Spin Density Waves in a Semiconductor Superlattice in a Tilted Magnetic Field

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Spin density waves in a semiconductor superlattice in a tilted magnetic field

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(Received 16 June 2011; revised manuscript received 19 October 2011; published 17 November 2011)

The ground state of a semiconductor superlattice (SL) placed in a tilted magnetic field is shown to exhibit a spin-density wave structure when the energy spectrum favors crossings between opposite-spin Landau minibands. The SL is modeled as an array of infinitely attractive quantum wells, whose single energy level is broadened into a miniband of width $\Delta$ when weak interwell tunneling is considered. In the presence of the Coulomb interaction, by tailoring the relationship between $\Delta$ and the cyclotron and Zeeman energies, the system transitions between paramagnetic, ferromagnetic, spin-density wave (SDW), and ferromagnetic-paramagnetic stripe ordering. These results are obtained by solving numerically a spin-density-wave gap equation derived at a consistent formalism. We find that for a given value of the difference between the Landau energy and the Zeeman splitting, the initial paramagnetic or ferromagnetic order becomes unstable with respect to the formation of a SDW for $\Delta$ within a certain range. At larger $\Delta$, the system exhibits alternate ferromagnetic-paramagnetic stripes. In the SDW regime, the fractional polarization is up to the order of several tens of percent.

DOI: 10.1103/PhysRevB.84.205321 PACS number(s): 73.21.Cd, 71.70.Ej, 71.45.Gm, 73.61.Ey

I. INTRODUCTION

In the presence of a magnetic field, an electron system—described in standard terms as a collection of $n$ particles per unit volume superimposed on a positive background—is known to exhibit various forms of magnetization that result from the interplay between the Coulomb repulsion and the Zeeman splitting. This phenomenology is even more interesting in systems of reduced dimensionality where quantum restrictions affect the energy spectrum.1 Under special circumstances, spin instabilities leading to long-range magnetic order can appear as a result of degeneracies in the single-electron energies of opposite spins. In GaAs-based two-dimensional (2D) structures the tilted-field geometry, where the applied external field is inclined under an angle with respect to the normal to the plane,2 offers the opportunity of creating such opposite-spin degeneracies by decreasing the value of the cyclotron frequency $\hbar\omega_c$, which depends on the normal component of the magnetic field, to values that are comparable with $\hbar\omega_s$, determined by the magnitude of the field. The latter is usually small in GaAs structures on account of the low value of the effective gyromagnetic factor $\gamma^*$. Early on, it was shown that when $\delta = \hbar(\omega_c - \omega_s)$ is small, many-body interactions can drive spin instabilities between the $\{0,\uparrow\}$ and $\{1,\downarrow\}$ Landau levels.3,4 A calculation of the total electron energy performed within the time-independent Hartree-Fock approximation for an electron liquid at high densities5 indicated that for positive values of $\delta$, the Coulomb interaction drives an abrupt paramagnetic (P) to ferromagnetic (F) transition, without any intermediate magnetic phases, such as spin-density waves (SDWs). In a simple, intuitive description, such an outcome can be understood as a consequence of the independence of the single-particle exchange energy on the 2D momentum $\mathbf{k}$. Ulterior experimental works supported this theoretical picture.6,7 Similar results have been reported to occur in quasi-2D quantum wires with parabolic confinement.8 The robustness of the first-order paramagnetic/ferromagnetic transition has been further explored in the case of the high-density limit in various other configurations.9,10

The fundamental premise for the formation of a SDW state in a simple Fermi system is the existence of a degeneracy between energy levels of opposite spins.11–13 Under these circumstances, the minimum energy of the interacting system in the presence of the exchange component of the Coulomb interaction is reached when a long-range order between electrons of opposite spins and of momenta displaced by the same vector $\mathbf{Q}$ appears. The energy is minimized by allowing for the rotation of the electron spins, such that the local spin polarization is a function of the momentum in phase space. In real space, this magnetic ordering is reflected by a net fractional polarization $\mathbf{P}(z)$, defined as the ratio of the difference in up and down spins to the total number of particles, which is changing continuously along the SL axis, such as in a spiral SDW:12

$$\mathbf{P}(z) = P (\hat{x} \cos Qz + \hat{y} \sin Qz).$$

While definitive proof for the spontaneous formation of a SDW in simple metals has yet to be found, cases of driven spin instabilities leading to stable SDW phases have been recorded in artificially created semiconductor heterostructures.14 Recent calculations found that at lower densities both paramagnetic and ferromagnetic configurations become unstable with respect to the formation of a SDW.15,16

The emergence of various magnetic phases developed in the presence of the Coulomb interaction have been identified theoretically and experimentally in double quantum well systems17–19 and superlattices (SLs).20 These developments originate in the changes induced in the single-particle energy.
spectrum and in the many-body interactions by a component of the electron motion along a direction perpendicular to the layers. This additional degree of freedom permits a larger flexibility in controlling the opposite-spin degeneracy in the momentum space, such that more propitious conditions for the realization of spin instabilities are obtained.

