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Spin instabilities in semiconductor superlattices

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The subband levels of quantum wells grown in a periodic array form minibands whose bandwidth Δ depends on the probability of interlayer tunneling. In the presence of a strong magnetic field, this system of minibands can exhibit various Coulomb-interaction-driven spin polarization instabilities at an integral value of the filling factor ν. We investigate in particular the Hartree-Fock phase diagram in the case in which the $n=0$ spin-up and $n=1$ spin-down Landau levels are separated by an energy smaller than Δ. A spin-density-wave ground state is shown to occur at filling factor $\nu=2$.

In the presence of a strong magnetic field, a single quantum well is known to exhibit a spin polarization instability at filling factor $\nu=2$ at a finite value of $\epsilon=\hbar(\omega_c-\omega_s)$, the energy separation between the upper spin state of the $n=0$ Landau level, $|0\uparrow\rangle$, and the lower spin state of the $n=1$ Landau level, $|1\downarrow\rangle$.[1] Quite generally, these instabilities result from electron-electron interactions in situations in which the exchange overcomes the correlation energy, and can lead to the stabilization of spin-polarized phases. Experimental evidence of such an interesting behavior has been reported by several groups.[2–4] It was, moreover, pointed out that in the presence of many flavors of electrons (as, for instance, in the case of multivalley degeneracy) the same system may undergo a spin-density-wave (SDW) instability.[5,6] An extensive study of the Hartree-Fock phase diagram for the multivalley configuration of Si inversion layers has been carried out in Ref. 7. A physically equivalent situation arises within the lowest Landau level when the $n=0$ and the $n=1$ energy levels are replaced by the symmetric and antisymmetric levels of a double quantum well.[8]

In this paper we extend the original work on a single quantum well[1] to a superlattice in which the Landau subbands are replaced by minibands whose energy depends on k_z, the wave number in the direction of the superlattice axis. The nature of the ground state is found to depend critically on the magnitude of the bandwidth Δ of the minibands. For small tunneling probability, the quasi-two-dimensional (quasi-2D) system undergoes a paramagnetic to ferromagnetic transition, as in the case of a 2D electron gas. For larger tunneling probability a critical value of the miniband width Δ_c occurs for which transitions from the lower miniband are energetically favorable. The resulting partial occupancy establishes a Fermi level at k_{F-} (k_{F+}) in the upper (lower) miniband. A SDW coupling between these two bands results at $Q=\pi/a$. This is an equivalent situation to that of a 3D electron gas in a strong magnetic field as studied by Celli and Mermin,[9] except that the superlattice has real minibands in which the periodic part of the Bloch function is not simply a constant. In addition, two different Landau levels as well as two different spin levels are involved. At $\epsilon=0$, the minibands $|0,k_y,k_z,\uparrow\rangle$ and $|1,k_y,k_z,\downarrow\rangle$ are degenerate, and each band is half-filled, and when the electron-electron interaction is considered, a rather standard Overhauser SDW (Ref. 10) with $Q=2k_F=\pi/a$ (where a is the superlattice period) occurs. For $|\epsilon|\gg\Delta$, the system has paramagnetic ($|0\downarrow\rangle$ and $|0\uparrow\rangle$ occupied) or ferromagnetic ($|0\downarrow\rangle$ and $|1\downarrow\rangle$ occupied) occupancy depending upon the sign of ϵ.

We model the superlattice as a periodic array of attractive δ-function potentials. For a single quantum well with potential $V(z)=-\lambda\delta(z)$, the bound-state energy and wave function are given by $\epsilon_0=-\hbar^2\kappa^2/2m$ and $\zeta(z)=\sqrt{\kappa}e^{-\kappa|z|}$, where $\kappa=m\lambda/\hbar^2$. For the superlattice we take the potential $V(z)=-\lambda\Sigma_l\delta(z-la)$, with l an integer. The miniband wave function and energy can be written (in a tight binding approximation) as

$$\psi(k_z,z)=\frac{1}{\sqrt{N}}\sum_l e^{ik_zla}\zeta(z-la) \tag{1}$$

and

$$\epsilon(k_z)=\epsilon_0(1+4e^{-\kappa a}\cos k_z a). \tag{2}$$

The wave function of Eq. (1) can be easily written in the standard Bloch form $\psi_{k_z}=e^{ik_zz}u(k_z,z)$, where $u(k_z,z)$ is a periodic function of z with period a. The complete function for a superlattice state is

$$|n,k_y,k_z,\sigma\rangle=e^{ik_zz}u(k_z,z)\phi_{nk_y}(x,y)\eta_\sigma. \tag{3}$$

