Novel Surface States and the Quantum Hall Effect in an Anisotropic Three-Dimensional System

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A theoretical study of the electronic level structure of tunneling semiconductor superlattices in the Hall configuration is presented. Our self-consistent calculations reveal that surface-type states associated with the depletion regions at the ends of the superlattice appear in the gap between Landau levels during Landau-level emptying. The surface-type states are pinned to the Fermi energy throughout the range of magnetic fields where the quantum Hall plateau occurs. Our results explain the Hall quantization index and the anomalously small activation energy observed recently by Störmer *et al.*

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Within the past few years, research on thin multilayer semiconductor structures has attracted a great deal of attention.[1,2] This work has been stimulated by the possibility of being able to synthesize systems with prescribed electronic properties which can be used to study a variety of very interesting physical phenomena. A prime example of such a system is the superlattice fabricated from layers of GaAs alternating with doped layers of AlGaAs. Since the latter material has a larger energy gap than GaAs, the electrons (or holes) donated by the ionized impurities are confined mainly to the GaAs regions. However, if the doped layers are thin, quantum tunneling occurs in the direction perpendicular to the layers, giving a three-dimensional character to the electrons. This system has been recently used by Störmer *et al.*[3] in a novel and stimulating quantum-Hall-effect experiment. Previously, the quantum Hall effect (QHE) had always been observed in systems where the electrons (or holes) have a purely *two-dimensional* character.[2,4] Well-known examples of such structures are the inversion layer in a metal-oxide-semiconductor field-effect transistor,[5] the interface of a single semiconductor heterojunction such as GaAs/AlGaAs,[6] and a layered semiconductor multiple quantum-well system.[7] However, Störmer *et al.*[3] demonstrated that the quantization of the Hall resistance persists in an electronic system which exhibits an anisotropic three-dimensional energy dispersion relation.[8]

In this Letter we report self-consistent calculations of the energy-level structure and corresponding charge distribution across a tunneling semiconductor superlattice in the presence of a large magnetic field. We predict an unusual behavior of the level structure as a function of the applied field. The levels undergo a complex, highly nonlinear global rearrangement with respect to the Fermi level every time that a Landau level is emptied. Most interestingly, this transition involves the creation of surface-type states (located mostly in the depletion region near the ends of the superlattice) which "peel off" from the band continuum and closely track the Fermi energy of the system. The calculated superlattice level structure allows us to explain important features observed in the QHE experiment,[3] such as the value of the Hall quantization index and, especially, the remarkably small activation energy of the Hall plateau. We also propose that the additional application of a potential difference across the superlattice chain in a QHE experiment would provide interesting information about the distribution of localized states *within* the levels.

The superlattice can be viewed as a set of N potential wells attractive to electrons and separated by finite barriers. The main features of the miniband structure, such as the bandwidths, are generally well represented by a simple Kronig-Penney model which uses the available experimental data such as the layer thicknesses and the alloy composition x (as in the case of the superlattice $GaAs/Al_xGa_{1-x}As$, to determine the potential barrier height).[1,9] However, a more detailed calculation of the electronic level structure should consider the existence of midgap states at both ends of the superlattice. The physical nature of these states is related to impurities in the substrate on which the superlattice is grown and/or to states associated with the termination of the layer growth. These midgap states at the ends of the superlattice chain strongly affect its electronic level structure by pinning the Fermi level of the system and producing depletion regions near the ends.[3,7]

In this calculation we make use of a basis of states belonging to the lowest electron miniband to describe electron propagation in the direction perpendicular to the superlattice layers (z direction). In order to work in real space, we transform from the miniband Bloch states to a representation in terms of a Wannier set (of tight-binding states) centered on the different GaAs layers. The corresponding Hamiltonian for the single miniband considered here is then given by

$$H_z = \sum_j (v_j c_j^\dagger c_j - t c_{j+1}^\dagger c_j - t c_j^\dagger c_{j+1}), \quad (1)$$

where c_j is the destruction operator associated with the tight-binding state in the layer j (=1 to N), and t is the nearest-neighbor hopping matrix element (spin indices

