Helical antiferromagnetic ordering in the lowest Landau level of a semiconductor superlattice

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When subjected to a tilted magnetic field, the ground state of a semiconductor superlattice (SL) with two identical quantum wells per unit cell is shown to exhibit different magnetic configurations that are dependent on the strength and direction of the field and the SL characteristics. Intra- and interunit cell tunneling between the wells, assumed to be infinitely attractive, generate an energy miniband structure of the lowest Landau level that, in cooperation with the Zeeman splitting, creates, at certain points in the momentum space, an energy difference between opposite-spin single-particle states that can be overcome by the Coulomb interaction. Within the Hartree-Fock approximation, we show that the minimum free energy is reached in ground states with different magnetic characteristics: ferromagnetic, helical antiferromagnetic (HAFM) or paramagnetic, depending on the system parameters and the external field. The HAFM phase results from an antiferromagnetic coupling of opposite electron spins that are rotated in respect to the $\hat{z}$ axis by an angle that varies continuously within the Brillouin zone between $[0,\pi/2]$. As a result, a finite polarization is registered in real space. The self-consistent equation satisfied by the inclination angle is solved numerically at $T = 0$ K for an array of SL parameters. Its solutions demonstrate that a continuous driven transition between ferromagnetic, HAFM, and paramagnetic states can be realized by adjusting the parameters of the system.

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I. INTRODUCTION

The complex interplay that occurs in electronic systems of reduced dimensionality between the Coulomb interaction and spin effects has long been recognized as a most interesting area of research.[1] The fundamental premise for the formation of a magnetically ordered state in a simple Fermi system is the existence of a degeneracy between energy levels of opposite spins.[2–4] 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 is realized. 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. When this long-range order is established between the electrons of same momentum, the magnetic phase corresponds to canted antierromagnetism (CAF), whereas when the electron momenta differ by the same value **Q**, a spin-density-wave (SDW) state is realized. If in metallic systems the required energetic degeneracy occurs only in certain cases, semiconductor heterostructures, whose band structure is engineered in the growth process, can present this opportunity frequently.

The emergence of various magnetic phases in the presence of opposite-spin energetic degeneracy is usually recognized from the analysis of spin instabilities. Early on, it was established that in a single GaAs quantum well system placed in a tilted the magnetic field, a geometry which allows for the Zeeman splitting to become comparable with the Landau-level spacing, spin transitions that occur between $|0,\uparrow\rangle$ and $|1,\downarrow\rangle$ are leading, in the presence of the Coulomb interaction, to an abrupt paramagnetic-ferromagnetic transition.[5,6] In a simple description, such an outcome can be understood as a consequence of the independence of the Coulomb interaction matrix element on the two-dimensional (2D) momentum **k** that leads to single-particle energies of fixed values. Ulterior experimental works supported this theoretical picture.[7,8] Further, the robustness of the ferromagnetic-paramagnetic phase transition was explored in the case of high-density limit in various other configurations.[9,10]

Extending the problem of spin instabilities in double-quantum-well systems[11,12] or multilayers[13,14] was based on the insight that the motion of the electrons in a direction perpendicular to the layers modifies the energy spectrum and enhances the many-body interactions. Experimental evidence of such phenomena was already obtained in the case of the double layer.[15] In this paper we discuss the existence of several magnetic phases in the case of a superlattice (SL) with two identical quantum wells per unit cell placed in a tilted magnetic field. In a simple description, this system is obtained by periodic replication, along a given spatial direction, of a double-quantum-well structure. Such a setup exploits the periodicity along the SL axis that is responsible, in the presence of tunneling between the wells, for the formation of a miniband spectrum and the existence of a Landau-level structure in the planes perpendicular on the SL axis, as established experimentally.[16] Ideally, the experimental realization of the theory discussed below involves SL with high mobility and thin barriers, to minimize disorder.

We show that in the miniband regime, the lowest Landau level can acquire an energetic configuration, largely controlled by the inter- and intraunit cell tunneling and the Zeeman interaction, which permits the realization of opposite-spin energetic degeneracy. In this instance, for a certain range on SL parameters, the free energy of the system is minimized by a helical antiferromagnetic (HAFM) long-range order,

characterized by pairing between electrons of equal momentum and opposite spins. The total spin of the pair is inclined versus the SL axis with an angle that varies continuously within the first Brillouin zone between 0 and $\pi/2$. This configuration represents a nontrivial spatial extension of the CAF ground state discussed in the case of a double-quantum-well system[11,12,17] and coupled multilayer structures.[14] The CAF state is realized by pairing electrons with the same momentum and opposite spins, whose total spin, however, is inclined at a constant angle. Moreover, we show that by adjusting the external parameters, the SL can be made to exhibit a ferromagnetic, paramagnetic, or a HFAM state. The transition into the HAFM from either paramagnetic or ferromagnetic order is of first order and is driven by the external magnetic field.

Below, we present in order a description of the system in Sec. II, followed by the analysis of the many-body problem in Sec. III. In Sec. IV the fundamental approximation and the ensuing self-consistent equations that control the solutions to the problem are presented, while in Sec. V we illustrate and discuss the results.

II. SYSTEM DESCRIPTION

The basic SL system considered in this problem is represented by a sequence of unit cells equally distributed along the $\hat{z}$ axis at a distance b. In each unit cell there are two infinitely attractive quantum wells, separated by a distance a ($a < b$), whose potential has strength $-\lambda$. This choice is justified by the fact that in this case there is only one significant bound state in the well, of energy $\epsilon_0 = -\hbar^2\kappa^2/2m^*$ and eigenstate $\nu(z) = \sqrt{\kappa}e^{-\kappa|z|}$, where $\kappa = 2m^*\lambda/\hbar^2$ (m^* is the effective mass).