In this paper we discuss the existence of a SDW ground state realized along the axis of a type-I semiconductor superlattice (SL) subject to a tilted magnetic field. The origin of such a phenomenon is the the interplay between the miniband structure, realized in the presence of tunneling between the wells, and the existence of a spin-polarized Landau level structure in the planes perpendicular on the SL axis. Semiconductor SLs have long served as a testing ground for theoretical studies of one-dimensional phenomena as they embody, through construction, the ideal crystal along a specific spatial direction. Given the opportunity to tailor their properties—specifically the energy spectrum—a SL system can be prepared in the most favorable state to support a certain phenomenon. Such characteristics can be particularly useful within the context of finding potential spintronic applications when a SL can be used to engineer states of a given magnetization. Here, we explore the possibility of realizing a definite polarization system by adjusting the parameters of a SL. More precisely, we show that in the presence of a tilted magnetic field, a SL can be made to exhibit a ferromagnetic, paramagnetic, spin-density wave, or ferromagnetic-paramagnetic stripe ground state. This arrangement is frequently used in situations where a comparable magnitude of the two energies is desired. When used in a superlattice, the tilted-field geometry determines a coupling of the motion in the $x$-$y$ planes and that along the SL axis through the in-plane component of the magnetic field. As a result, in the $x$-$y$ plane, the electron is subjected to a modified harmonic potential that depends on the layer index $s$, $e^2(B_x s a + B_y x)^2/2m^*$, while along the $z$ direction the center of the Landau orbits is displaced from $x = 0$ by $x_s = -(B_x/B_y)s a$. Under these circumstances, the exact solution for the single-particle eigenstate, obtained within the tight-binding approximation, is a Bloch function in the $(x,z)$ coordinates, multiplied by a plane wave along the $\hat{z}$ axis. In the following considerations we will approximate this result by its expression in the limit $B_x/B_y \ll 1$ when the in-plane and out-of-plane motions are decoupled. As we show below, this choice preserves the two significant features of the exact solution important for the problem at hand, namely the energy spectrum and the Bloch character along the $\hat{z}$ axis, while permitting a complete analytical treatment of the problem and thus a direct connection with the 2D case. In this sense, our theory generates an exact qualitative picture, but only semiquantitative results. Consequently, we write for the 3D eigenstate

$$\Psi_{n,l,k_x,k_y,\sigma}(x,y,z) = \zeta(z)\psi_{n,k_x,\sigma}(x,y)|\chi\rangle.$$ (2)

Equation (2) represents the product of a $z$-direction Bloch wave,

$$\zeta(z) = \frac{1}{\sqrt{N(1 + 2e^{-\kappa z})}} \sum_l v(z - la)e^{ik_la},$$ (3)

by a 2D state function of an electron in a magnetic field $B_z$,

$$\psi_{n,k_x}(x,y) = \frac{1}{\sqrt{L}} e^{ik_x l} u_n(x + k_x l^2),$$ (4)

and a spin $|\chi\rangle$ eigenstate. Here $u_n(x + l^2 k_x) = \frac{1}{\sqrt{2^n \sqrt{\pi_n}}} \exp[-(x + l^2 k_x)^2/2]\mathcal{H}_n(l^2 + l k_x)$. In these equations $l = \sqrt{\hbar c/\mu_B B_z}$ is the magnetic length, while $\mathcal{H}_n(x)$ is the Hermite polynomial of order $n$. Each Landau level is $N_l = L^2/(2\pi l^2)$ degenerate after $k_x$, the same number as the one given by the exact function. The momentum along the $\hat{z}$ direction is a valid quantum number, whose spectrum is given by $k_z = \frac{2\pi}{N_l} j (j = -N/2, N/2)$, when periodic boundary conditions are assumed. The normalization is done by assuming periodic boundary conditions for $k_x$ in a sample whose dimension along the $\hat{y}$ direction is $L$. In this case, $k_x$ is quantized, $k_x = \frac{2\pi}{L} j$, with $j \in (-\frac{L}{2}, \frac{L}{2})$.

The single-particle energy in a magnetic field associated with the eigenstate in Eq. (2), labeled by the relevant quantum numbers $n$, the Landau level, $k_x$, and $\sigma$, is obtained as

$$\epsilon_{n,k_x,\sigma} = \hbar \omega_c \left(n + \frac{1}{2}\right) + \frac{\Delta}{2} [1 - \cos(k_x a)] + \frac{1}{2} \gamma^* \mu_B \sigma B.$$ (5)

II. SYSTEM DESCRIPTION

The type-I SL system involved in this problem is described as a sequence of $N(N \to \infty)$ identical, infinitely attractive quantum wells of strength $-\lambda$ (of zero width, essentially 2D planes) displaced along the $\hat{z}$ axis at equal intervals $a$. In this setup, there is a single bound state in each well, of quantum wells of strength parameters, motion along the SL axis, when measured from the bottom broadened into minibands. The energy associated with the $N$ states is considered, realized along the axis of a type-I semiconductor superlattice. The flexibility in controlling the opposite-spin degeneracy in the layers. This additional degree of freedom permits a larger flexibility in controlling the opposite-spin degeneracy in the momentum space, such that more propitious conditions for the realization of spin instabilities are obtained.