Here $\phi_{nk_y}(x,y)=L^{-1/2}e^{ik_yy}H_n(x+k_yl)$, where $l=\sqrt{\hbar c/eB}$ is the magnetic length, $H_n(x)$ is the nth simple harmonic oscillator function, and η_σ represents the spin eigenfunction. The allowed values of k_y are $2\pi j/L$, with j an integer and L

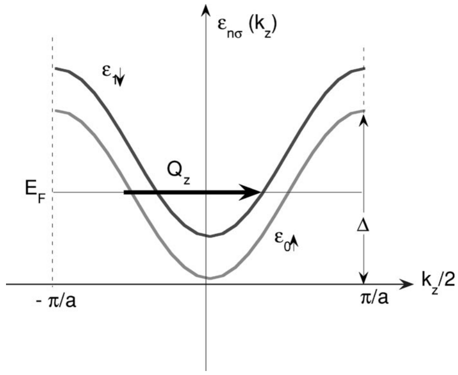

FIG. 1. Energy spectrum of the $|0,k_y,k_z,\uparrow\rangle$ and $|1,k_y,k_z,\downarrow\rangle$ minibands. The minimum interband transition energy is decreased from the value ϵ because of the finite bandwidth Δ. An instability to a SDW ground state can occur when ϵ becomes comparable to Δ.

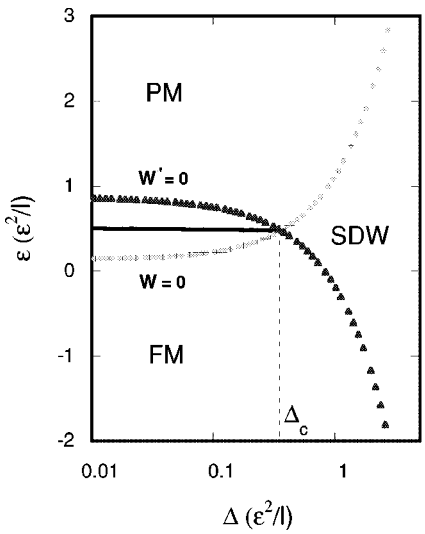

FIG. 2. Hartree-Fock phase diagram of the superlattice in the presence of a quantizing magnetic field. The nature of the ground state depends critically on the magnitude of the bandwidth Δ. At small Δ the system undergoes a paramagnetic to ferromagnetic transition. For values of Δ exceeding a critical value Δ_c a SDW ground state becomes possible.

the length for periodic boundary conditions in the y direction. $k_z = 2\pi j/Na$, where j is an integer in the range $\pm N/2$.

As shown in Fig. 1, the $|0\uparrow\rangle$ and $|1\downarrow\rangle$ minibands become almost degenerate when $\epsilon = \hbar(\omega_c - \omega_s)$ is made very small (for instance, by orienting the applied magnetic field in the appropriate direction). We anticipate then that when the bands overlap, the Hartree-Fock ground state of the superlattice will be characterized by a spin density wave. In this case the mechanism of formation for the SDW is the exchange interaction between electrons in states $|0,k_y,k_z,\uparrow\rangle$ and those in states $|1,k_y,k_z+Q,\downarrow\rangle$.

The existence a differential magnetic instability can be inferred from very simple considerations. When an electron from the $|0\uparrow\rangle$ miniband moves into the $|1\downarrow\rangle$ miniband, the energy of the transition can be seen as made up of three parts: the ''kinetic energy,'' which here is simply the energy gap between the two states in the absence of the electron-electron interactions, the exchange energy of the electron with all the other electrons with the same spin, and the binding energy of the electron and the hole which is left in the initial miniband.[11] The matrix element of the Coulomb interaction between electrons in minibands $|n,\vec{k}+\vec{Q},\sigma\rangle$ and $|m,\vec{k}',\sigma'\rangle$ is