The intraunit cell tunneling creates two energy eigenstates

$$\varphi_\alpha(z) = \frac{1}{\sqrt{2}}[\nu(z-a) + \alpha\nu(z+a)], \tag{1}$$

indexed by $\alpha = 1$ for the symmetric S state and $\alpha = -1$ for the antisymmetric A state. The corresponding energies are $\epsilon_\alpha = -\alpha\Delta_{SAS}/2$, where $\Delta_{SAS} = 4\epsilon_0 e^{-\kappa a}$. We assume that the SL parameters are chosen such that Δ_{SAS} is smaller than the Landau energy. Within the tight-binding approximation, the single-particle eigenstates are Bloch waves propagating along the SL axis,

$$\zeta_\alpha(k_z,z) = \frac{1}{\sqrt{N}}\sum_l e^{ik_z lb}\varphi_\alpha(z-lb), \tag{2}$$

normalized by

$$N_\alpha = \{1 + \alpha(1+2\kappa a)e^{-2\kappa a} + \alpha[1+\kappa(b-2a)] \times e^{-\kappa(b-2a)}\cos k_z b\}. \tag{3}$$

Equation (2) explicitly introduces the electron momentum along the $\hat{z}$ direction as a good quantum number, which on account of periodic boundary conditions assumes a quasicontinuum spectrum $k_z = \frac{2\pi}{Nb}j$ ($j = -\frac{N}{2}, \frac{N}{2}$). The single-particle energies are calculated by considering that tunneling is significant only between wells in adjacent cells. When measured in respect with the minimum in the lowest miniband, they are given by

$$\bar{\epsilon}_\alpha(k_z) = \alpha\left[-\frac{\Delta_{SAS}}{2} + \frac{\Delta}{2}(1-\cos k_z b)\right], \tag{4}$$

where the $+$ sign corresponds to S, while $-$ to A: $\Delta = 2\frac{m\lambda^2}{\hbar^2}e^{-\kappa(b-a)}$.

In the presence of a magnetic field of magnitude B, inclined in respect with the SL axis, the electrons with spin projection $\sigma = \{+1, -1\}$ acquire $\gamma^*\mu_B\sigma B/2$ Zeeman energy, where γ^* is the effective gyromagnetic factor, while their transverse motion is quantized in Landau levels spaced by the cyclotron energy eB_z/m^*, dependent only on the component of the field perpendicular on the x-y plane.[18] In the following considerations, all the electrons are considered to be in the lowest Landau level (LLL) whose index will not be explicitly declared henceforth.

The three-dimensional (3D) electronic eigenstate for an electron of momentum k_y, k_z and spin σ in a state α is obtained by multiplying Eq. (2) by the usual 2D wave function of the LLL inside each well (x-y motion) and the spin function χ_σ,

$$\Psi_{\alpha,k_y,k_z,\sigma}(x,y,z) = \zeta_\alpha(z)\frac{1}{\sqrt{L}}e^{ik_y l}\frac{1}{\sqrt{2\pi^{1/2}}}e^{-\frac{(x+l^2k_y)^2}{2l^2}}\chi_\sigma. \tag{5}$$

k_y is subject to periodic boundary conditions determined by L, the length of the sample in the y direction, its value being an integer multiple of $2\pi/L$. $l = \sqrt{\hbar c/eB_z}$ is the magnetic length. The are $N_L = L^2/(2\pi l^2)$ states indexed by k_y in each Landau level.

Finally, with input from Eq. (4), the corresponding single-particle energy is

$$\epsilon_{\alpha,k_z,\sigma} = \frac{\hbar\omega}{2} + \bar{\epsilon}_{\alpha,k_z} + \frac{1}{2}\gamma^*\mu_B B\sigma. \tag{6}$$

The result describes a sequence of Landau minibands spin split by the Zeeman interaction, a picture known to give realistic, semiquantitative results.[19] The interplay of the three energies introduced by the problem, Δ_{SAS}, $\gamma^*\mu_B$, and Δ, determine the miniband structure of the system depicted in Fig. 1 which, in the presence of the Coulomb interaction of the order $e^2/\varepsilon l$ (ε is the dielectric constant of the system) can lead to a specific magnetic phase. We are, in particular, targeting situations when a degeneracy between opposite-spin states occurs. It is easy to see from Eq. (4) that this happens at the edge of the Brillouin zone where the difference between the opposite-spin states in minibands $|A,k_z,\downarrow\rangle$ and $|S,k_z,\uparrow\rangle$ is reduced by both the Zeeman splitting and the band widening effect,

$$\delta = \left(E_{A,k_z,\downarrow} - E_{S,k_z,\uparrow}\right)|_{k_z=\pi} = \Delta_{SAS} - \Delta - \gamma^*\mu_B B. \tag{7}$$