In this paper we discuss the existence of a SDW ground state realized along the axis of a type-I semiconductor superlattice (SL) subject to a tilted magnetic field. The origin of such a phenomenon is the the interplay between the miniband structure, realized in the presence of tunneling between the wells, and the existence of a spin-polarized Landau level structure in the planes perpendicular on the SL axis. Semiconductor SLs have long served as a testing ground for theoretical studies of one-dimensional phenomena as they embody, through construction, the ideal crystal along a specific spatial direction. Given the opportunity to tailor their properties—specifically the energy spectrum—a SL system can be prepared in the most favorable state to support a certain phenomenon. Such characteristics can be particularly useful within the context of finding potential spintronic applications when a SL can be used to engineer states of a given magnetization. Here, we explore the possibility of realizing a definite polarization system by adjusting the parameters of a SL. More precisely, we show that in the presence of a tilted magnetic field, a SL can be made to exhibit a ferromagnetic, paramagnetic, spin-density wave, or ferromagnetic-paramagnetic stripe ground state. The existence of any of these states is conditioned by the selection of several parameters, such as the miniband width and the intensity of the magnetic field. These phases are stabilized in the presence of the Coulomb interaction, which is treated self-consistently within the Hartree-Fock approximation. Numerical solutions obtained at $T = 0$ K for the SDW gap equation outline the phase diagram of the system. The experimental realization of the theory discussed below involves SL with high mobility and thin barriers, to minimize disorder.

The paper starts by presenting a description of the system and single-particle properties, in Sec. II, followed by a discussion of the many-body Coulomb interaction in Sec. III. In Sec. IV the self-consistent SDW gap equation is derived. Its numerical solutions are later employed in Sec. V in describing the results.
Although the eigenstate in Eq. (2) is not exact, it generates an energy spectrum, described by Eq. (5), similar to the one detected experimentally in Ref. 21. This represents a sequence of Landau minibands spin-split by the Zeeman interaction. The validity of the approximation is constrained by the assumption that the in-plane and the \( \hat{z} \)-axis degrees of freedom can be decoupled. Beyond this limit, alternative methods for controlling the Zeeman splitting through the variation of the gyromagnetic factor \( \gamma^* \) can be pursued.24

In the following considerations, the same three indices \( \{n,k_z,\sigma\} \) will be used to label the minibands. The interplay of the three energies introduced by the problem, \( \hbar \omega_c, \gamma^* \mu_B B, \) and \( \Delta, \) determines the miniband structure of the system, which, in the presence of the Coulomb interaction of the order \( e^2/\epsilon l \) (\( \epsilon \) is the dielectric constant of the system), determines the magnetic structure of the ground state. In particular, here we explore the possible existence of a spin-density wave phase, known to appear when the degeneracy of two opposite-spin minibands favors a collective pairing of opposite spin states that differ by the same momentum \( \mathbf{Q}. \) In this problem, where the lowest lying states are contained within the minibands \( |0,k_z,\downarrow\rangle, |0,k_z,\uparrow\rangle, \) and \( |1,k_z,\downarrow\rangle, \) an SDW coupling is most likely realized between \( |0,k_z,\uparrow\rangle \) and \( |1,k_z + Q_z,\downarrow\rangle. \) We anticipate that paramount to the realization of the SDW phase is the role played by the momentum \( k_z, \) along the \( \hat{z} \) axis, on account of the previously established result that any coupling in the \( x-y \) plane leads only to a paramagnetic-ferromagnetic transition.3 This energetic arrangement is plotted in Fig. 1, where a potential SDW instability point is realized for a coupling vector \( Q_z = \pi/a \) when states at the edge of the Brillouin zone of \( |0,k_z,\uparrow\rangle \) becomes degenerate with those at the center of the Brillouin zone of \( |1,k_z,\downarrow\rangle. \) In the following considerations, we neglect the presence of the \( |1,k_z,\uparrow\rangle \) miniband which is considered to be separated by a significant Zeeman gap from \( |1,k_z,\downarrow\rangle. \)

III. THE MANY-BODY HAMILTONIAN

The existence of the spin instabilities discussed above needs to be placed, however, within the context of a many-body interactive system. Our analysis is concerned only with the three lowest lying minibands, \( |0,k_z,\downarrow\rangle, |0,k_z,\uparrow\rangle, \) and \( |1,k_z,\downarrow\rangle. \) While the bottom miniband, \( |0,k_z,\downarrow\rangle, \) does not participate in the formation of the SDW directly, its electrons provide an exchange interaction channel for the particles in \( |1,k_z,\downarrow\rangle. \) For simplicity, this miniband is assumed to be fully occupied and remains so even when a SDW state is being established. It is important to note that in the absence of tunneling, the particle density in the system is such that there are only two fully occupied Landau levels.

The electron states in the active minibands are represented by creation and destruction operators indexed by \( \{n,k_z,\sigma\}, \) \( c_{n,k_z,\uparrow}^\dagger \) and \( c_{n,k_z,\downarrow} \), with \( n = 0,1. \) This choice highlights the role played by \( k_z, \) in the formation of the SDW, knowing that the in-plane momentum does not lead to such a magnetic phase. We note that on account of translational symmetry along the SL axis, states whose \( k_z, \) differ by an integer multiple of the reciprocal lattice constant \( G = 2\pi/a \) are identical.

The noninteracting Hamiltonian \( H_0 \) is obtained by summing all the single-particle energies given in Eq. (5) over the momentum space,

\[
H_0 = \sum_{k_z} \epsilon_0 |0,k_z,\downarrow\rangle + \sum_{k_z} \epsilon_1 |0,k_z,\uparrow\rangle c_{0,k_z,\uparrow}^\dagger c_{0,k_z,\downarrow} + \sum_{k_z} \epsilon_1 |1,k_z,\downarrow\rangle c_{1,k_z,\downarrow}^\dagger c_{1,k_z,\uparrow}.
\]

In writing \( H_0, \) we recognized that the direct summation over the in-plane component of the electron momentum is equal to the degeneracy of the Landau level \( N_L, \) a constant that multiplies all the terms of the Hamiltonian, and consequently will be dropped from the calculation.

