LOW-DIMENSIONAL SYSTEMS AND SURFACE PHYSICS

Self-consistent calculation of Landau levels of a quasi-two-dimensional hole gas at a GaAs/AlGaAs *p*-type heterojunction

O. V. Volkov

Institute of Solid-State Physics, Russian Academy of Sciences, 142432 Chernogolovka, Moscow Region, Russia

(Submitted June 21, 1997; resubmitted October 29, 1997)
Fiz. Tverd. Tela (St. Petersburg) **40**, 1117–1125 (June 1998)

An efficient method is proposed for the self-consistent calculation of Landau levels of a quasi-two-dimensional hole gas at a GaAs/AlGaAs heterostructure in a perpendicular magnetic field. The method is based on transforming the Schroedinger and Poisson equations to a system of nonlinear differential equations which are then spatially discretized and solved by the method of relaxation. The method proposed is used to model the optical spectra for recombination of the quasi-two-dimensional hole gas with electrons localized at a δ layer of donors in an isolated *p*-type heterojunction. Particular attention is paid to effects associated with the dependence of the wave functions and shape of the potential well on the magnetic field, which have not been considered before. © *1998 American Institute of Physics.* [S1063-7834(98)03206-7]

In the course of the last few decades, there has been intense interest in fundamental physical phenomena observed in systems with low dimensionality. However, whereas the properties of quasi-two-dimensional (2D) electronic systems have been extensively studied using various experimental techniques, much less information has been obtained regarding the properties of 2D-hole systems. In essence this is because the effective mass of holes is considerably larger than that of electrons, and the nonparabolicity and anisotropy of the degenerate valence band leads to a complicated structure for the energy spectrum under size-quantization conditions. Despite the fact that a theoretical model for the valence band was constructed almost 40 years ago,[1,2] the fundamental implications of this model for a system of low dimensionality have been derived and understood only recently.[3–7] Thus, it was shown in Ref. 5 that Landau levels of a 2D-hole gas are not equidistant and in fact are quite nonlinearly spaced. Nevertheless, it is only recently that this complicated behavior has been observed directly in experiment, due to the smallness of the energy splittings between these levels. For the case of 2D electrons, study of the recombination of the electron gas with holes localized in a δ layer of acceptors located a certain distance from the heterojunction boundary has turned out to be an extremely useful way to probe the system physics.[8] In this case the luminescence spectrum is determined by the product of the density of states of the 2D-electron gas and the amplitude of the wave function in the δ layer, which determines the matrix element for the transition. Recently, analogous structures were obtained for a *p*-type heterojunction with a δ layer of donors. Studies of the recombination of 2D holes with electrons localized in the δ layer of donors make it possible to observe directly Landau levels of a hole gas for the first time.[9] The primary purpose of the analysis given below is to describe such a situation.

The problem of computing the energy spectrum of a 2D-hole gas in a perpendicular magnetic field has been studied by many authors.[4–7] All the numerical calculations to date have been made using matrix methods based on diagonalizing a Hamiltonian written in a basis made up of a certain set of functions which usually have a simple analytic form. The accuracy of this method depends on the number of basis functions and on the degree of completeness of the set chosen. The problem is especially complicated for the case of an isolated *p*-type heterojunction, since here the quantizing potential itself is determined by the quantities we want to solve for, i.e., the hole wave functions. This makes it necessary to repeat the diagonalization procedure iteratively many times, a procedure that converges very slowly. For this reason, authors usually do not discuss any effects connected with self-consistent calculations, nor do they treat the dependence of the potential shape on the magnetic field. In this paper a computational method is proposed that practically eliminates these inadequacies. The method is based on spatial discretization of the problem by first reducing it to a system of first-order nonlinear differential equations and then to a system of difference equations. This method makes it possible to solve the Schroedinger and Poisson equations simultaneously, thereby obtaining a self-consistent solution without additional iterations. In the sections that follow we will describe this method of solution, derive the starting system of equations, and address the problem of choosing boundary conditions. Then we will discuss the basic results of the calculation within this model and their connection with the observed recombination spectrum in a heterojunction with δ doping.

1. COMPUTATIONAL MODEL

Assume that we have already obtained a system of first-order differential equations corresponding to our physical system. Let us write it in the most general form

$$\mathbf{Y}' - \mathbf{F}(\mathbf{Y}) = \mathbf{0}, \tag{1}$$

where $\mathbf{Y}$ is an N-component solution vector. Let us pick out M equally spaced points z_k a distance h from one another within the spatial interval of interest (where z is the independent variable). Then we can approximate our system of differential equations by an equivalent system of difference equations for the $\mathbf{Y}_k$ values of the function we are looking for at the points z_k:

$$\mathbf{E}_k = \mathbf{Y}_k - \mathbf{Y}_{k-1} - \frac{h}{2}(\mathbf{F}(\mathbf{Y}_k) + \mathbf{F}(\mathbf{Y}_{k-1})) = \mathbf{0}. \tag{2}$$

Let us now define a new $N \times M$-component solution vector $\mathbf{Y}$ containing all the components of the vectors $\mathbf{Y}_k$; then we can write our system in the following simple form: $\mathbf{E}(\mathbf{Y}) = \mathbf{0}$. The general method for solving such a system (the relaxation method) is based on iterating Newton's method. Let us define an error vector $\mathbf{\Delta}_s = \mathbf{E}(\mathbf{Y}_s)$ after the s-th iteration. Then the next solution vector can be written based on the expression

$$\mathbf{Y}_{s+1} = \mathbf{Y}_s - \left[\frac{\delta \mathbf{E}}{\delta \mathbf{Y}}\right]^{-1} \mathbf{\Delta}_s. \tag{3}$$

The Jacobi matrix $\hat{\mathbf{S}} = \delta \mathbf{E}/\delta \mathbf{Y}$ for this problem is block-diagonal in form. We used the efficient algorithm described in Ref. 10 to invert this matrix. The advantages of this approach become more palpable when the problem is not limited to solution of the Schroedinger equation alone, since any other equations in the original system (1) that must be solved in combination with the Schroedinger equation can be incorporated as well. Furthermore, the eigenvalue problem is also solvable by simply including the additional equation $\lambda' = 0$ in the original system, where the eigenvalue λ (the energy in our case) is regarded as a function of the independence variable z. The procedure of iterating the solution of system Eq. (2) using Eq. (3), requires specification of a certain initial approximation. In our case we require a whole series of solutions with different physical properties, each of which should start from a different initial approximation. These are trivial to obtain in the limit of zero magnetic field and a planar quantizing potential with infinite barriers. We then change the parameters step by step so as to approach the limit we want, using the solution obtained at the previous step as an initial approximation for the next step. This procedure ensures that our solution will be continuous and that we can track its properties.