By appropriately adjusting the magnitude of the tunneling probability that controls Δ_{SAS} and Δ and, independently, the intensity of the magnetic field B, the difference can become comparable with the Coulomb exchange energy interaction, leading to the development of spin instabilities. This scenario was explored in Refs. 11,12 and 17, where, in the case of a single bilayer system, an incipient canted antiferromagnetic state was diagnosed from the softness of the poles of the spin-density response function. The extension of this problem to multilayer systems, discussed in Ref. 14, uses as a basis functions with

a layer index and considers a correlation parameter between adjacent layers. Moreover, in the absence of a minibandwidth to describe the energy spectrum, the relevant quantity in analyzing the transition remains the Zeeman splitting, which is always positive and needs to be greater or equal to a minimum value imposed by the electron interaction. In turn, the latter is dependent on the Zeeman splitting through the number of up and down electrons involved. In our approach, which follows the general outline of Ref. 13, the presence of k_z as a good quantum number imposed by the periodicity of the SL structure and the introduction of the miniband structure permit the realization of the single-state spin degeneracy through the variation of a parameter that is independent of the magnetic field. Thus, we obtain a continuous variation of the inclination angle of the antiferromagnetic coupling between 0 and $\pi/2$ throughout the Brillouin zone, resulting in a HAFM order. In this sense, our problem represents a nontrivial extension of the double-quantum-well situation.

III. THE MANY-BODY HAMILTONIAN

The properties of the SL described above are now studied within the context of a many-body interaction intermediated by the Coulomb repulsion, for values of the system parameters that favor the creation of spin instabilities. The Hamiltonian involves particles within the lowest three minibands, with electrons in $|S,k_z,\downarrow\rangle$ playing only a passive role, that of providing exchange interaction to electrons in $|A,k_z,\downarrow\rangle$, without being involved in the dynamics of the system. Their status is left unchanged by the formation of a HAFM order. The choice of electron operators and their dependence on momentum is based on the insight provided by the Coulomb interaction matrix element in 2D which was found to be independent of the in-plane momentum.[5,20] We anticipate that the special effect that the Coulomb interaction exerts in the case of the SL originates only in the coupling along the $\hat{z}$ axis. Consequently, the electron states are represented by creation and destruction operators indexed after the miniband k_z and spin orientation $c^{\dagger}_{\alpha,k_z,\uparrow}, c_{\alpha,k_z,\uparrow}$ $(\alpha = A,S)$. Because of translational symmetry along the SL axis, states whose k_z differ by an integer multiple of the reciprocal lattice constant $G = 2\pi/b$ are identical.

The kinetic (noninteracting) part of the total Hamiltonian H_0 is obtained by summing all the single-particle energies in Eq. (6):

$$H_0 = \sum_{k_z} \epsilon_{S,k_z,\downarrow} + \sum_{k_z,\alpha=A,S} \epsilon_{\alpha,k_z,\uparrow} c^{\dagger}_{\alpha,k_z\uparrow} c_{\alpha,k_z\uparrow}. \tag{8}$$

In writing H_0, we recognized that the direct summation over the in-plane components 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 part of the Hamiltonian is a sum over all momenta of the electrons scattered by the Coulomb interaction between initial states $\psi_{\alpha,k_z,k_y,\sigma}, \psi_{\beta,k_z+Q_z+q_z,k_y+Q_y+q_y,\sigma'}$ and final states $\psi_{\alpha,k_z+q_z,k_y+q_y,\sigma}, \psi_{\beta,k_z+Q_z,k_y+Q_y,\sigma'}$, given in Eq. (5). To focus the attention on the $\hat{z}$-direction scattering, the required summations after k_y (which generates N_L as above), q_y and Q_y are incorporated in the expression of the Coulomb interaction matrix element. Thus, we write

$$H_{\text{int}} = \frac{1}{2} \sum_{\alpha,\beta=A,S} \sum_{k_z,q_z,Q_z} \sum_{\sigma,\sigma'} v_{\alpha\beta}(k_z,q_z,Q_z) \times c^{\dagger}_{\alpha,k_z+q_z,\sigma} c^{\dagger}_{\beta,k_z+Q_z,\sigma'} c_{\beta,k_z+Q_z+q_z,\sigma'} c_{\alpha,k_z,\sigma}. \tag{9}$$

It is important to note that, because of the periodicity of the SL, the momentum exchanged by two interacting electrons along the $\hat{z}$ direction is defined only up to an integer multiple of $G = 2\pi/b$ 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 $q_z \longrightarrow q_z + nG$, where q_z is now strictly within the first Brillouin zone $q_z \in [-\pi/b,\pi/b]$.