The interaction Hamiltonian represents the sum of all Coulomb scattering processes that occur between initial states \( \psi_{n,k_z,k_x,\sigma,\Psi_{m,k_z+Q_z,q_z,\sigma}}, \) and final states \( \psi_{n,k+z_q,k_z+\tau,\sigma,\Psi_{m,k_z+Q_z,q_z,\sigma}}, \) given in Eq. (2), with a momentum exchange \( \{q_z,\tau\}. \) It is important to remark that the periodicity of the superlattice allows a definition of \( \tilde{q}_z, \) only up to an integer multiple of \( G = 2\pi/a \) when umklapp processes are being included. Since all the other terms in the expression of the Hamiltonian are explicitly periodic, it is useful to transform the interaction in a periodic function by performing the change \( \tilde{q}_z = q_z + s G, \) with \( q_z \) within the first Brillouin zone, \( q_z \in [-\pi/a,\pi/a]. \) Moreover, to focus the attention on the \( \hat{z} \)-direction scattering, the required summations after \( k_z \) (which generates \( N_L \) as above), \( q_z \) and \( Q_z, \) are incorporated in the expression of the Coulomb interaction matrix element. Thus, we write

\[
H_{int} = \frac{1}{2} \sum_{k_z,q_z,Q_z} \sum_{\sigma,\sigma'} v_{nm}(k_z,q_z,Q_z) \times c_{n,k_z+q_z+Q_z,\sigma}^\dagger c_{m,k_z,\sigma'} c_{m,k_z+q_z,\sigma} c_{n,k_z+Q_z,\sigma'}.
\]
where the Coulomb interaction matrix element is

\[
v_{nm}(k_x, q_z, Q_z) = \sum_{l} \sum_{q_y, Q_y} \int dr_1 \int dr_2 \frac{e^2}{|r_1 - r_2|} \psi_{m, k_x + q_y, k_z + q_z + sG, \mathbf{r}_1}^{*} \psi_{n, k_x + Q_y, k_z + Q_z + sG, \mathbf{r}_2}^{*} (r_1) \psi_{n, k_x, k_z, \mathbf{r}_1} (r_2). \tag{8}
\]

The computation of \(v_{nm}(k_x, q_z, Q_z)\) starts by replacing the Coulomb interaction with its 3D Fourier series, \(e^2/\varepsilon \to \sum_{q_y} 4\pi e^2/\varepsilon q_y^2\), which makes possible the factorization of the double 3D integral in Eq. (8) into a double integral along the \(\hat{z}\) axis, that defines the form factor, \(F(k_x, q_z + sG, Q_z)\), and a double integral in the 2D plane.

Along the \(\hat{z}\) axis, the form factor \(F(k_x, q_z, Q_z)\) is determined by the Coulomb interaction mediated superposition of the one-electron-wave functions given in Eq. (3),

\[
F(k_x, q_z, Q_z) = \sum_s \int_{-\infty}^{\infty} dz_1 \int_{-\infty}^{\infty} dz_2 \xi_{k_x, q_z}(z_1) \xi_{k_x + Q_y, q_z}(z_2) e^{iq_z(z_1 - z_2)} \xi_{k_x + Q_y, q_z}(z_2) \xi_{k_x + Q_y, q_z}(z_1), \tag{9}
\]

leading, after a straightforward calculation, to

\[
F(k_x, q_z, Q_z) = \left\{ 1 - 4(\kappa a)e^{-\kappa a} \cos \frac{Q_x a}{2} \cos \left( k_x - \frac{q_z}{2} + \frac{Q_z}{2} \right) a \left( \cos \frac{q_z a}{2} - \sin \frac{q_z a}{2} \right) \right\}. \tag{10}
\]

It is the dependence of \(F\) on \(k_x\), carried over into the Coulomb interaction matrix element, that will become a definite factor in the creation of the SDW state.

The in-plane form factor describes the momentum exchange in the \(x-y\) plane,

\[
A_{nm}(q_{0x}, q_y, Q_y) = e^{-q_{0x}^2/2(1 + q_{0x}^2 + q_y^2 + sG^2)} w_{nm}(\frac{q_{0x}^2 + q_y^2}{2}), \tag{11}
\]

with

\[
w_{nm}(x) = \left[ \delta_{n0} \delta_{m0} + \left( 1 - \frac{x}{2} \right) \delta_{n1} \delta_{m0} + \left( 1 - \frac{x}{2} \right)^2 \delta_{n1} \delta_{m1} \right].
\]

(\(\delta_{nm}\) is the Kronecker symbol.) We remark that \(A_{nm}\) is independent of \(k_x\), a result whose outcome is the constant value of the exchange interaction and absence of a SDW phase in pure 2D cases, when the system undergoes an abrupt ferromagnetic to paramagnetic transition.

