Energy spectrum of an electron in a semiconductor with a superlattice in a transverse magnetic field

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We determine the spectrum of an electron in a semiconductor having a one-dimensional superlattice, in a magnetic field of arbitrary strength and perpendicular to the periodicity direction. The variation of the electron energy spectrum with change of the magnetic field strength is studied in the range from weak fields, in which the effective-Hamiltonian method is valid, to strong fields in which the field affects strongly the electronic state in certain layers of the superlattice and for which the effective-Hamiltonian method is not valid.

I. INTRODUCTION

In ordinary crystals the intracrystalline and intra-atomic fields exceed substantially the experimentally attainable magnetic fields. The effective-Hamiltonian method can therefore be used in the calculations of the energy spectrum of the carriers.[1]

There is, however, an important class of materials in which both the "intracrystalline" and the "intra-atomic" fields are relatively weak. We have in mind semiconductors with superlattices, (SL), in which one-dimensional periodic modulation of the composition, and hence of the effective potential acting on the carriers, gives rise to quite narrow minibands of allowed energies, separated by energy gaps. Although these gaps greatly exceed the width of a miniband, they are nevertheless much narrower than the band gaps of ordinary semiconductors.[2] It is precisely because of the narrowness of the minibands in these materials that the "intracrystalline" fields turn out to be weaker by several orders than the corresponding fields in ordinary crystals. The "intra-atomic" fields are likewise weak, inasmuch as in semiconductors with SL the role of the "atoms" is assumed by the effective-periodic-potential wells whose width exeeds considerably the distance between the crystal atoms.

This raises the problem of finding the spectrum of the carriers in such magnetic fields, when the usual effective-Hamiltonian approximation no longer holds. The present paper is devoted to its solution.

First, based on the one-dimensional character of the effective SL periodic potential, we present a symmetry classification of the states and reduce the problem to one-dimensional. Next, using the smallness of the ratio of the allowed minibands to the gaps that separate them, i.e., to the weakness of the overlap of the wave functions localized in the neighboring wells of the SL potential, we obtain the basic equation that yields the eigenstates of an electron in an arbitrary magnetic field. We shall track the manner in which the carrier energy spectrum is transformed with increasing magnetic field from miniband Landau levels all the way to the spectrum of a "magnetized" carrier moving within the confines of an isolated SL potential well. We emphasize that owing to the narrowness of the allowed minibands compared with the gaps between them, the electron is trapped in an isolated SL potential well in magnetic fields considerably weaker than those needed for a substantial change of its "intra-atomic" motion.

II. DERIVATION OF FUNDAMENTAL EQUATION

Consider a semiconductor located in a magnetic field parallel to the z axis and having a one-dimensional SL whose periodic potential depends on the coordinate x. The Schrödinger equation obtained for the electron at the bottom of the conduction band after separating the motion in the field direction is of the form

$$\hat{\mathcal{H}}\psi=\left\{\frac{\hbar^2}{2m}\left[\left(i\frac{\partial}{\partial x}+\frac{y}{L_H^2}\right)^2-\frac{\partial^2}{\partial y^2}\right]+U(x)\right\}\psi=\varepsilon\psi, \tag{2.1}$$

$$L_H=(\hbar c/eH)^{1/2}, \quad U(x)=\sum_{l=-\infty}^{+\infty}u(x-al),$$

where m is the effective mass connected with the motion in the plane of the layer, L_H is the magnetic length, and $U(x)$ is the periodic potential of the SL. The gauge of the vector potential is chosen in a form that preserves the Hamiltonian invariant to translation along the x axis by the SL period a.

The symmetry of the two-dimensional Hamiltonian $\hat{\mathcal{H}}$ permits classification of its eigenstates. The Hamiltonian $\hat{\mathcal{H}}$ commutes with the operator $\hat{T}_a^x$ of translation by the SL period along the x axis, as well as with the operator

$$\hat{R}_d=\exp\left(-ixd/L_H^2\right)\hat{T}_d^y,$$

where $\hat{T}_d^y$ is the operator of translation by a segment d along the y axis. At

$$d=2\pi L_H^2/a \tag{2.2}$$

the operators $\hat{T}_a^x$ and $\hat{R}_d$ commute with each other. Let us find the set of common eigenfunctions of the operators, $\hat{\mathcal{H}}$, $\hat{T}_a^x$, and $\hat{R}_d$ for d defined by relation (2.2).