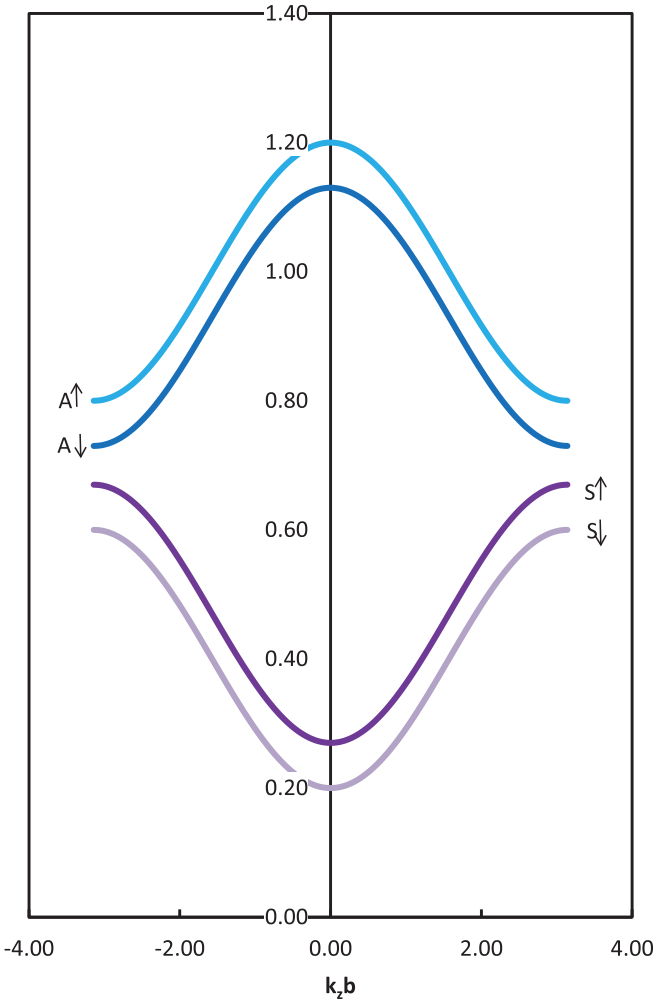

FIG. 1. (Color online) The band structure of a superlattice with two wells per unit cell in the presence of a tilted magnetic field that spin splits each miniband by $\gamma^*\mu_B B$. The minimum energy between the opposite spin minibands $|S,k_z,\uparrow\rangle$ and $|A,k_z,\downarrow\rangle$ is realized at the edge of the Brillouin zone, where $\delta = \Delta_{SAS} - \Delta - \gamma^*\mu_B B$ (measured in units of $e^2/\varepsilon l$). When the Zeeman splitting is much smaller than the minibandwidth, the system parameters are chosen such that $\delta = 0.382e^2/\varepsilon l$ describes a paramagnetic ground state.

We define therefore the Coulomb interaction matrix element to be

$$v_{\alpha\beta}(k_z,q_z,Q_z)=\sum_n\sum_{q_y,Q_y}\int d\mathbf{r_1}\int d\mathbf{r_2}\Psi^*_{\alpha,k_y+q_y,k_z+q_z+nG}(\mathbf{r_1})\times\Psi^*_{\beta,k_y+Q_y,k_z+Q_z}(\mathbf{r_2})\frac{e^2}{|\mathbf{r_1}-\mathbf{r_2}|}\times\Psi_{\beta,k_y+Q_y+q_y,k_z+Q_z+q_z+nG}(\mathbf{r_2})\Psi_{\alpha,k_y,k_z}(\mathbf{r_1}). \quad (10)$$

The computation of $v_{\alpha\beta}(k_z,q_z,Q_z)$ starts by replacing the Coulomb interaction with its 3D Fourier series $e^2/\varepsilon r\longrightarrow\sum_{\vec{q}_0}4\pi e^2/\varepsilon q_0^2$, which makes possible the factorization of the double 3D integral in Eq. (10) into a double integral along the $\hat{z}$ axis that defines the form factor $F_{\alpha\beta}(k_z,q_z,Q_z)$, and a double integral in the 2D plane that corresponds to the x-y interaction between two electrons in LLL.

$F_{\alpha\beta}(k_z,Q_z,q_z)$ results in the Coulomb interaction-mediated superposition of the one-electron wave functions in Eq. (2),

$$F_{\alpha\beta}(k_z,q_z,Q_z)=\int_{-\infty}^{\infty}dz_1\int_{-\infty}^{\infty}dz_2\zeta^*_{\alpha,k_z+q_z}(z_1)\zeta^*_{\beta,k_z+Q_z}(z_2)\times e^{iq_z(z_2-z_1)}\zeta_{\beta,k_z+Q_z+q_z}(z_2)\zeta_{\alpha,k_z}(z_1). \quad (11)$$

Three different types of form factors are possible in our system,

$$\begin{aligned}F^{SS}_{AA}(k_z,q_z,Q_z)&=\cos^2 q_za\pm 2e^{-2\kappa a}\cos q_za\left[\cos q_za-(1+2\kappa a)+2\kappa\frac{\sin q_za}{q_z}\right]\\&\pm 2e^{-2\kappa(b/2-a)}\cos q_za\cos\left[\left(k_z-\frac{q_z}{2}+\frac{Q_z}{2}\right)b\right]\cos\frac{Q_zb}{2}\\&\times\left\{\cos(b/2-a)q_z-[1+2\kappa\,(b/2-a)]\cos\frac{q_zb}{2}+2\kappa\frac{\sin q_z\left(\frac{b}{2}-a\right)}{q_z}\right\},\\F_{AS}(k_z,q_z,Q_z)&=\cos^2 q_za+2e^{-2\kappa(b/2-a)}\cos q_za\sin\left[\left(k_z-\frac{q_z}{2}+\frac{Q_z}{2}\right)b\right]\sin\frac{Q_zb}{2}\\&\times\left\{\cos(b/2-a)q_z-[1+2\kappa\,(b/2-a)]\cos\frac{q_zb}{2}+2\kappa\frac{\sin q_z\left(\frac{b}{2}-a\right)}{q_z}\right\},\end{aligned} \quad (12)$$

where the upper signs are assigned to the upper index.