From Eqs. (10) and (11) we write

\[
v_{nm}(k_x, q_z, Q_z) = \sum_s \sum_{q_y, Q_y} F(k_x, q_z + sG, Q_y) \sum_{q_{0x}, q_y} \frac{4\pi e^2}{q^2 + (q_z + sG)^2} A_{nm}(q_{0x}, q_y, Q_y). \tag{12}
\]

In Eq. (12) the summation over \(s\) can be done analytically,

\[
\sum_s \frac{4\pi e^2}{q^2 + (q_z + sG)^2} F(k_x, q_z + sG, Q_y) = \frac{2\pi e^2 a}{q} \sinh qa \cosh qa - \cos qa a \left( 1 - 4(\kappa a)e^{-\kappa a} \cos \frac{Q_x a}{2} \cos k_x a \cos^2 \frac{q_z a}{2} \left( 1 - \tanh \frac{qa/2}{qa/2} \right) \right). \tag{13}
\]

Further, we introduce the magnitude of the 2D exchanged momentum, \(q = \sqrt{q_{0x}^2 + q_y^2}\), and transform the sum over \(q_{0x}, q_y\) into an integral in cylindrical coordinates in the usual manner. With this, Eq. (12) attains its final form,

\[
v_{nm}(k_x, q_z, Q_z) = \frac{e^2 a}{8} \int \limits_{0}^{\infty} dq e^{-q^2/2} \sinh qa \cosh qa - \cos qa a \left( 1 - 4(\kappa a)e^{-\kappa a} \cos \frac{Q_x a}{2} \cos k_x a \cos^2 \frac{q_z a}{2} \left( 1 - \tanh \frac{qa/2}{qa/2} \right) \right) \left( \sum_{q_y} J_0(lQ_y) \right). \tag{14}
\]

\(J_0(lQ_y)\) is the Bessel function of zero order resulting from the angular integration of \(A(q_y, Q_y)\). The analysis of spin-flip excitations between the \(|0, \uparrow\rangle\) and \(|1, \downarrow\rangle\) in 2D indicates that a minimum transition energy is reached for \(Q_y, l = 1.2\). Based on this insight the same value is preserved in the following considerations and, consequently, the sum over \(Q_y\) in the expression of \(v_{nm}\) is dropped.
The formation of a SDW ground state is investigated within the Hartree-Fock (HF) approximation, a framework extensively used in studies of the properties of fully occupied Landau levels. The formal justification of this approximation centers on the fact that when $\epsilon^2 / 8 \ll \hbar \omega$, the electron excitations out of filled Landau levels can be treated in a perturbative approach. The transformation of the interaction Hamiltonian Eq. (7) in the Hartree-Fock approximation is well known, so here we will comment only on the most relevant aspects. Thus, with $\langle \ldots \rangle$ denoting an average over the ground state, a characteristic term of the interaction is factored into three different terms:

$$\langle c_{n,k,+q_z,+\sigma}^\dagger c_{m,k,+q_z,+\sigma}^\dagger c_{m,k,+q_z,-\sigma} c_{n,k,+q_z,-\sigma} \rangle$$

$$\langle c_{n,k,+q_z,+\sigma} c_{n,k,+q_z,-\sigma} \rangle$$

$$\langle c_{n,k,+q_z,+\sigma}^\dagger c_{m,k,+q_z,+\sigma}^\dagger c_{m,k,+q_z,-\sigma} \rangle \delta_{\sigma,\sigma'} \delta_{q_z,0} \delta_{\sigma,\sigma'}$$

$$\langle c_{n,k,+q_z,+\sigma}^\dagger c_{m,k,+q_z,+\sigma} c_{m,k,+q_z,-\sigma} \rangle \delta_{\sigma,\sigma'}$$

$$\langle c_{n,k,+q_z,+\sigma}^\dagger c_{m,k,+q_z,-\sigma}^\dagger c_{m,k,+q_z,-\sigma} c_{n,k,+q_z,+\sigma} \rangle.$$  (15)

The first term on the right-hand side of Eq. (15) is the direct interaction of the electrons on a given quasiparticle. The second is associated with normal exchange and requires that the interaction of the electrons on a given quasiparticle. The third term describes a SDW potential when the pairing vector $Q_z$ is identical for all the opposite spin pairs of electrons. Finally, the ground-state value of the interaction energy is

$$\langle H_{int} \rangle_{HF}$$

$$= -\frac{1}{2} \sum_{n,m=0}^\infty \sum_{k_z,\sigma} v_{nm}(k_z,q_z) \langle c_{n,k_z+q_z,+\sigma}^\dagger c_{m,k_z,+\sigma}^\dagger c_{m,k_z,-\sigma} c_{n,k_z,-\sigma} \rangle$$

$$\times \langle c_{m,k_z,-\sigma}^\dagger c_{n,k_z,+\sigma} \rangle \delta_{\sigma,\sigma'} \delta_{\sigma,\sigma'}$$

$$= -\frac{1}{2} \sum_{n,m=0}^\infty \sum_{k_z,\sigma} v_{nm}(k_z,q_z) \langle c_{n,k_z+q_z,+\sigma}^\dagger c_{m,k_z,+\sigma}^\dagger c_{m,k_z,-\sigma} c_{n,k_z,-\sigma} \rangle.$$  (16)

The terms that appear in Eq. (16) describe the exchange energy of the interactions of the electrons on $|0,k_z,\downarrow\rangle$ level, the exchange energy of the electrons on $|1,k_z,\downarrow\rangle$ levels, followed by the exchange of the $|0,k_z,\uparrow\rangle$ level, and the exchange of the $|1,k_z,\uparrow\rangle$ level. The latter term is present only if one assumes that the exchange of the particles of the type $\langle c_{1\downarrow}^\dagger c_{i}^{\downarrow} + Q_z \rangle \neq 0$. This is clearly not the case if one considers the usual electron distribution inside the Fermi sphere. But, if one envisions a state in which the average is different from zero, that state would describe a collective pairing of electrons of opposite spins and momenta $k_z$ and $k_z + Q_z$. This is the fundamental premise of the SDW formation.