Following Ref. 5, we start from the 4×4 Luttinger Hamiltonian[2] with an external magnetic field B parallel to the z axis, neglecting terms linear in the quasimomentum[4]:

$$\mathbf{H} = \begin{vmatrix} X^+ - 3Z & S^+ & R^+ & 0 \\ S & X^- - Z & 0 & R^+ \\ R & 0 & X^- + Z & -S^+ \\ 0 & R & -S & X^+ + 3Z \end{vmatrix}, \tag{4}$$

where

$$X^+ = P + Q, \quad X^- = P - Q, \quad Z = \frac{e}{2c} KB,$$

$$P = \frac{\gamma_1}{2}(k_z^2 + k^2), \quad k_\pm = k_x \pm i k_y,$$

$$Q = \frac{\gamma_2}{2}(-2k_z^2 + k^2), \quad k^2 = k_x^2 + k_y^2,$$

$$R = -\frac{\sqrt{3}}{2}\overline{\gamma} k_-^2 + \frac{\sqrt{3}}{2}\mu k_+^2, \quad \overline{\gamma} = \frac{1}{2}(\gamma_3 + \gamma_2),$$

$$S = \sqrt{3}\gamma_3 k_z k_-, \quad \mu = \frac{1}{2}(\gamma_3 - \gamma_2).$$

In this case, the wave function vector has the following form (the subscripts denote projections of the spin on the z axis):

$$\mathbf{\Phi} = \begin{vmatrix} \phi_{-3/2} \\ \phi_{-1/2} \\ \phi_{+1/2} \\ \phi_{+3/2} \end{vmatrix}. \tag{5}$$

When an external magnetic field B is applied along the direction z, the components of the quasimomentum in the plane no longer commute: $[k_x, k_y] = -ieB/(\hbar c) = -il^{-2}$, where $l = (\hbar c/eB)^{1/2}$ is the magnetic length. Let us introduce ladder operators according to the expressions

$$a^+ = \frac{l}{\sqrt{2}} k_+, \quad a = \frac{l}{\sqrt{2}} k_-, \quad N = a^+ a.$$

It is not difficult to show that these satisfy the relations $[a, a^+] = il^2[k_x, .k_y] = 1$. From this it follows that the operator N has eigenvalues 0, 1, 2, ... Let us denote the corresponding eigenfunctions by $\zeta_0, \zeta_1, \zeta_2, \ldots$; then these functions satisfy the following relations:

$$a^+ \zeta_{n-1} = \sqrt{n}\zeta_n, \quad a\zeta_n = \sqrt{n}\zeta_{n-1}. \tag{6}$$

Let us now rewrite the Hamiltonian (4) in terms of these ladder operators, neglecting the anisotropic term in R (which contains μ), which allows us to write the solution vector in a finite basis in what follows. As was shown in Ref. 5, inclusion of the anisotropy leads to the appearance of anticrossings among Landau levels with labels that differ by 4. Using the relation $N = (1/2)(l^2k^2 - 1)$, we can write the Hamiltonian (4) in the following form:

$$\mathbf{H} = \begin{vmatrix} \Phi_h - 3q & b^+ & -d^+ & 0 \\ b & \Phi_l - q & 0 & -d^+ \\ -d & 0 & \Phi_l + q & -b^+ \\ 0 & -d & -b & \Phi_h + 3q \end{vmatrix}, \tag{7}$$

where we have introduced the notation

$$\Phi_h=\frac{k_z^2}{m_h}+\frac{A}{l^2}\left(N+\frac{1}{2}\right),\quad \Phi_l=\frac{k_z^2}{m_l}+\frac{B}{l^2}\left(N+\frac{1}{2}\right),$$

$$q=\frac{K}{2l^2},\quad b=\frac{2s}{l}k_z a,\quad b^+=\frac{2s}{l}k_z a^+,$$

$$d=\frac{r}{l^2}a^2,\quad d^+=\frac{r}{l^2}a^{+2},$$

$$m_h=\left(\frac{\gamma_1}{2}-\gamma_2\right)^{-1},\quad m_l=\left(\frac{\gamma_1}{2}+\gamma_2\right)^{-1},$$

$$A=\gamma_1+\gamma_2,\quad B=\gamma_1-\gamma_2,$$

$$r=\sqrt{3}\overline{\gamma},\quad s=\sqrt{\frac{3}{2}}\,\gamma_3.$$

Here, m_h and m_l are the doubled effective masses of light and heavy holes. We will look for a solution in the form

$$\mathbf{\Phi}=\begin{vmatrix}\zeta_n(x,y)\psi_1(z)\\ -i\zeta_{n-1}(x,y)\psi_2(z)\\ -\zeta_{n-2}(x,y)\psi_3(z)\\ i\zeta_{n-3}(x,y)\psi_4(z)\end{vmatrix}, \tag{8}$$

where ζ_n are functions of the coordinates in the (x,y) plane corresponding to the Landau level with label n (eigenfunctions of the operator N), and ψ_i are functions of z alone that correspond to the various spin projections. This description corresponds to conservation of the sum of the spin and orbital angular momenta [compare with (5)], which holds in the presence of the spin-orbit interaction. Using Eq. (6), we can rewrite the Hamiltonian (7) in the form of a matrix that acts only on the columns of the function $\psi_i(z)$:

$$\mathbf{H}=\begin{vmatrix}\mathcal{E}_0 & -\frac{2Q}{l}\frac{\partial}{\partial z} & N/l^2 & 0\\ \frac{2Q}{l}\frac{\partial}{\partial z} & \mathcal{E}_1 & 0 & \frac{M}{l^2}\\ \frac{N}{l^2} & 0 & \mathcal{E}_2 & \frac{2P}{l}\frac{\partial}{\partial z}\\ 0 & \frac{M}{l^2} & -\frac{2P}{l}\frac{\partial}{\partial z} & \mathcal{E}_3\end{vmatrix}, \tag{9}$$

where we have made the substitution $k_z\to -i(\partial/\partial z)$ and used the notation

$$M=r\sqrt{(n-1)(n-2)},\quad N=r\sqrt{n(n-1)},$$

$$P=s\sqrt{n-2},\quad Q=s\sqrt{n},$$

$$E_0=\frac{A}{l^2}\left(n+\frac{1}{2}\right)-\frac{3}{2}\frac{K}{l^2},\quad E_1=\frac{B}{l^2}\left(n-\frac{1}{2}\right)-\frac{1}{2}\frac{K}{l^2},$$

$$E_2=\frac{B}{l^2}\left(n-\frac{3}{2}\right)+\frac{1}{2}\frac{K}{l^2},\quad E_3=\frac{A}{l^2}\left(n-\frac{5}{2}\right)+\frac{3}{2}\frac{K}{l^2},$$

$$\mathcal{E}_0=-\frac{1}{m_h}\frac{\partial^2}{\partial z^2}+E_0,\quad \mathcal{E}_1=-\frac{1}{m_l}\frac{\partial^2}{\partial z^2}+E_1,$$

$$\mathcal{E}_2=-\frac{1}{m_l}\frac{\partial^2}{\partial z^2}+E_2,\quad \mathcal{E}_3=-\frac{1}{m_h}\frac{\partial^2}{\partial z^2}+E_3.$$