The eigenfunctions of the operators $\hat{T}_a^x$ and $\hat{R}_d$ are numbered by the quantum numbers k_x and $\varkappa$, respectively:

$$-\pi/a\leqslant k_x<\pi/a, \quad -G/2\leqslant\varkappa<G/2, \tag{2.3}$$

where $G=2\pi/d=a/L_H^2$. The function $\psi_{k_x,\varkappa}(x,y)$ is of the form

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$$\psi_{k_x,\varkappa}(x,y)=\exp\left(i\varkappa y+i\frac{xy}{L_H^2}\right)$$

$$\times\sum_{r=-\infty}^{\infty}F_{k_x,\varkappa}(x+ar)\exp[i(Gy-k_xa)r]. \quad (2.4)$$

Substituting it in (2.1) we obtain the equation for $F_{k_x}\varkappa(x)$:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{m\omega_H^2}{2}(x+\varkappa L_H^2)^2+U(x)\right]F_{k_x,\varkappa}(x)$$

$$=\varepsilon F_{k_x,\varkappa}(x), \quad (2.5)$$

where $\omega_H = eH/mc$. We note that the energy ε and the functions $F_{k_x}\varkappa(x)$ are independent of k_x, and the degeneracy in k_x typical of motion in a magnetic field is present.[1]

The problem reduces thus to finding the spectrum and the eigenfunctions in a one-dimensional potential that is a superposition of the initial periodic potential on the quadratic potential due to the magnetic field. The energy spectrum in such a potential is discrete and the levels are numbered by the quantum numbers $n = 0,1,2,\ldots$. The energy depends on the position of the minimum of the quadratic potential, $-\varkappa L_H^2$, within the limits of the unit cell. To each quantum number there corresponds therefore an energy band $\varepsilon = \varepsilon_n(\varkappa)$. We shall call these bands magnetic. Clearly, as the periodic-potential amplitude tends to zero the magnetic bands contract to Landau levels with energy $\hbar\omega_H(n+1/2)$.

So far, the potential $U(x)$ was perfectly arbitrary. We now recognize that the influence of the SL potential on the electronic properties is most substantial when the widths of the allowed minibands obtained on spreading of the levels of the isolated potential wells on account of the tunneling are small compared with the energy gaps between them. This situation corresponds to a weak overlap of the wave functions of the electrons localized in neighboring potential wells, and are consequently well described in the tight binding approximation. Since the magnetic field compresses the wave function of the electron in the layer, the approximation becomes better the stronger the field. This circumstance permits (2.5) to be solved in the tight-binding approximation.

We represent the function $F^{\nu}_{\varkappa,n}(x)$in the form

$$F^{\nu}_{\varkappa,n}(x)=\sum_{l=-\infty}^{\infty}b^{\nu}_{\varkappa,n}(l)f^{\nu}_{\varkappa+Gl}(x-al), \quad (2.6)$$

where $f^{\nu}_{K}(x)$ is the eigenfunction of the level $\nu = 1,2,3,\ldots$ of the one-dimensional Schrödinger equation with potential $u(x)+m\omega_H{}^2(x+KL_H{}^2)^2/2$; this eigenfunction corresponds to an energy $E_\nu(K)$. This is the equation to which is reduced the problem of motion of an electron in an individual layer, with a momentum y-component equal to $\hbar K$. The resultant new quantum number ν is analogous to the number of the miniband. By the customary algebra of the tight-binding approximation we obtain an equation for the coefficients $b^{\nu}_{\varkappa,n}(l)$:

$$[E_\nu(\varkappa+Gl)-\varepsilon_n{}^{\nu}(\varkappa)]b^{\nu}_{\varkappa,n}(l)+\sum_{p\neq 0}\beta_p{}^{\nu}(\varkappa+Gl)\,b^{\nu}_{\varkappa,n}(l+p)=0, \quad (2.7)$$

where

$$\beta_p{}^{\nu}(K)=\langle f_K{}^{\nu}(x)\,|\,U(x)-u(x-ap)\,|\,f^{\nu}_{K+Gp}(x-ap)\rangle \quad (2.8)$$

are resonant integrals that decrease exponentially with increasing $|p|$ and have the property

$$\beta_p{}^{\nu}(K)=\beta_{-p}{}^{\nu}(-K). \quad (2.9)$$

Included in the energy $E_\nu(K)$ is an additional term equal to $\beta^{\nu}_{p=0}(K)$.