To understand the microscopic structure of an average of the type $\langle c_{i}^{\downarrow\dagger} c_{i}^{\downarrow} + Q_z \rangle$, a canonical Bogoliubov-Valatin (BV) transformation is performed. This introduces two new operators $\alpha_k$ and $\beta_k$ defined as

$$c_{k_z,\uparrow} = \cos \theta_k \alpha_k + \sin \theta_k \beta_k,$$

$$c_{k_z,\downarrow} = -\sin \theta_k \alpha_k + \cos \theta_k \beta_k,$$  (17)

where the angle $\theta_k$ is the variational parameter of the transformation. Substituting the electron operators by Eqs. (17) leads to an expression for the ground-state energy that depends on averages of the newly introduced operators, $\alpha_k$ and $\beta_k$. There are four types of terms that appear. Two represent the same particle averages, $(\alpha_k^\dagger \alpha_k)$ and $(\beta_k^\dagger \beta_k)$, and two mixed ones, $(\alpha_k^\dagger \beta_k)$ and $(\beta_k^\dagger \alpha_k)$. The first category can be easily associated with the occupation numbers of two new quasiparticles, while the second represents the excitation processes of these quasiparticles, absent in the ground state. Thus, by means of the BV transformation, the system of interacting electrons is transformed into a system of noninteracting quasiparticles.

As a function of the quasiparticle occupation numbers, $f_{1k} = (\alpha_k^\dagger \alpha_k)$ and $f_{2k} = (\beta_k^\dagger \beta_k)$, the ground-state energy becomes

$$\langle H \rangle_{HF} = \sum_{k_z} \left[ \epsilon_{0,k_z,\downarrow} + \epsilon_{0,k_z,\uparrow} \left( \cos^2 \theta_k f_{1k} + \sin^2 \theta_k f_{2k} \right) + \epsilon_{1,k_z,\downarrow} \left( \sin^2 \theta_k f_{1k} + \cos^2 \theta_k f_{2k} \right) \right]$$

$$- \frac{1}{2} \sum_{k_z,k_z'} \left[ v_{10}(k_z,k_z' - k_z,0) \left( \cos^2 \theta_k^2 f_{1k} + \sin^2 \theta_k^2 f_{2k} \right) \left( \cos^2 \theta_k^2 f_{1k} + \sin^2 \theta_k^2 f_{2k} \right) \right]$$

$$+ v_{11}(k_z + Q_z,k_z' - k_z,0) \left( \sin^2 \theta_k f_{1k} + \cos^2 \theta_k f_{2k} \right) \left( \sin^2 \theta_k f_{1k} + \cos^2 \theta_k f_{2k} \right)$$

$$+ 2 v_{10}(k_z,k_z' - k_z,0) \left( \sin^2 \theta_k f_{1k} + \cos^2 \theta_k f_{2k} \right)$$

$$- \frac{1}{4} \sum_{k_z,k_z'} v_{10}(k_z,k_z' - k_z,Q_z) \sin 2\theta_k \sin 2\theta_k \left( f_{1k} - f_{2k} \right) \left( f_{1k} - f_{2k} \right).$$  (18)

where $\theta_k$ is reached when $\partial \langle H \rangle_{HF} / \partial \theta_k = 0$. This condition generates the self-consistent SDW equation,

$$\tan (2\theta_k) = \frac{g(k_z)}{\epsilon_{1,k_z,\downarrow} + \epsilon_{0,k_z,\uparrow} - \epsilon_{0,k_z,\downarrow}}.$$  (19)
which expresses the dependence of the inclination angle on the ratio of two different energies. The numerator is the SDW gap function,

\[ g_k = \sum_{k'_z} v_{10}(k_z, k'_z - k_z, Q_z) \sin 2\theta_{k'_z}, \]  

(20)

while the denominator is the difference between two single-particle energies in the HF approximation,

\[ \tilde{\epsilon}_{0,k,\uparrow} = \epsilon_{0,k,\uparrow} - \sum_{k'_z} v_{00}(k_z, k'_z - k_z, 0) \cos^2 \theta_{k'_z}, \]  

(21)

for the electrons in the \(|0, k_z, \uparrow\rangle\) miniband and

\[ \tilde{\epsilon}_{1,k+Q_z,\downarrow} = \epsilon_{1,k+Q_z,\downarrow} - \sum_{k'_z} [v_{11}(k_z + Q_z, k'_z - k_z, 0) \sin^2 \theta_{k'_z} + v_{01}(k_z + Q_z, k'_z - k_z, 0)] \]  

(22)

for the electrons in the \(|1, k_z + Q_z, \downarrow\rangle\) miniband.

g_k is called the SDW gap since it represents the difference between the energy of the two quasiparticle states that exist in the SDW phase, as one can see by differentiating Eq. (18) with respect to the corresponding occupation numbers, \( f_{1k} \) and \( f_{2k} \), respectively:

\[ E_{1,2}(k_z) = \frac{1}{2} [\tilde{\epsilon}_{1,k+Q_z,\downarrow} + \tilde{\epsilon}_{0,k,\uparrow} + \sqrt{(\tilde{\epsilon}_{1,k+Q_z,\downarrow} - \tilde{\epsilon}_{0,k,\uparrow})^2 + g_k^2}]. \]  

(23)