After straightforward calculations, with input from (5) and (12) in Eq. (10), we obtain

$$\begin{aligned}v_{\alpha\beta}(k_z,Q_z,q_z)&=\frac{4\pi e^2}{\varepsilon}\sum_n F_{\alpha\beta}(k_z,q_z+nG,Q_z)\\&\times\sum_{Q_y,q_y,q_{0x}}\frac{e^{-\frac{l^2}{2}(q_y^2+2iq_{0x}Q_y+q_{0x}^2)}}{q_y^2+q_{0x}^2+(q_z+nG)^2}\\&=\frac{2e^2}{\varepsilon}\int_0^\infty dqe^{-q^2l^2/2}\\&\times\sum_n\frac{F_{\alpha\beta}(k_z,q_z+nG,Q_z)}{q^2+(q_z+nG)^2}\sum_{Q_y}J_0(lQ_y),\end{aligned} \quad (13)$$

where, in the second line, the summation over $\{q_y,q_{0x}\}$ was transformed into an integral in polar coordinates in the usual fashion, with $q=\sqrt{q_{0x}^2+q_y^2}$ and J_0 the Bessel function of zero order that results from the angular integration. This matrix element reflects the intermediate 2D-to-3D character of our system, a feature that permits the utilization of the Hartree-Fock approximation in discussing the existence of a spin-ordered state, as demonstrated in Refs. 2,3 and 21.

At this point, we anticipate that the most favorable choice for the formation of a long-range magnetic order corresponds to $Q_y,Q_z=0$, since, as one can see in Fig. 1, the difference between the opposite spin minibands $|k_z,S,\uparrow\rangle$ and $|k_z,A,\downarrow\rangle$ becomes small at the edge of the Brillouin zone. This selection is formally justified in the next section.

Consequently, in Eq. (13), $\sum_{Q_y}J_0(lQ_y)=1$, while the summation over n in the expression of the form factors generates

$$\begin{aligned}\tilde{F}^{SS}_{AA}(k_z,q)&=v_0\left\{\frac{1}{2}\left[1+\frac{\sinh(b-2a)q}{\sinh bq}+\frac{\sinh 2aq}{\sinh bq}\cos q_zb\right]\right.\\&\times\left[1\pm 2e^{-2\kappa a}\pm 2e^{-2\kappa(b/2-a)}\cos\left(k_z-\frac{q_z}{2}\right)b\cos\frac{q_zb}{2}\right]\\&\left.-\left[\frac{\sinh(b-a)q}{\sinh bq}+\frac{\sinh aq}{\sinh bq}\cos q_zb\right]\right.\end{aligned}$$

$$\times\left[\pm 2e^{-2\kappa a}(1+2\kappa a)\pm 2e^{-2\kappa(b/2-a)}[1+2\kappa(b/2-a)]\cos\frac{q_z b}{2}\cos\left(k_z-\frac{q_z}{2}\right)b\right]$$
$$\pm\kappa\frac{2\sinh qa}{q\sinh qb}\left[\sinh(b-a)q+\sinh qa\cos q_z b\right]$$
$$\times\left[2e^{-2\kappa a}-2e^{-2\kappa(b/2-a)}\cos\frac{q_z b}{2}\cos\left(k_z-\frac{q_z}{2}\right)b\right]$$
$$\pm e^{-2\kappa(b/2-a)}\frac{\sinh 2aq}{\sinh bq}\sin q_z b\sin\frac{q_z b}{2}\cos\left(k_z-\frac{q_z}{2}\right)b$$
$$\pm 2\kappa e^{-2\kappa(b/2-a)}\frac{\sin q_z b}{\sin\frac{q_z b}{2}}\left[\frac{\sinh^2\frac{bq}{2}}{q\sinh qb}+\frac{\sinh\frac{(b-a)q}{2}\sinh\frac{(b+a)q}{2}}{q\sinh qb}+\frac{\sinh^2\frac{qa}{2}}{q\sinh qb}\cos q_z b\right]$$
$$\times\cos\left(k_z-\frac{q_z}{2}\right)b\Bigg\}, \tag{14}$$

$$\tilde{F}_{AS}(k_z,q)=\frac{v_0}{2}\left[1+\frac{\sinh(b-2a)q}{\sinh bq}+\frac{\sinh 2aq}{\sinh bq}\cos q_z b\right], \tag{15}$$

where

$$v_0=\frac{b}{2q}\frac{\sinh qb}{\cosh qb-\cos q_z b}.$$

IV. HELICAL ANTIFERROMAGNETIC GROUND STATE

The formation of a HAFM ground state is investigated within the Hartree-Fock (HF) approximation, a framework extensively used in studies of the properties of fully occupied Landau levels.[5,17,20,22,23] The formal justification of this approximation centers on the fact that when $e^2/\varepsilon l \ll \hbar\omega_c$, the electron excitations out of filled Landau levels can be treated in a perturbative approach.[4] The transformation of the interaction Hamiltonian Eq. (9) in the HF approximation is well known,[4] so here we will comment only on the most relevant aspects. Thus, with $\langle\ldots,\ldots\rangle$ denoting the average over the ground state, a characteristic term of the interaction is factored into three different contributions:

$$\begin{aligned}\langle c^{\dagger}_{\alpha,k_z+q_z+Q_z,\sigma}c^{\dagger}_{\beta,k_z,\sigma'}c_{\beta,k_z+q_z,\sigma'}c_{\alpha,k_z+Q_z,\sigma}\rangle&\\ =\langle c^{\dagger}_{\alpha,k_z+q_z+Q_z,\sigma}c_{\alpha,k_z+Q_z,\sigma}\rangle\langle c^{\dagger}_{\beta,k_z,\sigma'}c_{\beta,k_z+q_z,\sigma'}\rangle&\\ -\langle c^{\dagger}_{\alpha,k_z+q_z,\sigma}c_{\beta,k_z+q_z,\sigma}\rangle\langle c^{\dagger}_{\beta,k_z,\sigma}c_{\alpha,k_z,\sigma}\rangle\delta_{Q_z,0}\delta_{\sigma,\sigma'}&\\ -\langle c^{+}_{\alpha,k_z+q_z+Q_z,\sigma}c_{\beta,k_z+q_z,\sigma'}\rangle\langle c^{\dagger}_{\beta,k_z,\sigma'}c_{\alpha,k_z+Q_z,\sigma}\rangle.&\end{aligned} \tag{16}$$