We have thus obtained the fundamental equation (2.7), which makes it possible to find the energy spectrum and the eigenfunctions of the electron in arbitrary magnetic fields. The explicit expression for the eigenfunction (2.4) is

$$\psi^{\nu}_{k_x,\varkappa,n}(x,y)=\exp\left(i\varkappa y+i\frac{xy}{L_H^2}\right)\sum_{r,l=-\infty}^{\infty}b^{\nu}_{\varkappa,n}(r)$$

$$\times\exp[i(k_xa-Gy)(l-r)]f^{\nu}_{\varkappa+Gr}(x-al). \quad (2.10)$$

III. SOLUTION OF FUNDAMENTAL EQUATION

When the main contribution to the wave function (2.10) is made by states of individual layers, for which the influence of the magnetic field on the electron motion inside the layer can be neglected, the fundamental equation is equivalent to the Schrödinger equation of the effective-Hamiltonian method. In this case the $E_\nu(K)$ dependence takes the form

$$E_\nu(K)\approx\varepsilon_\nu+\hbar^2K^2/2m, \quad (3.1)$$

where E_ν is the energy of the level ν in the potential $u(x)$, and the resonant integrals do not depend on K, since the individual-layer eigenfunctions that coincide with the eigenfunctions $f^{\nu}(x)$ corresponding to $H = 0$ do not depend on K. The summations over r and l in (2.10) become separated, and the wave function takes the form

$$\psi^{\nu}_{k_x,\varkappa,n}(x,y)=\exp(ixy/L_H{}^2)\,g^{\nu}_{k_x,\varkappa,n}(y)\,\varphi^{\nu}_{k_x-y/L_H{}^2}(x), \quad (3.2)$$

where

$$g^{\nu}_{k_x\varkappa,n}(y)=\left(\frac{2\pi}{a}\right)^{1/2}e^{i\varkappa y}\sum_{r=-\infty}^{\infty}b^{\nu}_{\varkappa,n}(r)\exp[i(Gy-k_xa)r], \quad (3.3)$$

$$\varphi^{\nu}_{k_x}(x)=\left(\frac{a}{2\pi}\right)^{1/2}\sum_{l=-\infty}^{\infty}\exp(ik_xal)f^{\nu}(x-al) \quad (3.4)$$

is the Bloch function of the miniband ν. The function $g^{\nu}_{k_x,\varkappa n}(y)$ satisfies the equation

$$\left\{-\frac{\hbar^2}{2m}\frac{d^2}{dy^2}+2\sum_{p=1}\beta_p{}^{\nu}\cos\left[\left(k_x-\frac{y}{L_H{}^2}\right)ap\right]\right\}$$

$$\times g^{\nu}_{k_x,\varkappa,n}(y)=[\varepsilon_n{}^{\nu}(\varkappa)-\varepsilon_\nu]g^{\nu}_{k_x,\varkappa,n}(y) \quad (3.5)$$

and the boundary condition

$$g^{\nu}_{k_x,\varkappa,n}(y+2\pi L_H{}^2/a)=\exp(2\pi i\varkappa L_H{}^2/a)\,g^{\nu}_{k_x,\varkappa,n}(y), \quad (3.6)$$

which follows from the definition (3.3). Equation (3.5) was obtained as a result of substituting the coefficients $b^{\nu}_{\varkappa,\eta}(r)$,

expressed in terms of $g^{\nu}_{k_x,\varkappa,n(y)}$, in the fundamental equation (2.7).