When the single-particle energies, written in the HF approximation, in the opposite spin minibands become degenerate, \( \tilde{\epsilon}_{1,k+Q_z,\downarrow} = \tilde{\epsilon}_{0,k,\uparrow} \), the two quasiparticle energies differ by \( g_k \). The stability condition for the SDW phase is \( \partial^2 (H)_{HF}/\partial \theta^2_k < 0 \), which is always realized when a solution to the gap equation is found, since

\[ \frac{\partial^2 (H)_{HF}}{\partial \theta^2_k} = -\sqrt{(\tilde{\epsilon}_{1,k+Q_z,\downarrow} - \tilde{\epsilon}_{0,k,\uparrow})^2 + g_k^2}. \]  

(24)

Equation (19) is a nonlocal, self-consistent equation, since solutions depend on the values of the inclination angle throughout the Brillouin zone. The starting point of the calculation is the replacement of the discrete sums by integrals over \( k_z \). When the expression of the Coulomb interaction is considered from Eq. (14), we obtain, after several simple manipulations, expressions for the gap function,

\[ g_k = -\frac{e^2}{\epsilon \alpha} \int_{-\pi}^{\pi} \frac{d(k'_z)}{2\pi} \int_0^\infty d(qa) e^{-[(qx)^2/2]} \sin 2\theta(k'_z) \times \tilde{F}(k_z, k'_z - k_z, Q_z) \left(1 - \frac{(qa)^2}{2}\right) J_0(l Q_z), \]  

(25)

and the single-particle energies in the denominator,

\[ \tilde{\epsilon}_{0,k,\uparrow} = \epsilon_{0,k,\uparrow} - \frac{e^2}{\epsilon \alpha} \int_{-\pi}^{\pi} \frac{d(k'_z)}{2\pi} \int_0^\infty d(qa) e^{-[(qx)^2/2]} \times \cos^2 \theta(k'_z) \tilde{F}(k_z + Q_z, k'_z - k_z, 0) \]  

(26)

V. RESULTS AND DISCUSSION

Solving the gap equation for arbitrary values of the tunneling probability requires an a priori selection for the input parameters of the problem. The most important is the coupling vector \( Q_z \). A convenient option, inspired by an educated guess that seeks to maximize the overlap between the two opposite-spin minibands, is \( Q_z = \pi/a \), the distance in the momentum space between the maximum energy measured at the edge of the Brillouin zone of the \(|0, k_z, \uparrow\rangle\) miniband and the minimum energy measured at the center of the Brillouin zone of the \(|1, k_z, \downarrow\rangle\) miniband. This \( a \) priori choice for \( Q_z \) corresponds to a commensurate SDW, similar to what happens in some chromium alloys.\(^{27}\) The other parameters that enter the gap equation are the tunneling probability \( e^{-\delta} \), the energy difference \( \delta = \hbar \omega - \gamma^* \mu_B B \), and the ratio of the superlattice constant to the magnetic length, \( l_{\text{a}} \), which in the following considerations is fixed at \( 10^{-1} \). All the energies are measured in units of \( e^2/\epsilon l \). A parametric representation for the miniband width of the form \( \Delta = 5.0 e^{-a e^2/\epsilon l} \) is justified by the insight provided by the analysis of single-particle excitations in this system\(^{20}\) which indicates that the magnetic phase transition to the SDW state happens only for \( \Delta \) larger than a critical value. This choice for \( \Delta \) allows us to access all the magnetic regimes for small values of the tunneling probability.

Numerical solutions obtained for the self-consistent gap equation showcase three different possible ground states that under the effect of increased interlayer tunneling become unstable with respect to the formation of the SDW ground state.

First, when \( \delta \) is low, here fixed at \( 0.2 e^2/\epsilon l \), and the bandwidth is small, the system presents ferromagnetic ordering, the only solution of Eq. (20) being \( \theta = \pi/2 \). This situation appears in Fig. 2 for values of the bandwidth below \( 1.0 \). This situation arises from the occupancy of the two lowest minibands \(|0, k_z, \uparrow\rangle\) and \(|1, k_z, \downarrow\rangle\).

As the tunneling, and correspondingly, the bandwidth increases, \( \theta \) deviates from the \( \pi/2 \) value, starting from the center of the Brillouin zone. For \( \Delta \in [1.0, 1.8] \), the angle modifications indicate the softening of the ferromagnetic ordering. This regime coincides with the opening on the gap, as seen in Fig. 3. The gap is almost constant throughout the Brillouin zone and reaches is maximum amplitude for values of the miniband width in the middle of the range, \( \Delta \sim 1.2 \).
FIG. 2. (Color online) Inclination angle in the first Brillouin zone of a superlattice for different values of the miniband width (measured in units of $e^2/\epsilon l$). The value $\delta = 0.2e^2/\epsilon l$ sets a ferromagnetic ground state in the absence of tunneling.

At large values of the miniband width, $\Delta \sim 2.0$, the coupling angle varies fast from 0 to $\pi/2$, signaling a paramagnetic to ferromagnetic spin reordering, reminiscent of what happens in a single 2D layer. The abrupt transition occurs exactly at $\pm \pi/2a$, half the length of the chosen coupling wave vector $Q_z$. In this regime, the system presents alternating ferromagnetic/paramagnetic stripes.

FIG. 3. (Color online) The gap function in the first Brillouin zone of a superlattice for different values of the miniband width (measured in units of $e^2/\epsilon l$). The value $\delta = 0.2e^2/\epsilon l$ sets a ferromagnetic ground state in the absence of tunneling.