The first term on the right-hand side of Eq. (16) is the direct interaction which is canceled by the positive background, always present in the analysis of electron systems to assure charge neutrality. The second is associated with normal exchange and requires that $\mathbf{Q}=\{Q_y,Q_z\}$ be zero and $\sigma=\sigma'$. The third term describes a spin-dependent pairing order when the pairing vector Q_z is identical for all the opposite spin pairs of electrons. It is nonzero only when, by *intuition* born out of some physical consideration, the ground state is *a priori* assumed to be described by a magnetic ordering different from the usual paramagnetic or ferromagnetic configurations. Since in our problem single-particle energies associated with opposite spins become equal in phase space at the direct superposition points between $|S,k_z,\downarrow\rangle$, and $|A,k_z,\uparrow\rangle$, we *choose* $\mathbf{Q}=0$ in this term also. Since Q_z ceases to be relevant, it will be dropped from the index array.

Consequently, the average interaction energy on a ground state that assumes $\langle c^{\dagger}_{S,k_z,\uparrow}c_{A,k_z,\downarrow}\rangle\neq 0$, estimated within the HF approximation, is

$$\begin{aligned}\langle H_{\rm int}\rangle_{\rm HF}=-\frac{1}{2}\sum_{\alpha,\beta=A,S}\sum_{k_z,q_z,\sigma}v_{\alpha\beta}(k_z,q_z)\langle c^{\dagger}_{\alpha,k_z+q_z,\sigma}c_{\alpha,k_z+q_z,\sigma}\rangle&\\ \times\langle c^{\dagger}_{\beta,k_z,\sigma}c_{\beta,k_z,\sigma}\rangle\delta_{\sigma,\sigma'}-\frac{1}{2}\sum_{k_z,q_z}v_{AS}(k_z,q_z)&\\ \times\langle c^{\dagger}_{A,k_z+q_z,\downarrow}c_{S,k_z+q_z,\uparrow}\rangle\langle c^{\dagger}_{S,k_z,\uparrow}c_{A,k_z,\downarrow}\rangle\ .&\end{aligned} \tag{17}$$

The terms that appear in Eq. (17) correspond, respectively, to the exchange energy between the electrons in each one of the minibands, as well as to the exchange between $|S,k_z,\downarrow\rangle$ and $|A,k_z,\downarrow\rangle$, and to the HAFM potential that is generated by the interaction of the electrons on $|S,k_z,\uparrow\rangle$ and those on $|A,k_z,\downarrow\rangle$.

The microscopic structure of an average of the type $\langle c^{\dagger}_{Sk_z\uparrow}c_{Ak_z\downarrow}\rangle$ in Eq. (17) is illuminated by performing a canonical Bogoliubov-Valatin (BV) transformation, whose purpose is, as in many other cases, to recast the system of interacting electrons into a noninteracting system of quasiparticles. Two new operators a_{k_z} and b_{k_z} are introduced:

$$\begin{aligned}c_{Sk_z\uparrow}&=\cos\theta_{k_z}a_{k_z}+\sin\theta_{k_z}b_{k_z},\\ c_{Ak_z\downarrow}&=-\sin\theta_{k_z}a_{k_z}+\cos\theta_{k_z}b_{k_z},\end{aligned} \tag{18}$$

where the angle θ_{k_z} is the variational parameter of the transformation $\theta_{k_z}\in[0,\pi/2]$. Equations (18) describe two independent quasiparticles whose spin projection changes continuously as a function of its momentum, within the first Brillouin zone. When written for electrons whose momentum

differs by a finite vector, Eqs. (18) lead to a SDW arrangement,[2] while when written for a constant angle θ describe the CAF phase, discussed in Ref. 17. The magnetic ordering anticipated in our problem is an extension of the CAF phase throughout the Brillouin zone.

By substituting the electron operators from the Eqs. (18), an expression for the ground-state energy is obtained which depends on averages of the newly introduced operators a_{k_z} and b_{k_z}. In this representation, quasiparticle occupation numbers correspond to $f_{1k_z} = \langle a^\dagger_{k_z} a_{k_z}\rangle$ and $f_{2k_z} = \langle b^\dagger_{k_z} b_{k_z}\rangle$, while $\langle a^\dagger_{k_z} b_{k_z}\rangle$ and $\langle b^\dagger_{k_z} a_{k_z}\rangle$ describe excitation processes of the quasiparticles.

As we inspect the ground-state properties, the latter will be neglected. The ground-state energy becomes