$$
\begin{aligned}
v_{nm}(k_z,\vec{q},\vec{Q}) &= \frac{e^2}{L}F(k_z,q_z,Q_z)\int_{-\infty}^{\infty}\frac{dq_x}{q^2}e^{(-l^2/2)(q_y^2+q_x^2-2iq_xQ_y)} \\
&\times\left\{\delta_{n,0}\delta_{m,0}+\left[1-\frac{l^2}{2}(q_y^2+q_x^2)\right]\delta_{n,0}\delta_{m,1}\right. \\
&\left.+\left[1-\frac{l^2}{2}(q_y^2+q_x^2)\right]^2\delta_{n,1}\delta_{m,1}\right\},
\end{aligned}
\tag{4}
$$

with $\vec{q} = \vec{k}' - \vec{k}$ and $\delta_{n,m}$ the Kronecker delta. The form factor $F(k_z,q_z,Q_z)$ describes the exchange of momentum along the z direction. Assuming small tunneling probability, an approximate expression for $F(k_z,q_z,Q_z)$ is obtained:

$$
\begin{aligned}
F(k_z,q_z,Q_z) &= \frac{2\pi}{a^2}\left(\frac{4\kappa^2}{4\kappa^2+q_z^2}\right)^2\left\{1-2\kappa a e^{-\kappa a}\sin\left(\frac{q_z a}{2}\right)\right. \\
&\times\cos\left[\left(k_z+\frac{q_z}{2}+\frac{Q_z}{2}\right)a\right]\left[\sin\left(\frac{Q_z a}{2}\right)\right. \\
&\left.\left.-\frac{2\kappa}{q_z}\cos\left(\frac{Q_z a}{2}\right)\right]\right\}.
\end{aligned}
\tag{5}
$$

By summing over the exchanged momentum $\vec{q}$, one obtains the exchange energy and the electron-hole binding energy.[11] The latter is $\gamma_{nm}(k_z,Q_y,Q_z) = -\Sigma_{q_y,q_z}v_{nm}(\vec{k},\vec{q},\vec{Q})$, whereas the former is simply $\epsilon_{nm}^{ex}(k_z) = \gamma_{nm}(k_z,0,0)$. The exciton energy involving the states $|0,k_y,k_z,\uparrow\rangle$ and $|1,k_y+Q_y,k_z+Q_z,\downarrow\rangle$ is given by

$$
\begin{aligned}
W = \epsilon - \frac{\Delta}{2}[\cos(k_z+Q_z)a - \cos k_z a] - \gamma_{00}(k_z,0,0) \\
+\gamma_{01}(k_z,0,0) + \gamma_{01}(k_z,Q_y,Q_z).
\end{aligned}
\tag{6}
$$

The paramagnetic ground state becomes differentially unstable for $W \leqslant 0$. The first electronic states to experience this instability are those with $k_z = \pi/a$ (at the maximum energy in the lower band) interacting with $k_z = 0$ (at the minimum in the upper band) so that $Q_z = \pi/a$ also. Using these values of k_z and Q_z, and by setting $lQ_y = lQ_{yc} = 1.25$ (the value for which the 2D instability occurs), we plot the curve $W = 0$ in the ϵ,Δ plane in Fig. 2 where, for illustration purposes, we have also chosen $a = 0.5l$. Above this curve, the paramagnetic occupancy (of $|0\downarrow\rangle$ and $|0\uparrow\rangle$) is a stable Hartree-Fock solution for the interacting system.

For large negative values of ϵ and for negligible tunneling, electrons occupy $|0\downarrow\rangle$ and $|1\downarrow\rangle$ minibands and the ground state is ferromagnetic. The energy of an exciton involving the states $|1,k_y,k_z,\uparrow\rangle$ and $|0,k_y+Q_y,k_z+Q_z,\downarrow\rangle$ consists of the "kinetic energy" $-\epsilon$, the lost exchange $-\gamma_{11}(k_z,0,0)-\gamma_{01}(k_z,0,0)$, and the electron-hole binding energy $\gamma_{01}(k_z,Q_y,Q_z)$. Clearly the ferromagnetic ground state becomes differentially unstable when the exciton energy

$$\tilde{W}=-\epsilon-\frac{\Delta}{2}[\cos(k_z+Q_z)a-\cos k_z a]-\gamma_{11}(k_z,0,0)$$
$$-\gamma_{01}(k_z,0,0)+\gamma_{01}(k_z,Q_y,Q_z) \tag{7}$$