The amplitude of the spin-density wave, the fractional polarization, is calculated from Eqs. (1) and (17) and obtained to be

$$P = \sum_{k_z} \left( |c_{k_z\uparrow} c_{-k_z\uparrow} - c_{k_z\downarrow} c_{-k_z\downarrow}|^0 \right) = \sum_{k_z} \sin 2\theta_{k_z}. \quad (28)$$

As before, in this calculation we do not consider the contribution of the electrons in the lowest miniband, $|0, k_z, \downarrow\rangle$, which provide a uniform spin-down contribution. As depicted in Fig. 4, the fractional polarization peaks within the interval of miniband widths for which the SDW is established and becomes zero at either of the extremities of the bandwidth interval.

At large values of $\delta$, for example $0.7e^2/\epsilon l$, and low tunneling, the system is in a paramagnetic state, as shown in Fig. 5, where the inclination angle $\theta$ is 0 throughout the Brillouin zone. This corresponds to a paramagnetic initial ordering when the two lowest fully occupied minibands are $|0 \downarrow\rangle$ and $|1 \uparrow\rangle$. This situation persists for as long as the bandwidth remains small. As the tunneling increases, the inclination angle follows suit at the edge of the zone, while remaining low in the center. The progression continues for a limited interval of $\Delta$ values and ends in the same stripe phase when an alternative paramagnetic/ferromagnetic ordering is established. Figures 5–7 describe the evolution of the inclination angle, the gap function, and of the fractional polarization, respectively.

A paramagnetic ground state of a GaAs SL was obtained experimentally in Ref. 21 where a filling factor of 2 was found for a perpendicular magnetic field $B_{\perp} = 8.6$ T. In that case, the miniband width of the SL, estimated based on the Kronig-Penney model, was found to be $\approx 2.5$ meV. This value represented just a fraction of 0.18 of the Coulomb interaction energy which for the same system parameters is $e^2/\epsilon l \sim \ldots$
FIG. 5. (Color online) The inclination angle in the first Brillouin zone for different values of the miniband width, $\delta = 0.7(e^2/\epsilon l)$. From an initial paramagnetic state, the system evolves in a SDW state, while for large values of the miniband width a sequence of paramagnetic-ferromagnetic stripes are exhibited.

13 meV. For the realization of a SDW state, the miniband width needs to be larger than a critical value. A Kroning-Penney simulation suggests that a good candidate would be a SL with a well width of about 125 Å (compared with 188 Å), a barrier width of 25 Å (compared with 38 Å), and a barrier height of 130 meV (compared with 144 meV) to generate a miniband width of about 16 meV that is approximately $1.2e^2/\epsilon l$.

FIG. 6. (Color online) The gap function, in $e^2/\epsilon l$ units, is plotted within the first Brillouin zone for different values of the miniband width (in $e^2/\epsilon l$); $\delta = 0.7e^2/\epsilon l$ corresponds to a paramagnetic ground state at weak tunneling.

FIG. 7. Fractional polarization as a function of $\Delta$ (expressed in $e^2/l$ units) for $\delta = 0.7e^2/\epsilon l$.

FIG. 8. (Color online) The inclination angle within the first Brillouin zone as a function of $\Delta$ (in $e^2/\epsilon l$ units) for $\delta = 0.5e^2/\epsilon l$. Even at weak tunneling, the system exhibits a SDW ordering on account of a modified Coulomb interaction. As the tunneling increases, the system presents an alternate sequence of paramagnetic-ferromagnetic stripes.
A very interesting situation is found to occur at intermediate values of the separation energy, $\delta = 0.5(e^2/\varepsilon_l)$. As our results show, even at weak tunneling, the inclination angle, the gap function, and the fractional polarization indicate the existence of a stable SDW phase. It is important to point out that while the tunneling is weak, it is not zero and the system retains its superlattice characteristic through a small but finite value of $\Delta$, and the periodicity along the superlattice axis. The main consequence of this situation is the change undergone by the Coulomb matrix element, which is modified from its 2D form by the $\hat{z}$-axis form factor. In this respect, the situation is entirely different from the pure 2D case when for similar values of $\delta$ the system is ferromagnetic, at large $\delta$ is paramagnetic, and both states become unstable leading to the formation of a SDW phase for a certain range of values of the miniband width. At high tunneling levels, the ground state is described by an alternating sequence of paramagnetic-ferromagnetic stripes. Since the system parameters that favor such a behavior in the case of the superlattice can be chosen with considerable liberty, we believe that this problem can serve as an experimental test case of the manifest action of the long-range Coulomb interaction in determining magnetic characteristics.

In conclusion, we have obtained numerical solutions to the SDW gap equation of a superlattice in the presence of a tilted magnetic field at $T = 0$ K, when for low tunneling values, the ground state of the system is determined by the value of the energy difference between the cyclotron frequency and Zeeman splitting. At low $\delta$ the system is ferromagnetic, at large $\delta$ is paramagnetic, and both states become unstable leading to the formation of a SDW phase for a certain range of values of the miniband width. At high tunneling levels, the ground state is described by an alternating sequence of paramagnetic-ferromagnetic stripes. Since the system parameters that favor such a behavior in the case of the superlattice can be chosen with considerable liberty, we believe that this problem can serve as an experimental test case of the manifest action of the long-range Coulomb interaction in determining magnetic characteristics.