Now our problem is to obtain a system of first-order differential equations from this second-order differential operator. The easiest method, i.e., treating the first derivatives ψ_i' as unknown functions, is somewhat inconvenient here since these functions will not be continuous at the boundary between GaAs and AlGaAs. In order to satisfy the requirement of continuity, let us construct new unknown functions by operating on the vector ψ with the velocity operator $v_z=(i/\hbar)(\mathbf{H}z-z\mathbf{H})$. The continuity of the functions v_z will be a consequence of the law of conservation of particle number. Substituting the Hamiltonian of the form

$$\mathbf{H}=A\frac{\partial^2}{\partial z^2}+B\frac{\partial}{\partial z}+C,$$

into the velocity operator, we obtain by analogy with Ref. 11

$$v_z=\frac{i}{\hbar}\left(2A\frac{\partial}{\partial z}+B\right). \tag{10}$$

Now we can write the complete system of first-order differential equations for the functions ψ and $\tilde{\psi}=v_z\psi$. The first four equations are obtained directly from Eq. (10), while the next four are obtained by differentiating the first and substituting the expressions obtained for the second derivatives ψ''

into the original operator (9):

$$\begin{cases} \psi_1' - m_h\left(\tilde{\psi}_1 - \frac{Q}{l}\psi_2\right) = 0, \\ \psi_2' - m_l\left(\tilde{\psi}_2 + \frac{Q}{l}\psi_1\right) = 0, \\ \psi_3' - m_l\left(\tilde{\psi}_3 + \frac{P}{l}\psi_4\right) = 0, \\ \psi_4' - m_h\left(\tilde{\psi}_4 - \frac{P}{l}\psi_3\right) = 0, \\ \tilde{\psi}_1' - \left[\left(A(n+\frac{1}{2}) - m_l Q^2 - \frac{3}{2}K\right)\frac{1}{l^2} + u - \epsilon\right] \\ \quad \times\psi_1 + m_l\frac{Q}{l}\tilde{\psi}_2 - \frac{N}{l^2}\psi_3 = 0, \\ \tilde{\psi}_2' - \left[\left(B(n-\frac{1}{2}) - m_h Q^2 - \frac{1}{2}K\right)\frac{1}{l^2} + u - \epsilon\right] \\ \quad \times\psi_2 - m_h\frac{Q}{l}\tilde{\psi}_1 - \frac{M}{l^2}\psi_4 = 0, \\ \tilde{\psi}_3' - \left[\left(B(n-\frac{3}{2}) - m_h P^2 + \frac{1}{2}K\right)\frac{1}{l^2} + u - \epsilon\right] \\ \quad \times\psi_3 - m_h\frac{P}{l}\tilde{\psi}_4 - \frac{N}{l^2}\psi_1 = 0, \\ \tilde{\psi}_4' - \left[\left(A(n-\frac{5}{2}) - m_l P^2 + \frac{3}{2}K\right)\frac{1}{l^2} + u - \epsilon\right] \\ \quad \times\psi_4 + m_l\frac{P}{l}\tilde{\psi}_3 - \frac{M}{l^2}\psi_2 = 0, \end{cases} \tag{11}$$

where u is the electrostatic potential and ϵ is the energy eigenvalue. For the case $n=0$, all the components of the wave function (8) except those with spin $-3/2$ equal zero. In this case, only the first and fifth equations remain in the system (11), and the state is a pure spin state. For $n=1$, there are two, and for $n=2$ there are three nonzero spin components, and system (11) contains four and six equations, respectively. These have two or three solutions, corresponding to different spin sublevels. All the remaining states have four nonzero spin components in all, and the system (11) admits four different solutions. Nevertheless, in the limit $B=0$ all the solutions become pure with respect to spin. The spin projection corresponding to the nonzero component of the wave function that remains in this limit can also be assigned to a Landau level. In this case, the solutions with spin $\pm 3/2$ will correspond to heavy holes, while those with spin $\pm 1/2$ correspond to light holes. Following Ref. 12, we will use, along with the Landau level label N, an additional label i for the component $\zeta_i(x,y)$ that dominates the solution vector (8) in the limit $B\to 0$, i.e., n, $n-1$, $n-2$, $n-3$ for states with spin $-3/2$, $-1/2$, $+1/2$, $+3/2$ respectively. In this system of notation, all the Landau levels have four spin sublevels apiece, with two corresponding to heavy and two to light holes.

In order to obtain a complete system of equations that describe the problem under study, we should include in the system the Poisson equation for the potential u, which is a second-order equation. We can transform it to a first-order equation by integrating over the coordinate z. The integral of the square of the wave function which enters into this equation will be used as yet another unknown function χ which satisfies the equation $\chi' = |\psi|^2$. Finally, the last equation is for the eigenvalue ϵ. Thus, we obtain

$$\begin{cases} u' + 4\pi\dfrac{e^2}{\varepsilon}[n_s(p_l\chi + \rho_l - 1) + N_i z - N_s] = 0, \\ \chi' - \psi_1^2 - \psi_2^2 - \psi_3^2 - \psi_4^2 = 0, \\ \epsilon' = 0. \end{cases} \tag{12}$$