becomes negative. As before, this first occurs for values of the momentum at the edges of the Brillouin zone, $k_z=\pi/a$, and for a momentum transfer $Q_z=\pi/a$. In Fig. 2, the curve $\tilde{W}=0$ delimits the region below which the ferromagnetic occupancy (of $|0\downarrow\rangle$ and $|1\downarrow\rangle$) is a stable Hartree-Fock solution. The two dashed curves cross at $\Delta=\Delta_c$. In the weak tunneling regime of $\Delta<\Delta_c$, the paramagnetic occupancy occurs for $W>0$, while the ferromagnetic occupancy obtains for $\tilde{W}<0$. The paramagnetic to ferromagnetic transition occurs for $W\leqslant\epsilon\leqslant\tilde{W}$, just as it does for a 2D system.[1] Which of these possible solutions is more stable is determined by comparing the corresponding Hartree-Fock total energies just as in the single-layer case. This leads to the solid line separating paramagnetic and ferromagnetic states in Fig. 2. At higher tunneling values, when $\Delta>\Delta_c$, the miniband broadening determines the appearance of an intermediate ground state characterized by a spatially varying local magnetic moment. As we show below a possible candidate is a SDW ground state.

The nature of the ground state can be analyzed by introducing the Hamiltonian of the interacting system,

$$H=\sum_n\sum_{k_z}\epsilon_{n,k_z,\sigma}c^\dagger_{n,k_z,\sigma}c_{n,k_z,\sigma}+\frac{1}{2}\sum_{n,m}\sum_{\vec{k},\vec{q},\vec{Q},\sigma,\sigma'}v_{nm}$$
$$\times(\vec{k},\vec{q},\vec{Q})c^\dagger_{n,\vec{k}+\vec{Q}+\vec{q},\sigma}c^\dagger_{m,\vec{k},\sigma'}c_{m,\vec{k}+\vec{q},\sigma'}c_{n,\vec{k}+\vec{q},\sigma}. \tag{8}$$

Here n and m take only the values 0 and 1, and the first term of the Hamiltonian is the kinetic energy. The second describes the Coulomb interaction between electrons in minibands $|n,\vec{k}+\vec{Q},\sigma\rangle$ and $|m,\vec{k},\sigma'\rangle$. A possible Hartree-Fock SDW ground state is obtained from the coherent mixing of states of opposite spins from the $|0,\vec{k},\uparrow\rangle$ and $|1,\vec{k}+\vec{Q},\downarrow\rangle$ minibands. The $|0,\vec{k},\downarrow\rangle$ miniband is considered fully occupied (and remains such) and does not enter the dynamics of the system. Linear-independent operators describing this state are obtained from $c_{\vec{k}}$ through a standard canonical transformation,[1]

$$c_{0,\vec{k},\uparrow}=\cos\theta_{\vec{k}}a_{\vec{k}}+\sin\theta_{\vec{k}}b_{\vec{k}}, \tag{9}$$

$$c_{1,\vec{k}+\vec{Q},\downarrow}=-\sin\theta_{\vec{k}}a_{\vec{k}}+\cos\theta_{\vec{k}}b_{\vec{k}}. \tag{10}$$

The spin inclination angle of each pair of states, $\theta_{\vec{k}}$, and the new quasiparticle spectrum are determined by minimizing the total Hartree-Fock energy of the system. By defining the quantity $g_{\vec{k}}$ as

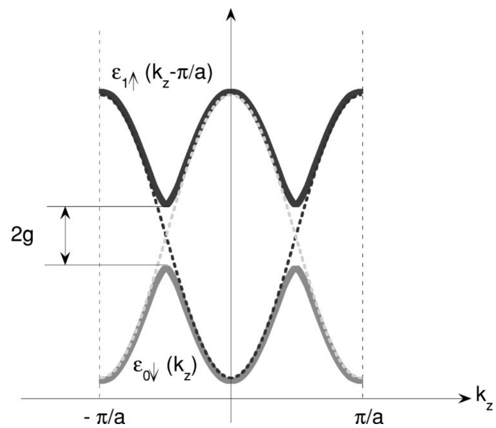

FIG. 3. Quasiparticle spectrum of the superlattice in a linear SDW state. A gap $2g$ opens up at $k_z=Q_z/2a$. Here we have taken $\epsilon=0$.