$$\begin{aligned}\langle H\rangle_{\rm HF} = &\sum_{k_z}\left[\epsilon_{S,k_z,\downarrow} + \epsilon_{S,k_z,\uparrow}\left(\cos^2\theta_{k_z} f_{1k_z} + \sin^2\theta_{k_z} f_{2k_z}\right) + \epsilon_{A,k_z,\downarrow}\left(\sin^2\theta_k f_{1k_z} + \cos^2\theta_{k_z} f_{2k_z}\right)\right]\\
&-\frac{1}{2}\sum_{k_z,k_z'}\Big[v_{SS}(k_z,k_z'-k_z,0)\left(\cos^2\theta_{k_z} f_{1k_z} + \sin^2\theta_{k_z} f_{2k_z}\right)\left(\cos^2\theta_{k_z'} f_{1k_z'} + \sin^2\theta_{k_z'} f_{2k_z'}\right)\\
&+ v_{AA}(k_z,k_z'-k_z,0)\left(\sin^2\theta_{k_z} f_{1k_z} + \cos^2\theta_{k_z} f_{2k_z}\right)\left(\sin^2\theta_{k_z'} f_{1k_z'} + \cos^2\theta_{k_z'} f_{2k_z'}\right)\\
&+ 2v_{AS}(k_z,k_z'-k_z,0)\left(\sin^2\theta_{k_z} f_{1k_z} + \cos^2\theta_{k_z} f_{2k_z}\right)\Big]\\
&-\frac{1}{4}\sum_{k_z,k_z'} v_{AS}(k_z,k_z'-k_z,\pi/b)\sin 2\theta_{k_z}\sin 2\theta_{k_z'}(f_{1k_z} - f_{2k_z})(f_{1k_z'} - f_{2k_z'}),\end{aligned} \tag{19}$$

with $k_z' = q_z + k_z$. Equation (19) is quite general and can be used to describe the system at all temperatures. At $T = 0$ K, the ground state corresponds to $f_{1k_z} = 1$, while $f_{2k_z} = 0$. Under these circumstances, a minimum of $\langle H\rangle_{\rm HF}$ as the function of θ_{k_z}

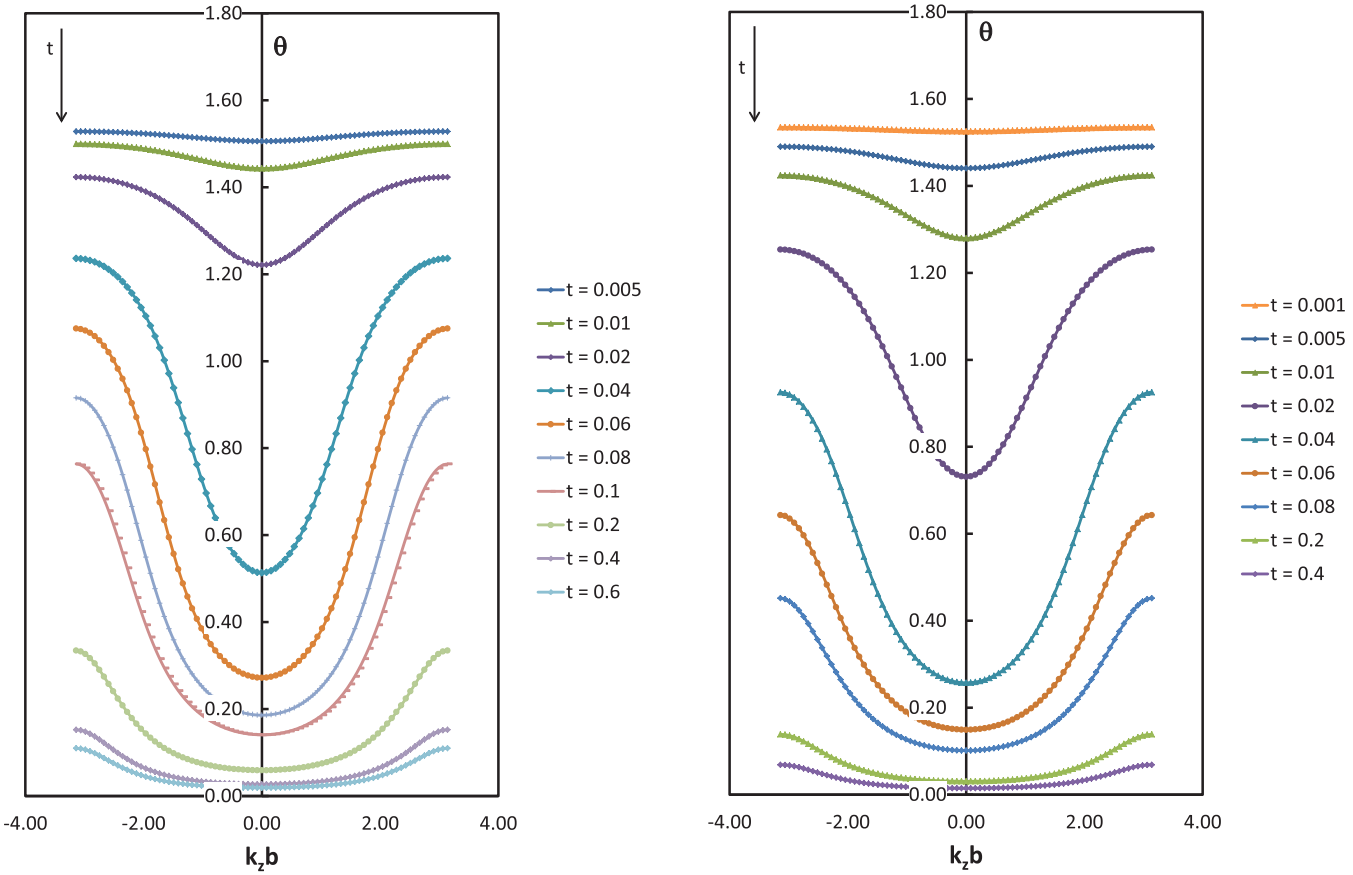

FIG. 2. (Color online) The inclination angle in the first Brillouin zone of a superlattice plotted as a function of the tunneling probability, for the same value of $\gamma^*\mu_B B = 0.1e^2/\varepsilon l$ in (a) and for $\gamma^*\mu_B B = 0.05e^2/\varepsilon l$ in (b). t increases in the direction of the arrow.

