Spin splitting in the spectrum of two-dimensional electrons due to the surface potential

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We consider spin splitting in the spectrum of two-dimensional electrons (Tamm state, quantum film, and inversion layer) due to interaction with the short-range surface potential. The calculation is done in the isotropic approximation of the effective mass.

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The dynamics of a conduction electron in a bounded semiconductor is described in the **k·p** approximation by the equation

$$(\hat{\epsilon} + \hat{\mathbf{v}}\cdot\mathbf{p})\psi_\lambda = E_\lambda \psi_\lambda , \tag{1}$$

supplemented by a short-range (length on the order of the lattice constant a) surface potential with boundary conditions for a set of envelopes ψ_λ. The total electron wave function is usually expressed by the columns of ψ_λ.[1] The boundary condition for ψ_λ is obtained below in the effective mass approximation for an ideal surface (given by the equation $z = z_0$) from the requirement

$$\int d^2x \{ \psi_\lambda^+ \hat{v}_z \psi_\nu + (\hat{v}_z \psi_\lambda)^+ \psi_\nu \}|_{z=z_0} = 0, \tag{2}$$

for the hermiticity of Eq. (1). This approach corresponds to the zero radius potential technique[2] and was used to deduce the spin-free boundary condition.[3] In Eqs. (1) and (2) $\mathbf{p}$ is the momentum operator, the diagonal matrix $\hat{\epsilon}$ determines the position of the band extrema, and $\hat{\mathbf{v}}$ is the nondiagonal velocity matrix in terms of the band number; the effective mass m is assumed to be small in comparison with the mass of a free electron.

When the energy E_λ is close to an extremum in the conduction band ϵ_c (below $\epsilon_c = 0$) and only the spinor $\phi_\lambda^{(c)}$ is large in the multicomponent function ψ_λ, the Hamiltonian in Eq. (1) reduces to the form $p^2/2m$ by the transformation $\psi_\lambda = e^{\hat{s}}\phi_\lambda$ (explicit form of the operator $\hat{s}$, see Ref. 1), and condition (2) is spin-dependent

$$\begin{aligned} \int d^2x \{ & \phi_\lambda^{(c)+} (p_z/m + \sum_i \hat{\beta}_{zi}\, p_i) \phi_\nu^{(c)} \\ & + [(p_z/m + \sum_i \hat{\beta}_{zi}\, p_i) \phi_\lambda^{(c)}]^+ \phi_\lambda^{(c)} \}|_{z=z_0} = 0 \end{aligned} \tag{3}$$

through the tensor

$$\hat{\beta}_{zi} = \sum_n \frac{v_{cn}^z v_{nc}^i - v_{cn}^i v_{nc}^z}{\epsilon_c - \epsilon_n} \tag{4}$$

The tensor (4) that defines the g-factor for the conduction electron, [1,4] is obtained from the anticommutator $\hat{v}_z\hat{S} + \hat{S}\hat{v}_z$ that occurs when the expansion $\psi_\lambda = (1 + \hat{S}_{111})\phi_\lambda$ is substituted into Eq. (2). The terms of Eq. (4) are expressed by the spin matrices

$$\beta_{zi} = \frac{\chi}{2m}(\sigma_z\sigma_i - \sigma_i\sigma_z), \tag{5}$$

where the coefficient χ is equal to the ratio of the spin splitting of the electron spectrum in a magnetic field to a diamagnetic one, and is small for the case of weak spin-orbit interaction. For the Keino band spectrum model $\chi = 1/2$ for a large spin-orbit splitting (such a case is realized in InSb), while for the Dirac model (used in describing the electron spectrum of lead [5] and bismuth [6] chalcogens) $\chi = 1$, i.e., in a number of meterials the spin-dependent interaction with the surface is not small.

For the case of a translationally-invariant surface $\phi_\lambda^{(c)} = \bar{\phi}_\lambda|\mathbf{p}_\parallel\rangle$, where $|\mathbf{p}_\parallel\rangle$ is a two-dimensional plane wave, while for the z-coordinate dependent spinor $\bar{\phi}_\lambda$ the set of conditions obtained from Eq. (3) is ($\mathbf{p}_\parallel$ and $\mathbf{p}'_\parallel$ are two-dimensional momenta corresponding to the states λ and ν, and $\mathbf{e}_z$, is a unit vector along the OZ-axis)

$$\delta_{\mathbf{p}_\parallel \mathbf{p}^*_\parallel}\{\bar{\phi}^+_\lambda(p_z + i\chi\vec{\sigma}[\mathbf{e}_z\times\mathbf{p}_\parallel])\bar{\phi}_\nu$$
$$+[(p_z + i\chi\vec{\sigma}[\mathbf{e}_z\times\mathbf{p}_\parallel])\bar{\phi}_\lambda]^+\bar{\phi}_\nu\}|_{z=z_0} = 0. \tag{6}$$

Diagonalizing Eq. (6) with respect to spin, [7] we obtain $\bar{\phi}_\lambda = \exp[i\pi/4(\sigma_x\cos\phi + \sigma_y\sin\phi)]\theta_\lambda|\Sigma\rangle$, where $\mathbf{p}_\parallel = (p_\parallel\cos\phi, p_\parallel\sin\phi)$, $|\Sigma\rangle$is the eigenfunction of the operator $\sigma_z(\sigma_z|\Sigma\rangle = \Sigma|\Sigma\rangle$, and the quantum number $\Sigma = \pm 1$ determines the spin projection on the axis perpendicular to $p_\parallel$). The scalar function θ_λ satisfies the equation $(p_z^2/2m)\theta_\lambda = [E_\lambda - (p_\parallel^2/2m)]\theta_\lambda$ with the boundary condition for the logarithmic derivative at the surface

$$(p_z + i\chi\Sigma p_\parallel + ip_0)\theta_\lambda|_{z=z_0} = 0. \tag{7}$$

In the transition from the bilinear form (6) to (7), the momentum p_0 independent of the quantum numbers λ characterizing the surface properties appears as the case is in Ref. 3. [1] Here this momentum is not explicitly related to the surface potential and must be determined from the experimental data.