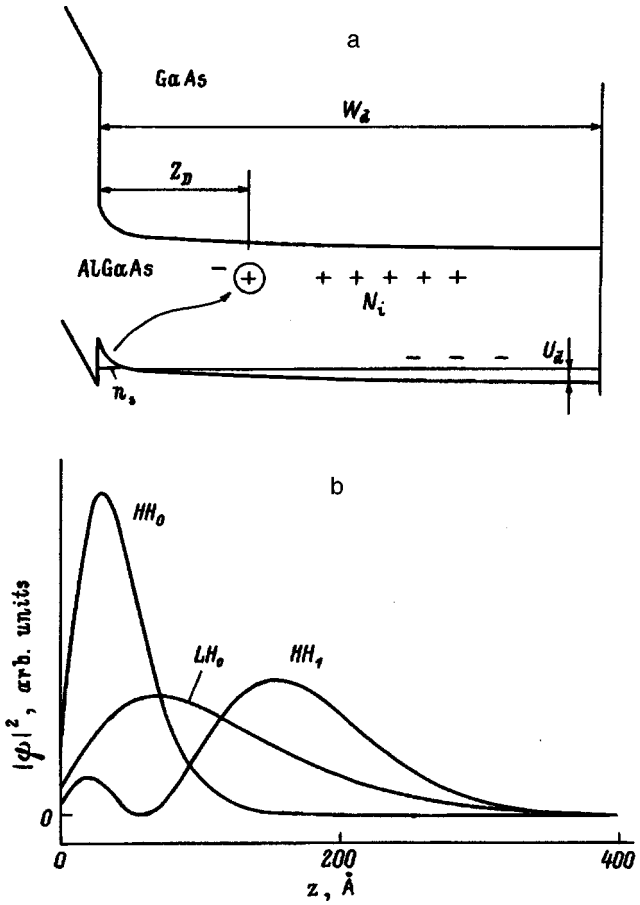

FIG. 1. a) Structure of bands near the heterojunction and basic model parameters. b) Square of the wave function in zero magnetic field plotted versus distance to the heterojunction for the size-quantized subbands HH_0, LH_0 and HH_1.

Here we have introduced the following notations: n_s is the density (per unit surface area) of the hole gas, ε is the dielectric permittivity, l is a label that enumerates a given energy level, p_l is the fraction of the overall number of holes that belongs to the l-th energy level ($\Sigma p_l = 1$), χ is the integral of the wave function density ($\chi(z\to-\infty)=0$, $\chi(z\to+\infty)=1$) and ρ_l is the integral of the wave function density averaged over all the remaining levels, i.e., $\rho_l = \Sigma_{i\neq l} p_i\chi_i$, N_i is the bulk density of charged impurities in the depletion layer, and N_s is the total number of charged impurities in the depletion layer per unit heterojunction area. For this we have $N_s = W_d N_i$, where W_d is the width of the depletion region.

As is well-known, under conditions of steady-state photoexcitation the potential behind the heterojunction very rapidly becomes flat due to neutralization of the depletion layer charge.[13] In this case, the quasi-Fermi level of the holes measured from the top of the valence band will equal half the binding energy of an acceptor: $U_d \approx 15$ meV (Fig. 1a). The width of the depletion layer can be estimated from the first equation in (12) if we do not include the hole charge and impose the equation $u(W_d) = U_d$. Thus, we obtain $W_d = (U_d\varepsilon/2\pi e^2 N_i)^{1/2}$. For $N_i \approx 10^{15}\,\mathrm{cm}^{-3}$ this gives $W_d \approx 1500$ Å.

It is possible to solve Eqs. (11) and (12) using the relaxation method described above only along a finite segment of

the z axis. It is convenient to pick as this segment the region of width W_d between the heterojunction boundary and the region of constant potential. As we shall show below, for a constant potential there exists a simple algorithm for constructing boundary conditions for the wave function that takes into account its penetration of the barrier. In this case, for the left-hand boundary, i.e., in AlGaAs, we also shall assume the potential is a constant, since the interval over which its varies considerably exceeds the penetration depth of the wave function. In this approximation the wave function $\mathbf{y}=\{\psi,\tilde{\psi}\}$ is a solution to the differential equation $\mathbf{y}'+A\mathbf{y}=\mathbf{0}$ with a matrix A that is independent of z. The boundary conditions required to solve Eqs. (11) and (12) on the interval $[0,W_d]$ are made up to two parts. First of all we should guarantee that the wave function attenuates at the barrier. For this we must obtain matrix projection operators onto the subspaces of eigenvectors of the matrix A whose eigenvalues have positive and negative real parts. It is easy to obtain a matrix $\tilde{A}$ (as the solution to the equation $\tilde{A}^2=A^2$) that differs from A only by the sign of certain eigenvalues. Let us choose these signs such that the real parts of all the eigenvalues will be positive. Then the matrix projection operators are obtained according to the expression $A^{\pm}=A\pm\tilde{A}$. The second boundary condition includes the integral of the wave function density χ. At the right edge of the integral we can set this integral equal to unity, since the amplitude of the wave function is negligibly small there. However, for the right-hand boundary we require an exact computation. In the most general case $\chi=\int y^T D y dz$, where D is a quadratic form. The problem reduces to calculating the integral

$$\int_0^{\infty} y^T D y dz = y_0^T I_0^{\infty}(A,D) y_0,$$

where I_0^{∞} is the matrix of the unknown quadratic form. When the matrix A is z independent, we can write the solution vector y with the help of a matrix exponential, by which we understand the sum of the corresponding series, as follows: $y(z)=e^{-Az}y_0$. Then $I=\int e^{-A^T z} D e^{-Az} dz$. Integrating by parts and taking into account that during the integration we have $e^{-Az}\to 0$ at the infinite limit, we obtain the following recursion relation that allows us to compute I_0^{∞} to any prespecified accuracy:

$$I_0^{\infty}(A,\,D)=\frac{1}{2}DA^{-1}+\frac{1}{2}I_0^{\infty}(A,\,D-A^T DA^{-1}). \tag{13}$$

Now we can write the necessary boundary conditions at the left and right boundaries in the following form:

$$\begin{cases} A_0^+ y_0 = 0, \\ \chi_0 - y_0^T I_0 y_0 = 0, \\ u_0 = 0, \end{cases} \quad \begin{cases} A_1^- y_1 = 0, \\ \chi_1 = 1, \end{cases} \tag{14}$$

where the labels 0, 1 denote parameters that are computed at the left- and right-hand boundaries respectively. The procedure for self-consistent calculation of the shape of the potential requires computation of the integrated density function $\rho_l(z)$ and the occupation numbers p_l at each magnetic field step. The occupation numbers should be calculated from the capacity of the Landau levels, which depends on magnetic field. In this case it is understood that the occupation factor ν is smaller than the total number of levels M involved in the calculation. In the range of magnetic fields where this condition is not satisfied, we can set all the p_l equal to M^{-1} as a first approximation. However, this approach leads us to a completely incorrect result in the limit of zero magnetic field, since in this case all the holes will have $\mathbf{k}=0$. In order to resolve this problem, we make use of the following concept. At a certain magnetic field B_x, where $\nu<M$, let us fix the factor $(2N+1)/(2l^2)$ in the Hamiltonian and decrease the magnetic field while keeping all the occupation numbers p_l constant. In the limit $B\to 0$ this corresponds to $N\to\infty$, where the level N transforms into a state with $(k^2/2)=(2N+1)(eB_x)/(2\hbar c)$. The two spin sublevels transform into two spin dispersion branches.[4,6] Equal occupation numbers of Landau levels will correspond to equal fractions of states that are equidistant with respect to k^2. In this case we will not necessarily obtain the exact value of the Fermi energy in zero field, but the approximate shape of the potential well will be entirely satisfactory. The shape of the potential well in the range $0<B<B_x$ can be kept in memory and used for the next calculation of energy levels.