are suppressed and summations over them are understood). The terms with v_j represent the self-consistent potential felt by the electrons. We take v_j to be a Coulombic potential[10] calculated from Poisson's equation

$$v_{j+1}-2v_j+v_{j-1}=4\pi e^2 a(\rho_+-\rho_j)/\varepsilon, \quad (2)$$

where ρ_+ is the positive background density, ρ_j is the areal electronic density of layer j, a is the superlattice period, and ε is the average semiconductor dielectric constant. The boundary conditions at both ends of the superlattice are chosen to take into account the midgap states mentioned above. In the present scheme, the potential values at the ends are kept fixed with respect to the Fermi energy μ of the system. At one end, we set $v_{N+1}=\mu+\delta$, with a constant value of δ which mimics the effect of states at the free surface of the superlattice structure. The other end is assumed to be attached to an impurity-free buffer, of thickness L, followed by a doped substrate region which also provides midgap states at this end of the structure. Therefore, $v_0=v_1+(v_{N+1}-v_1+\delta'-\delta)a/L$, where we have assumed the buffer to be free of any charges, and the potential at its far end is given by $\mu+\delta'$, with a constant δ'.

In the case of a magnetic field along the z axis, $\mathbf{B}=B\hat{\mathbf{z}}$, the intralayer motion is characterized by a Landau-level number n, and a spin index, with eigenvalues

$$\varepsilon_{n\sigma}=(n+\tfrac{1}{2})\hbar\omega_c+g\mu_B B\sigma, \quad (3)$$

where $\omega_c=eB/m$ is the cyclotron frequency, m is the electronic effective mass, μ_B is the Bohr magneton, $\sigma=\pm\frac{1}{2}$ is the spin z projection, and g is the Landé factor appropriate to the system.[11] The corresponding level degeneracy per unit area is given by $(2\pi a_c^2)^{-1}$, where $a_c=(\hbar/eB)^{1/2}$ is the magnetic length. The electronic density per layer appearing in Eq. (2) can then be written as

$$\rho_j=(1/2\pi a_c^2)\sum_{mn\sigma}|b_j^m|^2 I_{mn\sigma}, \quad (4)$$

where b_j^m is the jth coefficient of the transverse-motion eigenvector of H_z with eigenvalue ε_m. The coefficients $I_{mn\sigma}=\{1-\mathrm{erf}[(\varepsilon_{mn\sigma}-\mu)/\Gamma\sqrt{2}]\}/2$, with $\varepsilon_{mn\sigma}=\varepsilon_{n\sigma}+\varepsilon_m$, take into consideration the impurity broadening of the levels via a Gaussian function of rms half-width Γ, and neglect the typically small thermal broadening present in experiments (i.e., $\Gamma\gg kT$).

Equations (2)–(4), together with the diagonalization of H_z in Eq. (1), are numerically solved self-consistently. In Fig. 1 we show the resulting level structure as a func-