Equation (3.5) is equivalent to the Schrödinger equation of the effective-Hamiltonian method[3] for a particle with a dispersion law

$$\varepsilon_\nu(\mathbf{k})=\frac{\hbar^2}{2m}(k_y^2+k_z^2)+2\sum_{p=1}^{\infty}\beta_p^{\nu}\cos k_x ap \tag{3.7}$$

the gauge of the vector potential being chosen in the form $\mathbf{A}=(-H_y,0,0)$. It is of the form of the Schrödinger equation for a particle moving in a periodic "potential" whose role is played by the dispersion law in the miniband ν.

Let us discuss the characteristic features of the spectrum $\varepsilon_n^{\nu}(\varkappa)$. It is convenient for this purpose to transform to the dimensionless coordinate $\xi=ya/L_H^2$ and represent Eq. (3.5) in the form

$$\left\{-\frac{1}{2}\left(\frac{H}{H_1^{\nu}}\right)^2\frac{d^2}{d\xi^2}+\sum_{p=1}^{\infty}\frac{\beta_p^{\nu}}{\Delta_\nu}\cos[(\xi-\xi_0)p]\right\}g^{\nu}_{k_x,\varkappa,n}(\xi)$$

$$=\frac{\varepsilon_n^{\nu}(\varkappa)-\varepsilon_\nu}{\Delta_\nu}\,g^{\nu}_{k_x,\varkappa,n}(\xi), \tag{3.8}$$

$$\xi_0=k_x a,$$

$$H_1^{\nu}=\frac{\hbar c}{ea^2}\left(\frac{m}{m_\nu}\right)^{1/2}\approx 6\cdot 10^4\left(\frac{m}{m_\nu}\right)^{1/2}\left(\frac{10^{-6}\text{ см}}{a}\right)^2\text{Oe},$$

where H_1^{ν} is the "intracrystalline" field connected with the miniband ν; $2\Delta_\nu$ is the width of this miniband; $m_\nu=\hbar^2/a^2\Delta_\nu$ is the effective mass in it.

In this equation the quantity $(H_1^{\nu}/H)^2$ plays the role of the dimensionless mass and the amplitude of the periodic "potential" is equal to unity. When $H<H_1^{\nu}$ the dimensionless mass is large, the particle is "heavy," and behaves almost as a classical one. At low energies it is localized mainly in one of the wells of the periodic "potential." In this case one can use the tight-binding approximation to analyze Eq. (3.8), i.e., the levels in the isolated wells of the "potential" are found, and account in then taken of their spreading into magnetic bands because of the finite penetrability of the barriers. The "potential"near the minima is then approximated by a quadratic expansion, corresponding to the use of the effective mass approximation in the miniband. The spectrum obtained thereby describes miniband Landau levels smeared out because of the periodicity of the "potential"[1]:

$$\varepsilon_n^{\nu}(\varkappa)=\varepsilon_\nu-\Delta_\nu+\hbar\omega_H^{\nu}(n+1/2)-(-1)^n\eta_n^{\nu}\cos 2\pi\frac{\varkappa L_H^2}{a},$$

$$n=0,1,2,\ldots, \tag{3.9}$$

where $\omega_H^{\nu}=eH/c(mm_\nu)^{1/2}$; $2\eta_n^{\nu}$ is the width of the nth magnetic band in the miniband ν.

In this case the magnetic bands are narrow compared with the energy bands between them.

For high energies $\varepsilon_n^{\nu}(\varkappa)$ the equidistance of the levels in the isolated wells is violated on account of the deviation of the "potential" of the isolated well from quadratic, and their smearing increases, since the overlap of states localized in neighboring wells increases. These factors can be neglected for those n which satisfy the inequality.

$$n<H_1^{\nu}/H-1. \tag{3.10}$$

This inequality can be rewritten in the form

$$\varepsilon_n^{\nu}(\varkappa)<\varepsilon_\nu. \tag{3.11}$$

For energies $\varepsilon_n^{\nu}(\varkappa)>\varepsilon_n+\Delta_\nu$ the periodic "potential" in (3.8) becomes a small perturbation and one can use the weak-binding approximation. This is equivalent to reducing the infinite system of coupled equations obtained for the coefficients $b\,\varkappa,n(l)$ from (2.7) to a single equation, when $\varepsilon_n^{\nu}(\varkappa)$ is located in the interior of the magnetic band, or to a system of two equations when $\varepsilon_n^{\nu}(\varkappa)$ is located at the edge. In this case the spectrum is of the form