In order to compare the results of this calculation with data from optical experiments, it is necessary to obtain expressions for the quantities observed in these experiments, i.e., the intensity and degree of polarization of the recombination light. We shall ignore the actual shape of the wave function of an electron bound to a donor, which is similar to the ground state of a hydrogen atom, and approximate it by an inverse- exponential dependence in the z direction: $|e_D\rangle=\exp(-|z-z_D|/a_D)$, where z_D is the coordinate of the δ-layer and a_D is the Bohr radius. To accuracy up to a numerical factor, the intensity of luminescence in the $\sigma+$ and $\sigma-$ polarizations for a level with label l can be written in the form

$$\begin{cases} I_l^+ = p_l\left[\dfrac{3}{4}\langle\psi_1|e_D^-\rangle+\dfrac{1}{4}\langle\psi_2|e_D^+\rangle\right], \\ I_l^- = p_l\left[\dfrac{3}{4}\langle\psi_4|e_D^+\rangle+\dfrac{1}{4}\langle\psi_3|e_D^-\rangle\right], \end{cases} \tag{15}$$

where $|e_D^{\pm}\rangle$ are wave functions of an electron in the z direction with two directions of spin; the matrix elements $\langle\psi_i|e_D^{\pm}\rangle$ are understood to be integrals over the variable z. Here we have taken into account that the optical transition matrix element connected with the spin is three times larger for heavy holes than it is for light holes.[14] In this case the selection rule for the spins is the following: the difference between spins of an electron and hole should equal ± 1 [compare Eqs. (8) and (5)]. Neglecting the spin splitting of the electron and its polarization, we can set $|e_D^{\pm}\rangle=|e_D\rangle$, and then the total intensity of circularly polarized light will equal

$$I_l^{\sigma}=\frac{p_l}{4}[3\langle\psi_1|e_D\rangle+\langle\psi_2|e_D\rangle+\langle\psi_3|e_D\rangle+3\langle\psi_4|e_D\rangle], \tag{16}$$

while the degree of polarization is

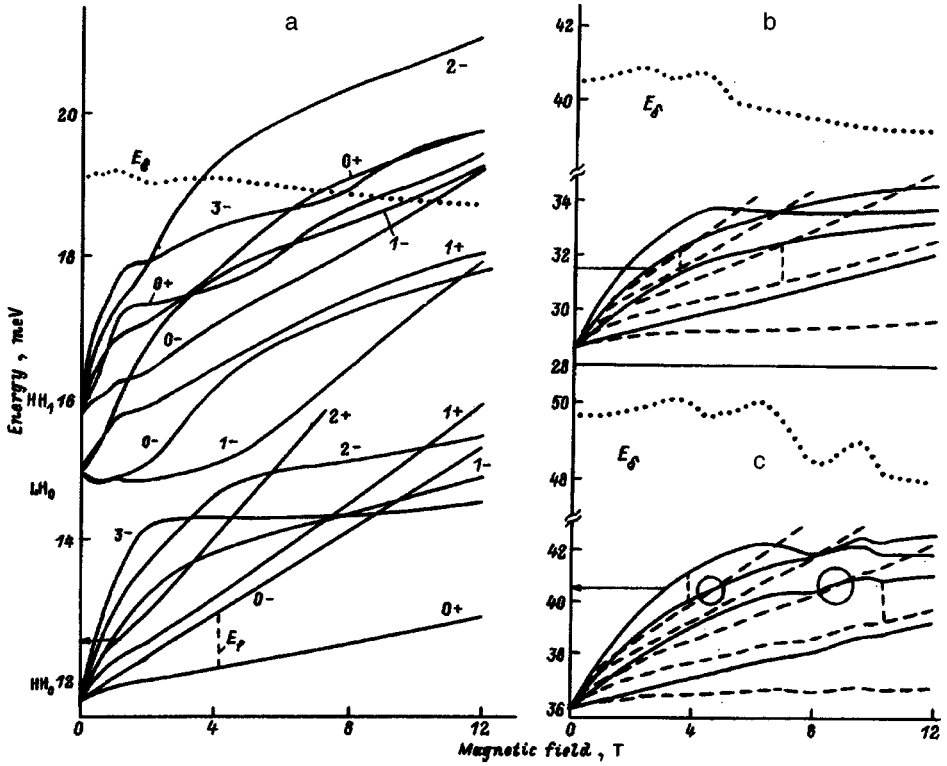

FIG. 2. a—Energy levels of a 2D hole gas plotted versus magnitude of the magnetic field for three size-quantized subbands at a concentration of $1\times10^{11}\,\mathrm{cm}^{-2}$. Also shown is the position of the Fermi level E_f and the magnitude of the electrostatic potential at the δ layer U_δ. The position of the Fermi level in zero magnetic field is denoted by arrows. b, c—Energy levels of the ground-state heavy-hole subband at concentrations of 5×10^{11} and $7.5\times10^{11}\,\mathrm{cm}^{-2}$ respectively. Also shown is the dependence of U_δ on magnetic field, which reflects the filling and emptying of levels with different spins, denoted by solid $(-)$ and dotted $(+)$ curves. The circles denote the pinning region of the energy levels.

$$\rho_l=\frac{I_l^+-I_l^-}{I_l^++I_l^-}$$
$$=\frac{3\langle\psi_1|e_D\rangle+\langle\psi_2|e_D\rangle-\langle\psi_3|e_D\rangle-3\langle\psi_4|e_D\rangle}{3\langle\psi_1|e_D\rangle+\langle\psi_2|e_D\rangle+\langle\psi_3|e_D\rangle+3\langle\psi_4|e_D\rangle}. \qquad (17)$$

For linearly polarized light, the difference in spins should be zero, and the spin matrix element should equal 1/2.[14] Accordingly, we obtain for the intensity $I_l^\pi=(p_l/2)[\langle\psi_2|e_D\rangle+\langle\psi_3|e_D\rangle]$. In these calculations we start from the following choice of parameters[6]: $\gamma_1=6.85$, $\gamma_2=2.1$, $\gamma_3=2.9$, $K=1.2$, and $\varepsilon=12.5$.

