$

$$E_{0,0,0} = E_{\pm 1,0,0} = -4\mathrm{Ry}^*/9, \quad (16)$$

where $\pm$ sign is equal to the sign of the flux $\Phi = \pm 1/2$ and $r_0 = 3\hbar^2\kappa/2Ze^2 m_t$.

It can be seen that the topological interaction reduces the binding energy of Coulombic centers and repels the wave function out of the dislocation core, thus justifying the application of the effective mass approximation to the description of such centers. It is worth noting that the reduction of the impurity binding energy near the dislocation line might convert some deep multiply charged impurities into shallow ones whose description is possible in the effective mass approximation.

Equations (11)–(16) are applicable only for spherically symmetric valleys, an approximation that is good in some cases (PbS, PbSe). However, in many other semiconductors, valleys are strongly anisotropic (Si,Ge,diamond). A general analytical solution of Eqs. (14) and (15) for anisotropic valleys has not been found. However, we can obtain an exact solution in a case of very strong anistropy, when $m_l \to \infty$. In this case, the Hamiltonian for a Coulombic impurity at the dislocation line takes the form

$$H(\nabla,\mathbf{r}) = -(\hbar^2/2m_l)(\delta_{\alpha\beta} - k_\alpha k_\beta/k^2) \times [\nabla_\alpha - i\beta_{\gamma\alpha}(\mathbf{r})k_\gamma][\nabla_\beta - i\beta_{\gamma\beta}(\mathbf{r})k_\gamma] - Ze^2/\kappa r \quad (17)$$

if we neglect the deformation-potential interaction. We assume instead that it can be accounted for as a perturbation (for a screw dislocation oriented along the valley axis this interaction disappears).

In a cylindrical system of coordinates, related to the valley, the Hamiltonian, after the gauge transformation

$$\Psi \to \Psi\exp\{i[\mathbf{ku}(\mathbf{r}) - \mathbf{kb}\varphi(\mathbf{r})/2\pi]\},$$
$$\nabla \to \nabla + i\beta^T(\mathbf{r})\mathbf{k} - (\mathbf{kb})\nabla\varphi(\mathbf{r})/2\pi, \quad (18)$$

where $\varphi(\mathbf{r})$ is the angle coordinate, takes the form

$$H = -(\hbar^2/2m_t)\{\partial^2/\partial\rho^2 + (1/\rho)(\partial/\partial\rho) + (1/\rho^2)[i\partial/\partial\varphi + (\mathbf{kb})/2\pi]^2\} - Ze^2/\kappa\sqrt{\rho^2+z^2}. \quad (19)$$

The wave functions that satisfy the Schrödinger equation with this Hamiltonian can be found in the same way as for Eq. (9),

$$\Psi_{m,n}(\rho,\varphi,z) = A\delta(z)e^{im\varphi}e^{-\rho/2\rho_0}(\rho/\rho_0)^{|m-\Phi|} \times L_n^{2|m-\Phi|}(\rho/\rho_0), \quad (20)$$

where $\rho_0 = 2\hbar^2\kappa(n+|m-\Phi|)/Ze^2 m_t$, the quantum numbers m, n take values $0, 1, 2$, and the normalizing constant A is

$$A = \{n!\}^{1/2}/\rho_0\{2\pi(2|m-\Phi|+2n+1) \times \Gamma(2|m-\Phi|+n+1)\}^{1/2}. \quad (21)$$

The corresponding energies are

$$E_{m,n} = -\mathrm{Ry}^*/(n+|m-\Phi|+1/2)^2. \quad (22)$$

When the flux Φ takes values $\pm 1/2$ (the usual case for a band extremum at the edge of Brillouin zone and a Burgers vector equal to the shortest lattice repeat) the main state is doubly degenerate and the corresponding wave functions and binding energy are

$$\Psi_{0,0}(\rho,\varphi,z) = \delta(z)\rho^{1/2}e^{-\rho/2\rho_0}/2\sqrt{\pi}\rho_0^{3/2},$$
$$\Psi_{\pm 1,0}(\rho,\varphi,z) = e^{\pm i\varphi}\delta(z)\rho^{1/2}e^{-\rho/2\rho_0}/2\sqrt{\pi}\rho_0^{3/2}, \quad (23)$$

$$E_{0,0} = E_{\pm 1,0} = -\mathrm{Ry}^*, \quad (24)$$

where $\pm$ sign is equal to that of the flux and $\rho_0 = \hbar^2\kappa/Ze^2 m_t$.