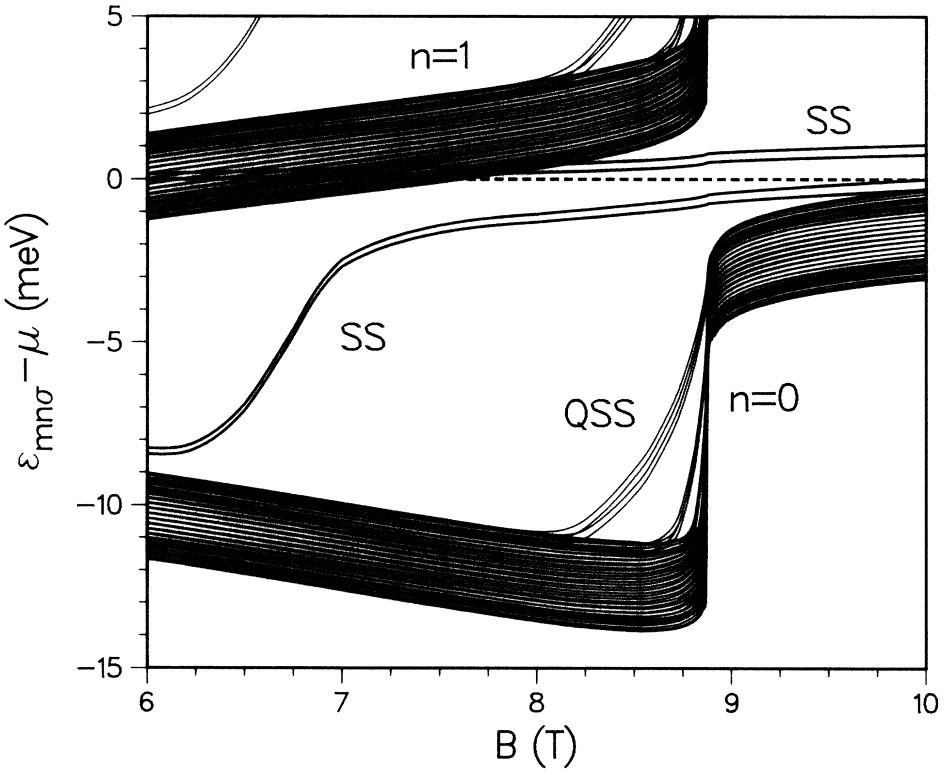

FIG. 1. Level structure of superlattice for lowest Landau indices ($n=0,1$) and high fields; only the center of each broadened level is shown ($\Gamma=1$ meV). Fermi level appears dashed. SS denotes surface states, appearing in doublets because of spin, and correspond to $\sigma=\pm\frac{1}{2}$, $n=0$, and $m=24,25$. For QSS see text. 48 $nm\sigma$ levels lie below μ at $B\simeq 9$ T.

tion of the magnetic field for a GaAs/AlGaAs superlattice with thirty layers, the case studied in the experiment of Ref. 3.[12] The eigenvalues $\varepsilon_{mn\sigma}$ are plotted relative to μ for a region of magnetic field in which the second Landau *band* ($n=1$) is being emptied (only the center of each broadened level is shown). In addition to the expected Landau bands due to the z dispersion of the electrons (bandwidth $W \simeq 4t$ in the case of large N), there are states that "peel off" from the quasicontinuum to lie in the gap region between the Landau bands. These states [denoted by SS in Fig. 1 and belonging to the $n=0$ Landau band with $\sigma = \pm\frac{1}{2}$ and $m=24,25$] arise because of the inhomogeneous self-consistent Coulomb potential associated with the depletion regions near the ends of the superlattice chain and, most interestingly, closely track the Fermi level over a wide range of magnetic fields. The eigenvectors corresponding to these states which lie in the Landau gap are strongly peaked near one of the ends of the chain, and decay rapidly (within about two GaAs layers) towards the interior. Other states (denoted by QSS in Fig. 1) also show a tendency to peel off from the continuum (and correspondingly show eigenvectors having a somewhat enhanced amplitude near one of the ends), but only for a small range of magnetic fields. They promptly rejoin the band, and recover their "bulklike" character. Notice that in Fig. 1 there are only 48 $mn\sigma$ levels below μ at $B \simeq 9$ T, out of the 60 levels corresponding to the $n=0$ Landau band. The other $n=0$ levels are not occupied (or only partially so, as in the case of the upper SS doublet) since they are associated with the depletion layers at the ends of the superlattice. The highest ten levels in the $n=0$ band are at too high an energy to be visible in Fig. 1.

Figure 1 also shows the quite sudden highly nonlinear rearrangement of most of the level structure with respect to μ, occurring close to the value of B at which the band $n=1$ is emptied completely. This unique behavior is a consequence of the self-consistent interactions, and would not appear in a noninteracting-electron scheme. The global level rearrangement occurs every time that a Landau band empties, but with decreasing "jump" amplitude for increasing n, because of the decreasing fractional charge of each band with respect to the total.[13] In addition, Fig. 1 shows that the surface states SS remain almost stationary in energy across the global level rearrangement (other than the expected systematic slow drift with respect to μ, which changes their fractional occupation). Indeed, the surface states must dominate the behavior of the quasiparticle excitations near the Fermi level of the system in this regime, and are thus of the utmost importance for the QHE experiment.