2. RESULTS AND DISCUSSION

The calculations show that for the chosen values $U_d=15$ meV and $N_i=10^{15}\,\mathrm{cm}^{-3}$ (Fig. 1a) three size-quantized levels are present in the potential well: a lower heavy-hole level HH_0, a lower light-hole level LH_0, and the first size-quantized heavy-hole level HH_1. Figure 1b shows the dependence of the square of the wave function $|\psi|^2=\psi_1^2+\psi_1^2+\psi_3^2+\psi_4^2$ on the coordinate z for zero magnetic field. The Landau levels for these three size- quantized subbands in the range of magnetic fields from 0 to 12T at a concentration of $n_s=1\times10^{11}\,\mathrm{cm}^{-2}$ are shown in Fig. 2a. This figure shows the position of the Fermi level E_f. It is clear from the figure that the pure-spin Landau level $0-$ in the HH_0 subband is not the lowest in energy, since the level $0+$ is located considerably below it. Out of the entire set of levels only $0-$ remains more or less linear over the entire range of magnetic fields: its deviation from linearity is due only to changes in the shape of the potential well. The largest nonlinearity in the HH_0 subband is for level $N-$ (for $N>0$), which increases with increasing N. In Fig. 3 we show the dependence of the square of the wave function $|\psi|^2$ on coordinate z for Landau levels H_03-, L_00+ and H_13-, i.e., the three subbands, in fields 1, 5, and 12T. It is clear from this figure that the nonlinearity of the $N-$ level in the HH_0 subband is unambiguously associated with the strong dependence of the wave function on magnetic field. Conversely, the level $N+$ behaves practically linearly with respect to field. Its wave functions differ only slightly from the wave function $0-$ over the entire range of magnetic fields.

The light-hole Landau levels of the subband LH_0 differ by a still larger nonlinearity even in the range of small fields. Qualitatively this is explained by the presence in the Hamiltonian (9) of terms proportional to $l^{-1}=\sqrt{B}$, which act on the wave function component with spin $\pm1/2$ and are dominant in the small-field range. In this case, even the sign of the g factor for light holes turns out to be opposite the sign of the g factor for heavy holes: levels with negative projection of the spin lie lower in energy. Furthermore, levels $0-$ and $0+$ have larger energy than $1-$ and $1+$ (although for higher labels this is no longer true). This anomaly is probably explained by the fact that these levels have an incomplete set of spin components. As is clear from Fig. 3, the wave function for level $0+$ changes significantly with increasing magnetic field, its maximum shifts to the right, which also causes an increase in energy. The other levels behave analogously. The figure reveals the nonmonotonic character of the change in shape of the wave function as well, connected with the appearance of new zeros as the magnetic field increases. This feature, which is characteristic of all the hole levels except the few with an incomplete set of spin components, can be described as follows: the number of zeros of the wave function increases continuously with increasing magnetic field

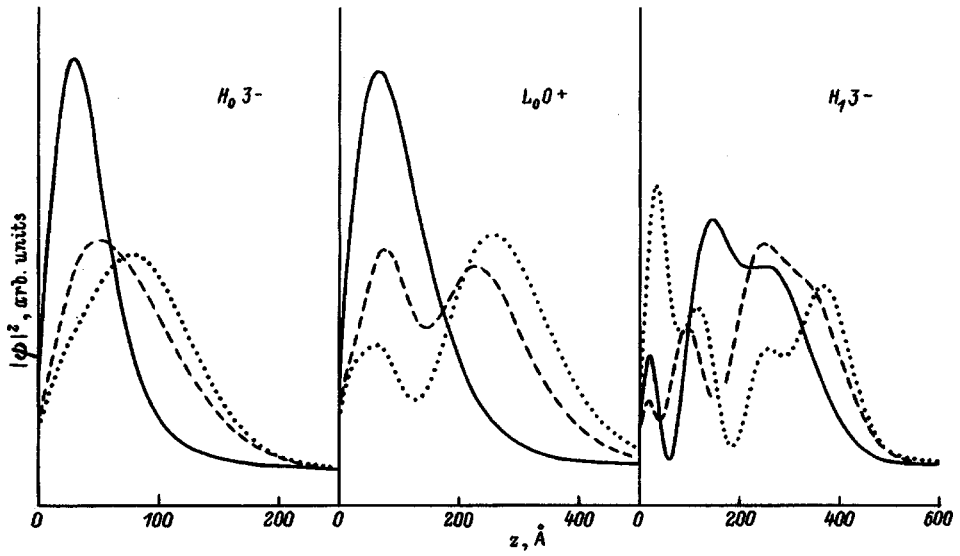

FIG. 3. Square of the wave function plotted against distance to the heterojunction for Landau levels of three size-quantized subbands in magnetic fields of 1T (solid curve), 5 T (dashed curve), and 12 T (dotted curve) at a concentration of 5×10^{11} cm^{-2}.

roughly as $\sqrt{B}$, with a coefficient that depends on the label of the level. This is explained qualitatively by the presence of a term with $S\sim k_z k_-$ in the Hamiltonian (4), which mixes the motion in the plane of the potential well with the motion normal to it. If, however, we revert to the dispersion law for zero magnetic field,[3] then the behavior of the new zeros will be connected with the appearance of anticrossings of various size-quantized subbands. The Landau levels are constructed out of states with $k^2\sim B$, while the energy of the size-quantized subbands is proportional to n^2. Accordingly, the anticrossings appear for $k^2\sim n^2$, from which it is clear that the number of zeros should increase like k and $\sqrt{B}$. The Landau levels of the HH_1 subband have a still more complicated structure. Here the g factor again has a reversed sign, but it does not depend as strongly on magnetic field as for the case of the light holes. This phenomenon is apparently explained by the interaction with the low-lying subband of light holes. Although essentially the Landau levels of various subbands do not have sharply expressed anticrossings and can intersect each other, the overall character of their field dependence reflects anticrossings that existed in the dispersion. The wave functions of Landau levels of this subband begin to depend strongly on magnetic field even at fields of 1T (Fig. 3). This probably reflects the increasing importance of the cross term $S\sim k_z k_-$ in the Hamiltonian (4) as k_z increases.