$$\varepsilon_n^{\nu}(\varkappa)=E_\nu(k(\varkappa,n)), \tag{3.12}$$

where

$$k(\varkappa,n)=\varkappa+Gp(\varkappa,n),$$

$$p(\varkappa,n)=(-1)^n[(2n+1-(-1)^n)/4]\,(\varkappa/|\varkappa|)$$

for energies in the interior of the nth magnetic band and

$$\varepsilon^{\nu}_{n+(1\pm 1)/2}(\varkappa)=1/2\{E_\nu(k(\varkappa,n))+E_\nu(k(\varkappa,n+1))$$

$$\pm[[E_\nu(k(\varkappa,n))-E_\nu(k(\varkappa,n+1))]^2+4(\beta^{\nu}_{n+1})^2]^{1/2}\} \tag{3.13}$$

for energies at the edges of the $(n+1)$st gap that separates the magnetic bands n and $(n+1)$. The spectrum comprises broad magnetic bands separated by narrow gaps. At almost all energies the dispersion law $\varepsilon_n^{\nu}(\varkappa)$ coincides with the corresponding section of the dispersion law $E_\nu(K)$ of an electron in an isolated layer. Exceptions are narrow intervals near the gaps.

From the condition for the applicability of the weak coupling approximation follows the inequality

$$n>(H_1^{\nu}/H)^2, \tag{3.14}$$

which determines the numbers n of the magnetic bands for which the approximation is valid, and the satisfaction of the inequality for $n=1$ means that the approximation is valid also for $n=0$. In the derivation of the inequality (3.14) we have assumed that

$$|\beta^{\nu}_{n+1}|\approx 1/2\Delta_\nu\delta_{n,0},$$

since the resonant integrals decrease exponentially with increasing n.

When $H>H_1^{\nu}$, the dimensionless mass in (3.8) is small, the particle is "light," and the energy needed for its localization over a length on the order of the period of the potential becomes larger than the amplitude of the potential. In this case the weak binding approximation is valid for all energies $\varepsilon_n^{\nu}(\varkappa)$ in accord with (3.14). In these magnetic fields the miniband character of the energy spectrum is violated, since the neighboring-layer states, the tunneling between which leads to the dispersion law in the miniband, go out of resonance. The electrons are trapped by the magnetic field inside the

layers corresponding to the wells of the SL periodic potential.

So far we have neglected the possible influence of the field on the state of the electron in an isolated well of the SL potential. This is justified when the magnetic fields and the energies of the electron are not too large. The values of the numbers n of the magnetic bands at which this is valid satisfy the inequality

$$n<2(H_2^\nu/H)^2[1-(H/H_2^\nu)^2]^{1/2}, \quad H_2^\nu=(mc^2\delta\varepsilon_\nu/e^2\overline{x_\nu^2})^{1/2}, \tag{3.15}$$

where H_2^ν is the "intra-atomic" field connected with the level ν: $\delta\varepsilon_\nu$ is the modulus of the energy difference between the level ν and the level closest to it in energy; $\overline{x_\nu^2}$ is the mean square of the coordinate x in the νth state at $H=0$. It can be seen from (3.15) that the fields $H>H_2^\nu$ influence substantially the νth "atomic" state. From the definitions of the fields H_1^ν and H_2^ν it follows that

$$H_2^\nu=H_1^\nu(\delta\varepsilon_\nu/\Delta_\nu)^{1/2}(a^2/\overline{x_\nu^2})^{1/2}>H_1^\nu, \tag{3.16}$$

since $a^2>\overline{x_\nu^2}$ and $\delta\varepsilon_\nu\gg\Delta_\nu$. It follows from (3.14)–(3.16) that in those cases when the influence of the field on the state of the electron in isolated wells is substantial, the infinite system of coupled equations for the coefficients $b_{\varkappa,n}^\nu(l)$, which is obtained from the fundamental equation (2.7), reduces to one equation or to a system of two equations, depending on the electron energy. The $\varepsilon_n(\varkappa)$ spectrum is defined as before by expressions (3.12) and (3.13), in which, however, the $E_\nu(K)$ dependence is no longer described by expression (3.1) but is obtained from the solution of the problem of the isolated layer in a magnetic field. In addition, the resonant integrals depend now on the y component of the electron momentum $\hbar K$ in the layer and of the magnetic field, so that β_{n+1}^ν in (3.13) must be replaced by $\beta_{n+1}^\nu(-G(n+1)/2)$. Since the magnetic field clamps the wave function of the electron in thewell, enhancing its localization, the resonance integrals decrease exponentially with increasing field :$\beta\propto\exp[-H/(\hbar c/ea^2)]$, and consequently the gaps between the magnetic bands decrease.