Let us now discuss the consequences of the calculated level structure for the QHE. In the usual two-dimensional electron systems, at low temperatures and large magnetic fields, the Hall resistance is quantized according to $\rho_H = \hbar/e^2\nu$, where ν is an integer to a very high experimental accuracy,[4-7] while the longitudinal resistance nearly vanishes. The Hall plateaus are understood in terms of the Fermi level's lying in a region of localized states which exist in the tails of each broadened 2D level.[4] The integer ν is a topological invariant[4,14] which is identified with the number of Landau levels l (counting spin) having their extended states below the Fermi level. In a single 2D system $\nu = l$, whereas in a multiple-quantum-well stack $\nu = ls$, where s is the number of wells in the stack. On the other hand, both experimental[15] and theoretical[16] evidence suggests that the energy range of extended states in the middle of each 2D level is very narrow. Moreover, since the impurities and disorder which produce localized states in a typical 2D system are also present in the case of a superlattice, we expect that the broadened levels $\varepsilon_{mn\sigma}$ will show similar characteristics. Indeed the experimentally observed value $\nu = 48$ of the QHE index reported by Störmer *et al.*,[3] for the plateau centered at $B \simeq 8.9$ T, is completely consistent with identification of ν with the number of broadened levels $\varepsilon_{mn\sigma}$ whose centers lie below the Fermi energy in our calculation (see Fig. 1) for a reasonable choice of model parameters.[12] The surface states SS have a strong 2D-like character, being nearly confined to a single GaAs layer, and lying outside of the bulklike energy bands. It is thus reasonable to suppose that, in common with 2D systems,[15,16] the SS also have only a very narrow range of extended states at the middle of the broadened $\varepsilon_{mn\sigma}$ level. Correspondingly, the activation energy Δ of the QHE plateau should be given by the separation between μ and the *closest extended surface level.* (Note that there are localized states right at μ which come from the tails of the nearby levels as a result of the finite level broadening Γ.[12]) We find $\Delta \lesssim 0.5$ meV. This value is over an order of magnitude smaller than the activation energy which one would expect in the absence of surface states (since then one would estimate $\Delta \simeq \hbar\omega_c - W \simeq 13$ meV, as is explained in Ref. 3). Thus our calculations provide a plausible answer to the puzzle of the very small experimentally observed activation energy $\Delta_{exp} \simeq 0.26$ meV.[3] Precise agreement with experiment can be attained here by small variations of the constants δ and δ', or by reduction of Γ to $\simeq 0.5$ meV, but this would be somewhat artificial since one expects other effects also to have an impact on this fine tuning.[10,11] The above interpretation of the QHE experiment in terms of the calculated level structure also answers the question raised by Störmer *et al.*[3] as to why an integer QHE is observed experimentally in this system even though there is unequal filling with electrons of the superlattice quantum wells in the region of the depletion layers.

It is interesting to notice that variation of the total electronic density by the application of a voltage across the superlattice (possibly in a backsided-gate configuration[17]) would affect the value of Δ, as well as the number

of levels below μ, changing the Hall quantization index in a concurrent QHE experiment. This could provide a direct experimental map of the distribution of extended and localized states within the surface levels, as well as information on the mixing of spin doublets which seems to affect the widths of QHE plateaus.[18] This information is of great current interest,[4,19] and experimental work in this direction would certainly be very stimulating.

In summary, we have calculated the electronic level structure of a semiconductor superlattice as a function of the magnetic field in a Hall configuration. Self-consistent interactions produce a global level rearrangement at the emptying of the Landau bands which is preceded by the peeling off of surface states from the band continuum. These surface states track the Fermi level in the region of the Hall plateaus, and are vital in understanding the main features of the QHE experiment.

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