As the concentration of the hole gas increases, the change in the shape of the wave functions in a magnetic field begins to affect the shape of the potential well more and more strongly, since levels turn out to be occupied with larger and larger labels for the same field. In order to estimate the scale of this shape change of the potential, in Fig. 2 we show the magnetic field dependence of the potential for the δ- layer $U_\delta = u(z_D)$ by a dotted curve. At a concentration of 5×10^{11} cm^{-2} (Fig. 2b), the occupation of level $N-$ of the subband HH_0 is found to have a strong effect on the shape of the potential well in the range of fields where its wave functions begin to shift to the right due to the appearance of new zeros. Occupation of this level turns out to leads to broadening of the potential well and to an increase in U_δ and the energy of the higher-lying size- quantized subbands due to the overall increase in the difference of potentials between the left and right edges of the potential well. When the Fermi level eventually passes through this level, its emptying is accompanied by an abrupt change in the shape of the well and a corresponding decrease in the energy of the higher-lying levels. It is clear from Fig. 2b that the oscillations in fields of 2.5 and 4.5T are unambiguously related to emptying of Landau levels $2-$ and $1-$ respectively. The subsequent smooth falloff in U_δ at large fields is apparently connected with the fact that the wave function of level $0+$ has a tendency to be compressed with increasing magnetic field. One more interesting phenomenon connected with changes in the shape of the potential well takes place when levels $N-$ and $M+$ intersect while the Fermi level lies within one of the two. At a concentration of 7.5×10^{11} cm^{-2} (Fig. 2c) this happens twice: in a field of 4.7T, where levels $2-$ and $4+$ intersect, and in a field of 9T, where levels $1-$ and $2+$ intersect. As the hole levels intersect, their populations begins to redistribute. As a result, the occupation of level $N-$ increases, while that of $M+$ decreases. However, since the wave function of level $N-$ is considerably broader than that of $M+$, this leads to a change in the shape of the potential well, which is apparent in the increase in U_δ. However, because the wave function of level $N-$ is considerably broader, it reacts strongly to this change, and its energy increases. The feedback that arises decreases the occupation of this level, and as a result a pinning of these two levels takes place: within a certain interval of magnetic field they remain very close to one another, and only the occupation of the levels changes. All of this is accompanied by the appearance of distinctive features in U_δ and in the energy of the higher-lying levels. Of course, a correct calculation of this situation requires choice of a specific hole temperature. The scheme described above for calculating the occupation numbers p_l is implicitly zero-temperature, and leads to computational instability in the case of pinning. The simplest method of removing this instability was used, i.e., introducing a linear

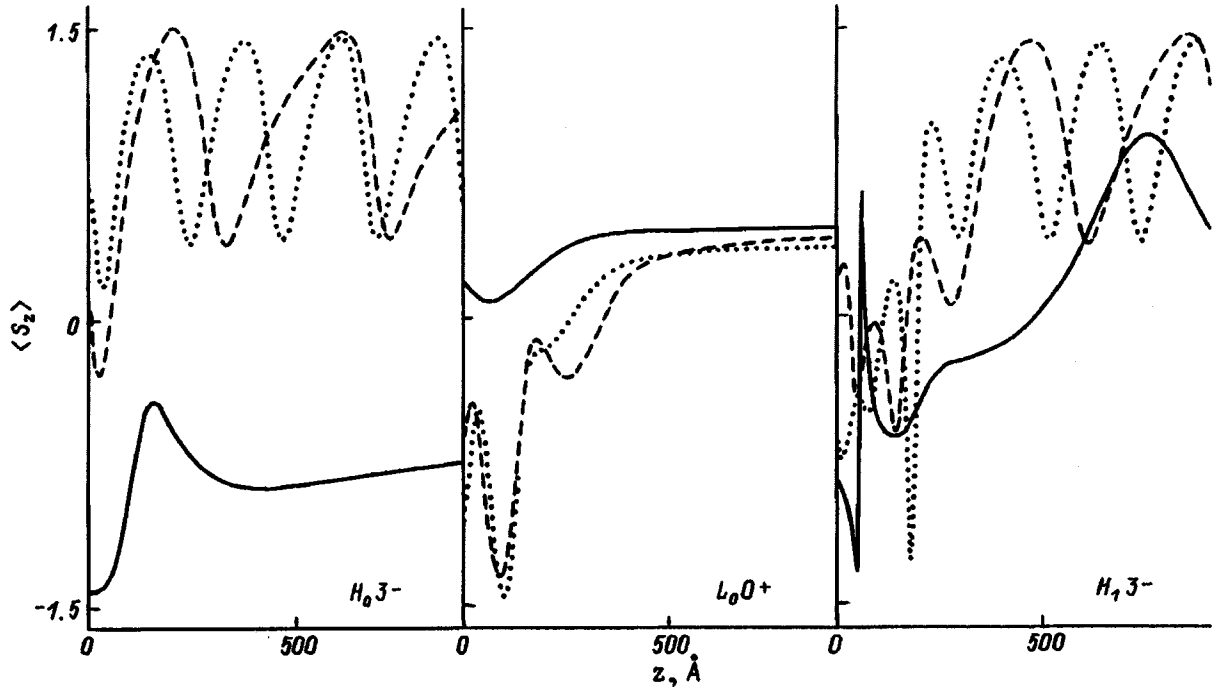

FIG. 4. Dependence of the average spin on the distance to the heterojunction for the levels shown in Fig. 3.

washing-out of the Fermi level over a fixed energy interval.

Figure 4 shows the dependence of the average spin $\langle S_z \rangle$ on coordinate z for the Landau levels shown in Fig. 3, which were calculated from the expression

$$\langle S_z \rangle = \frac{-\frac{3}{2}\psi_1^2 - \frac{1}{2}\psi_2^2 + \frac{1}{2}\psi_3^2 + \frac{3}{2}\psi_4^2}{\psi_1^2 + \psi_2^2 + \psi_3^2 + \psi_4^2}.$$

As is clear from this figure, the average spin of all the levels (except for the pure-spin level $0-$ for heavy holes) exhibits a strong dependence both on the magnitude of the magnetic field and on coordinates. The spin of level $3-$ undergoes nonattenuating oscillations in both subbands, which spread with unchanged period even into the region of the potential barrier where the wave functions are strongly attenuated. Here is yet another interesting property of the hole wave functions: they can attenuate in the barrier in an oscillatory manner, and the period of these oscillations depends only weakly on the potential energy. This is explained qualitatively by the presence of the cross term $S \sim k_z k_-$ in the Hamiltonian (4), which adds a real part that is potential-independent to the imaginary part of k_z in the below-barrier region.