If the layers that produce the wells of the LS periodic potential are so wide that the localization length of the νth state in the well exceeds the localization length $2L_H(2\nu)^{1/2}$ of the state of the Landau oscillator in the attained magnetic field, the isolated layer contains ν intralayer Landau levels in such a field. This means that for the first ν states of the layer at small K the energies $E_\nu(K)$ do not depend on K and are equal to $\hbar\omega_H(\nu-1/2)$. It follows therefore [see (3.11)] that for these ν the $\varepsilon_n^\nu(\varkappa)$ spectrum in the first miniband ($n=0$) contains an interval of values of $\varkappa$ near the origin, on which $\varepsilon_{n=0}^\nu(\varkappa)=\hbar\omega_H(\nu-1/2)$.

IV. CONCLUSION

We have thus arrived at the following picture of the energy spectrum of an electron in a magnetic field perpendicular to the direction of the periodicity of the SL. The entire field-variation interval is divided into three regions by two characteristic magnetic fields:"intracrystalline" H_1^ν and "intra-atomic" H_2^ν (see Fig. 1). When $H<H_1^\nu$, the $\varepsilon_n^\nu(\varkappa)$ spectrum has four characteristic regions. This spectrum

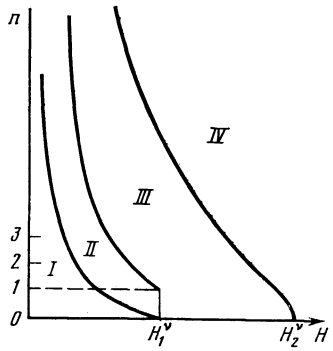

FIG. 1.

constitutes the miniband Landau level for magnetic bands belonging to the region I, corresponding to

$$n<H_1^\nu/H-1.$$

Corresponding to region II, which is a transition region, are

$$H_1^\nu/H-1<n<(H_1^\nu/H)^2.$$

In regions III and IV the $\varepsilon_n^\nu(\varkappa)$ spectrum coincides at almost all energies with the spectrum of an electron in an isolated layer. Pertaining to region III are magnetic bands for which the influence of the field on the states of the electron in an isolated layer is negligibly small. Here

$$(H_1^\nu/H)^2<n<2(H_2^\nu/H)^2\times[1-(H/H_2^\nu)^2]^{1/2}.$$

The influence of the field on the state of an electron in an isolated layer is substantial for magnetic bands of region IV, to which correspond

$$n>2(H_2^\nu/H)^2[1-(H/H_2^\nu)^2]^{1/2}.$$

When $H_1^\nu<H<H_2^\nu$, the first two regions are absent and only the last two are present. When $H>H_2^\nu$ only the last region remains.

The theory expounded above is applicable not only to semiconductors with SL, but also to layered and intercalated crystals. A distinguishing feature of these materials is a strong anisotropy of the conductivity; the conductivity along the layer is several orders larger than the conductivity in the direction perpendicular to the layers. This is due to the weak overlap of the wave functions of the electrons localized in the neighboring layers. As a result of this circumstance, the intracrystalline fields connected with the motion of the electron in this direction are weak, meaning that the characteristic magnetic field H_1 is weak, and the electrons can be trapped in the layers by a magnetic field parallel to the planes of the layers. On the other hand, the characteristic intra-atomic fields in these materials are strong, $\sim 10^8$–10^9 Oe, as in ordinary crystals, since the layers corresponding to the wells of a one-dimensional periodic potential are atomic in size.

[1])The subscript k_x will be hereafter omitted wherever this leads to no misunderstanding.

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