The spin-dependent interaction with a smooth (at distances on the order of a) external field has the form of a spin-orbit component [8] and leads to small effects (in terms of the parameter $\bar{E}/\epsilon_g$, where $\bar{E}$ is the characteristic energy of the conduction electron, and ϵ_g is the width of the forbidden band). The main difference between Eq. (7) and the results for a smooth field is the fact that the short-range potential (in similarity with a constant magnetic field) changes the spin state of the conduction electrons, and in the "nonrelativistic" limiting case $\bar{E}/\epsilon_g \to 0$. Below, we shall find spin splitting in the spectrum of moving ($p_\parallel \neq 0$) electrons localized at the surface described by Eq. (7).

We shall obtain the solution for a shallow Tamm state on the surface $z_0 = 0$, having augmented the problem with the boundary condition $\theta_{\lambda|z\to+\infty} = 0$. The dispersion equality for the Tamm state $E_{p_\parallel \Sigma}$ and the depth of its localization $K_{p_\parallel}^{-1}\Sigma$ ($\theta_\lambda \sim e^{-K_{p_\parallel \Sigma} z}$) is given by the equations

$$E_{p_\parallel}\Sigma = -\frac{(\hbar K_{p_\parallel \Sigma})^2}{2m} + \frac{p_\parallel^2}{2m}, \quad \hbar K_{p_\parallel \Sigma} = p_o + \chi \Sigma p_\parallel, \tag{8}$$

and the region of its occurrence is determined by the condition $p_0 + \chi \Sigma p_\parallel > 0$. The resulting spectrum (and also the one considered below) is linear at small $p_\parallel$, which leads (as in the three-dimensional case [9]) to the occurrence of an extremum loop that is large at $\chi \sim 1$. For the Dirac model the spectrum (8) is linear in terms of $p_\parallel$; transition to the quadratic spectrum is provided by the contribution of the remote bands dropped from Eq. (1).

In studying dimensional quantization in a film of thickness d the boundary conditions (7) are set on both surfaces (the characteristic momenta are denoted by $p_\pm$). The dispersion law is given by the equation $E_\lambda = [(\hbar K_\lambda)^2 + p_\parallel^2]/2m$, where K_λ is determined by the equation

$$\operatorname{ctg} K_\lambda d = \frac{p_+ p_- - (\chi p_\parallel)^2 - \chi \Sigma p_\parallel (p_+ - p_-)}{\hbar K_\lambda (p_+ + p_-)} - \frac{\hbar K_\lambda}{p_+ + p_-}. \tag{9}$$

When the right-hand side of Eq. (9) is large, the solutions are nearly quasiclassical ($K_\lambda d \approx n\pi$) and are split weakly in terms of spin. The spin splitting is not small only for the region $\hbar \bar{K} \sim \sqrt{p_+ p_-}$ (for small $p_\parallel$), where the quasiclassical approximation does not work. The value for $\Delta K = |K_{\Sigma=+1} - K_{\Sigma=-1}|$ is obtained in the form

$$\hbar \Delta K \sim \frac{\text{const}}{\bar{K} d} \chi p_\parallel \frac{p_+ - p_-}{p_+ + p_-} \tag{10}$$

while for a symmetric film the splitting does not occur. In the anti-symmetrical case ($p_+ = -p_-$) the solutions are always quasi-classical. The imaginary root of Eq. (9) describes the change in the Tamm state spectrum in the film.

For an electron in the inversion layer the dimensionless energy ϵ_λ ($\epsilon_\lambda = [E_\lambda - (p_\parallel^2/2m)]/[(\hbar/l)^2/2m]$, where the characteristic length l is defined as $l^{-3} = -2meE_s/\hbar^3$, $e<0$, and E_s is the uniform surface field) is determined by the dispersion equation

$$\frac{p_o + \chi \Sigma p_\parallel}{\hbar/l} Ai(-\epsilon_\lambda) - Ai'(-\epsilon_\lambda) = 0. \tag{11}$$

In the quasiclassical energy region $\epsilon_\lambda \gg 1$ the use of the asymptotic Airy function $Ai(x)$ yields a small spin splitting of the level $\Delta\epsilon \approx [\text{const}/\epsilon_\lambda^{1/2}][\chi p_{11}/(\hbar/1)]$. For the strongly-bound Tamm state $\epsilon_\lambda \ll -1$ the result in [8] is obtained. For $|\epsilon_\lambda| \sim 1$ the order of magnitude of the spin splitting is determined by the parameter $\chi p_\parallel/(\hbar/l)$.

The numerical solution of the dispersion equations (9,11) allows us to calculate similar [10] spectral characteristics of the absorption of electromagnetic radiation due to spin splitting. The region of negative effective masses $[(d^2E_\lambda/dp_\parallel^2)<0]$ is large for a large radius of the extremum loop. Thus, in materials with $\chi\sim 1$ anomalies of the collective and kinetic effects on the two-dimensional electron are possible.

[1]Because of the factor $\delta_{p_\parallel p'_\parallel}$, in Eq. (6), p_0 may depend on $p_\parallel$. Since the surface potential is short-range, this dependence is small in terms of the parameter $p_\parallel a/\hbar$. The dependence of p_0 on Σ is insignificant because of the invariance of the problem with respect to the operation of time reversal at $p_\parallel=0$.

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