The phenomena discussed above should be directly visible in the optical properties of this system, i.e., the intensities and polarizations of the luminescence lines. The dependence of the intensity of recombination light on magnetic field for the two ground-state heavy-hole levels $0-$ and $0+$ is shown in Fig. 5a. For this calculation we use Eq. (16) and the following parameters of the electron wave function at the donor: $z_D = 500$ Å, $a_D = 80$ Å. As is clear from the figure, the intensity of the luminescence of the pure spin level $0-$ behaves quite trivially: first it increases linearly

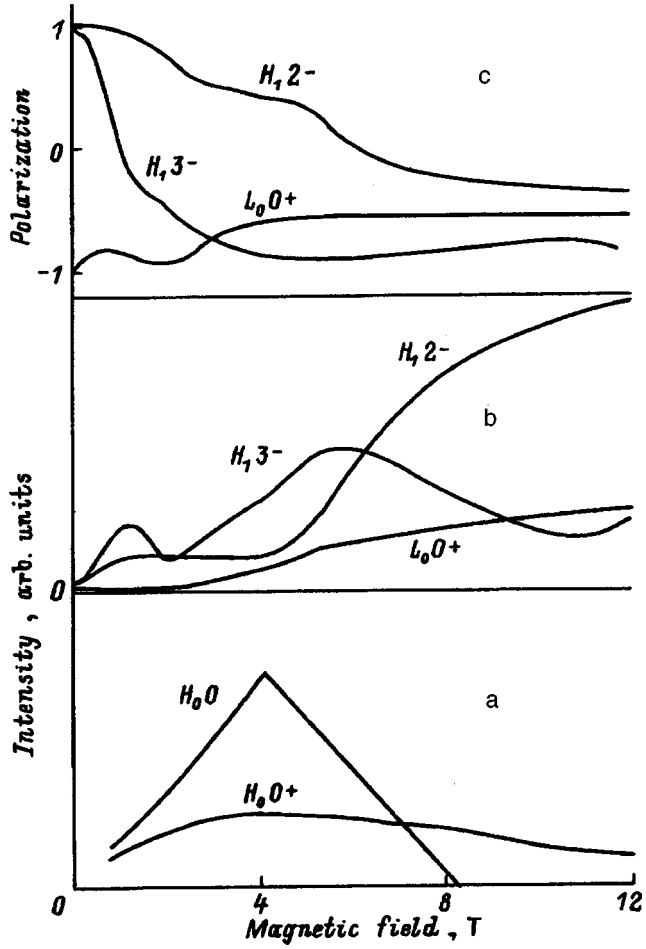

FIG. 5. a—Dependence of the luminescence intensity from the ground-state subband level HH_0 on the magnitude of the magnetic field at a concentration of 2×10^{11} cm^{-2}. b, c—Dependence of the intensity and degree of polarization of the luminescence from Landau levels of the upper size-quantized subband that are most active in recombination on the magnitude of the magnetic field for a concentration of 5×10^{11} cm^{-2}.

with field, proportional to the increase in capacity of the level, and then falls off, also linearly, proportional to its emptying. The intensity of the luminescence from level $0+$ depends on field in a more complicated way. Here the increase due to the increased capacity of the level competes with the falloff due to the weak compression of the level with increasing magnetic field. However, the effects described above are manifested in the most dramatic way in the intensity and polarization of luminescence from nonequilibrium occupied levels of the higher-lying subbands. Figures 5b and 5c show the field dependences of the intensity and degree of polarization of recombination light from the most luminescence-active Landau levels of the excited subbands at a concentration of $5\times10^{11}\,\mathrm{cm}^{-2}$. These oscillations in intensity and degree of polarization are connected with changes in the shape of the wave functions and the potential well, and also with the oscillations of the average spin discussed above. Reference 9 gives a more detailed comparison of the calculations with experimental results.

Thus, the method given here is a very effective instrument for calculating hole wave functions, especially when this requires a self-consistent calculation of the shape of the potential well caused by the holes themselves. It was used to calculate energy levels and wave functions for 2D holes in an isolated p-type heterojunction in a perpendicular magnetic field at various 2D hole concentrations. We have shown that the wave functions corresponding to different hole quantized states exhibit a strong dependence on magnetic field, which is enhanced with increasing level energy and depends appreciably on the level spins. We have demonstrated that at high hole-gas concentrations effects of occupation and emptying of different-spin levels of the ground-state heavy- hole subband lead to a change in the shape of the potential well and pinning of the energy levels. We have discussed the processes of recombination of 2D holes with electrons bound to a δ layer of donors near the heterojunction. We have shown that the change in shape of the wave functions of holes in a magnetic field is accompanied by an increase in the number of zeroes of the wave function and oscillations in the average spin, leading to oscillations in the intensity and polarization of the recombination light.

The author is grateful to V. E. Bisti, and also to I. V. Kukushkin and V. E. Zhitomirskiĭ for fruitful discussions in connection with the theoretical model and the results obtained using it.

This work was carried out with the support of the Russian Fund for Fundamental Research (Grant 96-02-16177) and INTAS (Grant 95-IN/RU-675).

[1] J. M. Luttinger and W. Kohn, Phys. Rev. **97**, 869 (1955).
[2] J. M. Luttinger, Phys. Rev. **102**, 1030 (1956).
[3] M. I. D'yakonov and A. V. Khaetskiĭ, Zh. Éksp. Teor. Fiz. **82**, 1584 (1982) [Sov. Phys. JETP **55**, 917 (1982)].
[4] D. A. Broido and L. J. Sham, Phys. Rev. B **31**, 888 (1985).
[5] S.-R. Eric Yang, D. A. Broido, and L. J. Sham, Phys. Rev. B **32**, 6630 (1985).
[6] U. Ekenberg and M. Altarelli, Phys. Rev. B **32**, 3712 (1985).
[7] E. Bangert and G. Landwehr, Surf. Sci. **170**, 593 (1986).
[8] I. V. Kukushkin and V. B. Timofeev, Adv. Phys. **45**, 147 (1996).
[9] O. V. Volkov, V. E. Zhitomirskii, I. V. Kukushkin, W. Dietsche, K. V. Klitzing, A. Fischer, and K. Eberl, Phys. Rev. B **56**, 7541 (1997).
[10] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, in *Numerical Recipes in C* (Cambridge Univ. Press, 1992).
[11] R. Eppenga, M. F. H. Schuurmans, and S. Golak, Phys. Rev. B **36**, 1554 (1987).
[12] B. B. Goldberg, D. Heiman, M. J. Graf, D. A. Broido, A. Pinczuk, C. W. Tu, J. H. English, and A. C. Gossard, Phys. Rev. B **38**, 10 131 (1988).
[13] I. V. Kukushkin and V. B. Timofeev, Zh. Éksp. Teor. Fiz. **92**, 258 (1987) [Sov. Phys. JETP **65**, 146 (1987)].
[14] C. R. Pidgeon and R. N. Brown, Phys. Rev. **146**, 575 (1966).

Translated by Frank J. Crowne