Thus, we have found, making a number of reasonable approximations, that the topological interaction reduces the binding energies of carriers to Coulombic impurities for off-center valleys in semiconductors. The reduction of the binding energy to Coulombic impurities located at the dislocation line is by more than a factor of 2 in the case of an isotropic carrier mass and by a factor of 4 in the case of highly anisotropic valleys. The topological interaction pushes the energy levels of multiply charged deep impurities toward the band edges and might allow, in some cases, their description as shallow impurities

in effective mass approximation. The dislocation cores should not significantly affect the bound states since their wave functions given in Eqs. (11), (15), (20), and (23) all go to zero at the dislocation line.

The theory developed in the present Letter is applicable for off-center valleys with $|\mathbf{k}| > \sqrt{m^* \mathrm{Ry}^*/\hbar}$. In the opposite case, for example, for the central valley with $\mathbf{k} = 0$, the first-order term $i\beta^T\mathbf{k}$ in Eq. (4) vanishes and the second-order terms $\beta\nabla$ should be retained in the course of the $\mathbf{kp}$-perturbation procedure. For a model case of the tight-binding Hamiltonian with the distortion-independent transfer matrix, this leads exactly to the Hamiltonian found by Kawamura [2]. It was shown by Zempo, on the basis of this Hamiltonian, that for the central valley the terms of order $\beta\nabla$ reduce the binding energy of carriers to screw dislocations [11]. For this reason we expect a reduction of the binding energy of carriers to Coulombic impurities located at the dislocation line for the central valley as well, but this reduction should be much less than that for off-center valleys since $|\nabla|/|\mathbf{k}| \sim \sqrt{a^2 m^* \mathrm{Ry}^*/\hbar^2} \ll 1$, where a is the lattice constant.

The phenomenon of the topological interaction of impurities with dislocations discussed in this Letter has not been investigated yet experimentally. One possible manifestation of this phenomenon is blueshift of donor-acceptor-pair recombination luminescence in diamond in the vicinity of dislocations [12–14]. A detailed theoretical investigation into this particular case will be performed in a forthcoming paper.

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[1] Y. T. Rebane, Phys. Rev. B **52**, 1590 (1995).
[2] K. Kawamura, Z. Phys. B **29**, 101 (1978).
[3] R. A. Brown, J. Phys. F **9**, L241 (1979).
[4] K. Kitahara, K. Nakazato, and H. Araki, in *Topological Disorder in Condensed Matter,* edited by F. Yonezava and T. Ninomiya (Springer-Verlag, Berlin, 1982), p. 153.
[5] H. Teichler, Phys. Lett. **87A**, 113 (1981).
[6] H. Teichler and H. Veth, J. Phys. (Paris), Colloq., Suppl. **44**, C4-93 (1983).
[7] G. L. Bir and G. E. Pikus, *Symmetry and Strain-Induced Effects in Semiconductors* (Wiley, New York, 1974).
[8] C. Herring and E. Vogt, Phys. Rev. **101**, 944 (1956).
[9] M. Kretzschmar, Z. Phys. **185**, 97 (1965).
[10] S. Olairu and I. I. Popescu, Rev. Mod. Phys. **57**, 339 (1985).
[11] Y. Zempo, J. Phys. Soc. Jpn. **54**, 1023 (1985).
[12] N. Yamamoto, J. C. H. Spence, and D. F. Fathy, Philos. Mag. B **49**, 609–629 (1984).
[13] J. A. Freitas, Jr., P. B. Klein, and A. T. Collins, Appl. Phys. Lett. **64**, 2136 (1994).
[14] L. H. Robins and D. R. Black, J. Mater. Res. **9**, 1298 (1994).