$$g_{\vec{k}}=\sum_{\vec{q}}v_{01}(\vec{k},\vec{q},\vec{Q})\sin 2\theta_{\vec{k}+\vec{q}}[f(E^-_{\vec{k}+\vec{q}})-f(E^+_{\vec{k}+\vec{q}})], \tag{11}$$

$\theta_{\vec{k}}$ is obtained by solving the self-consistent equation

$$\tan 2\theta_{\vec{k}}=\frac{g_{\vec{k}}}{(\tilde{\epsilon}_{1,\vec{k}+\vec{Q},\downarrow}-\tilde{\epsilon}_{0,\vec{k},\uparrow})}. \tag{12}$$

Here $\tilde{\epsilon}_{n,k_z}$ is the single particle energy with inclusion of exchange, and the occupation probabilities of the new states $f(E^{\pm}_{\vec{k}})$ are given by the usual Fermi function evaluated for the quasiparticle energies

$$E^{\pm}_{\vec{k}}=\frac{1}{2}[(\tilde{\epsilon}_{1,\vec{k}+\vec{Q},\downarrow}+\tilde{\epsilon}_{0,\vec{k},\uparrow})\pm\sqrt{(\tilde{\epsilon}_{1,\vec{k}+\vec{Q},\downarrow}-\tilde{\epsilon}_{0,\vec{k},\uparrow})^2+g^2_{\vec{k}}}]. \tag{13}$$

$E^{\pm}_{\vec{k}}$ differ from the normal-state solutions only in the vicinity of $\vec{k}=-Q/2$, where a gap equal to $2g$ opens up in the energy spectrum. This is shown in Fig. 3 where the spin-up band has been displaced by $\Delta k_z=Q_z=\pi/a$. The overlapping bands would cross, but the SDW exchange coupling opens up gaps at the crossings.

Equation (12) admits three solutions for the angle $\theta_{\vec{k}}$. The solutions $\theta_k=0$ and $\theta_k=\pi/2$ correspond, respectively, to the paramagnetic and ferromagnetic states of the system. The third solution, which we will label as $\theta^*_{\vec{k}}$, corresponds to a SDW state and is a differentially stable solution when $\epsilon<\Delta$. This can be surmised either from Overhauser original paper[10] or from the result of Ref. 9 where it was shown that, for a three-dimensional electron gas in the presence of a magnetic field, a linear SDW solution has lower energy than the paramagnetic state (when many Landau levels are assumed to be occupied) independently of the specific form of the repulsion potential.[12] This would correspond in our case to independence of the result of the exact form of $v_{10}(\vec{k}-\vec{k}')$ in Eq. (12).

The magnetic moment associated with the SDW will be proportional to $(\hat{x}\cos Q_z z+\hat{y}\sin Q_z z)\sin 2\theta_{\vec{k}}$. This oscillatory magnetization must be added to the uniform magnetization associated with the fully occupied $|0\downarrow\rangle$ Landau level, which is parallel to the direction of the applied magnetic field (considered for simplicity to be parallel to the superlattice axis).

Very recently Brey investigated the magnetic phases of a superlattice in which only the $n=0$ Landau level was considered.[13] In this case, the spin splitting $\hbar\omega_s$ appears in the theory in place of our $\hbar(\omega_c-\omega_s)$. This spin splitting is always positive and must be greater or equal to a minimum value dictated by the electron concentration and the integral filling factor. Brey's treatment makes use of the basis function with a layer index l in contrast to our use of a miniband wave vector k_z, and has no discussion of the miniband width Δ in relation to the energy scale $\hbar\omega_s$. Nevertheless, a canted antiferromagnetic state is found when the tunneling amplitude and the layer separation satisfy certain conditions. We have shown here that the canted antiferromagnetic phase, which occurs when the two open bands overlap, is simply the Overhauser SDW studied by Mermin and Celli. For materials in which the spin and cyclotron splittings are of comparable magnitude, the flexibility of adjusting the parameter $\epsilon=\hbar(\omega_c-\omega_s)$ in both magnitude and sign afforded by the present model should be important for the experimental observation of these transitions. The transformation of the quasi-2D subband levels into minibands makes the connection between two- and three-dimensional systems more apparent, and also allows us to use the proofs of Refs. 9 and 10 that, within the Hartree-Fock approximation, a SDW state will have lower energy than the paramagnetic state independently of the exact form of the interaction.

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