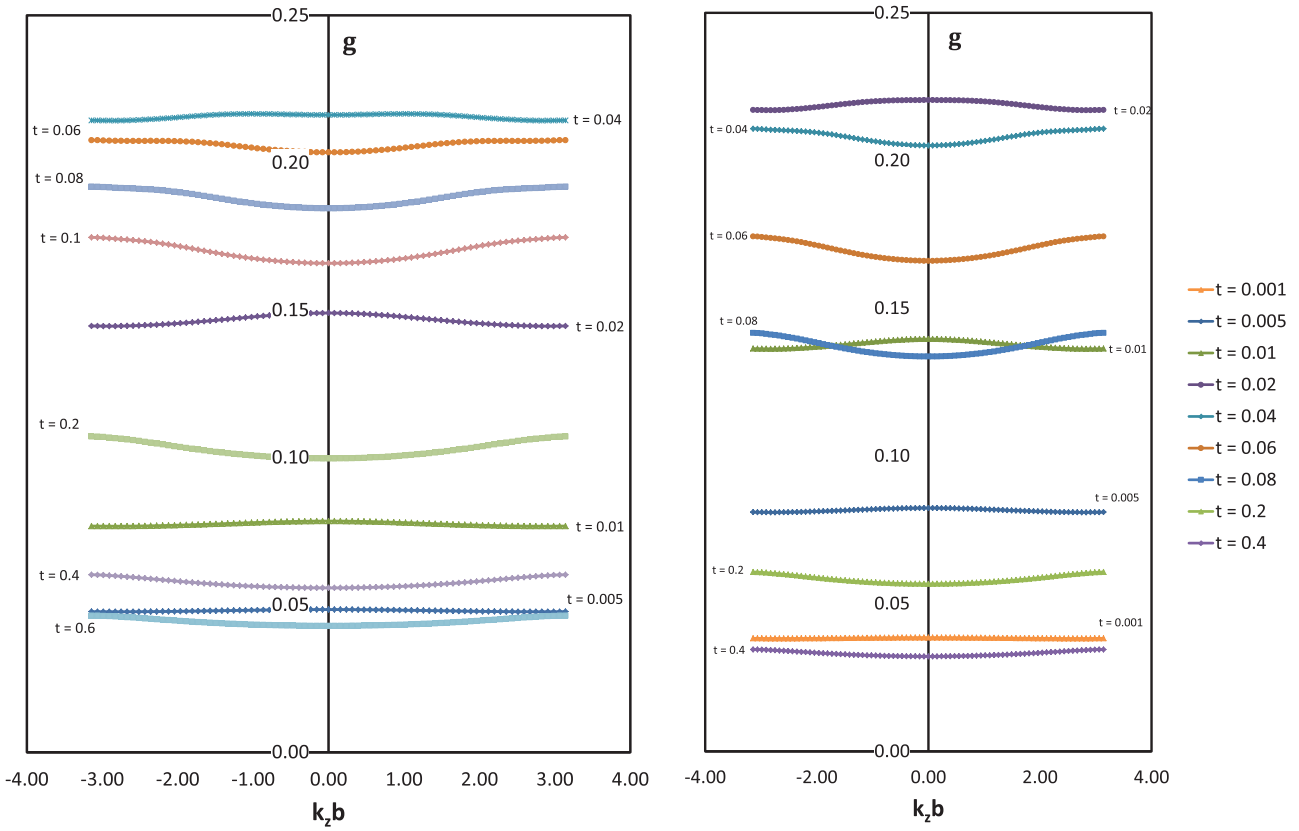

FIG. 3. (Color online) The gap function, expressed in $e^2/\varepsilon l$, in the first Brillouin zone of a SL plotted as a function of the tunneling probability, for the same value of $\gamma^* \mu_B B$ fixed at 0.1 $e^2/\varepsilon l$ in (a) and at 0.05 $e^2/\varepsilon l$ in (b).

is reached when $\partial\langle H\rangle_{\rm HF}/\partial\theta_{k_z} = 0$. This condition generates a self-consistent equation for the angle θ_{k_z}. We introduce the single-particle energies in the HF approximation for the electrons in the $|S,k_z,\uparrow\rangle$ and $|A,k_z,\downarrow\rangle$ minibands,

$$\tilde{\epsilon}_{S,k_z,\uparrow} = \epsilon_{S,k_z,\uparrow} - \sum_{k_z'} v_{SS}(k_z,k_z'-k_z)\cos^2\theta_{k_z'},$$
$$\tilde{\epsilon}_{A,k_z,\downarrow} = \epsilon_{A,k_z,\downarrow} - \sum_{k_z'}\left[v_{AA}(k_z,k_z'-k_z)\sin^2\theta_{k_z'} + v_{AS}(k_z,k_z'-k_z)\right], \tag{20}$$

and write the inclination angle equation in its consecrated form

$$\tan\left(2\theta_{k_z}\right) = \frac{g_{k_z}}{\tilde{\epsilon}_{A,k_z,\downarrow} - \tilde{\epsilon}_{S,k_z,\uparrow}}. \tag{21}$$

The gap function g_{k_z} is defined by

$$g_{k_z} = \sum_{k_z'} v_{AS}(k_z,k_z'-k_z)\sin 2\theta_{k_z'}. \tag{22}$$

Equation (21) is a nonlocal, self-consistent expression, since the solution is dependent on the values of the inclination angle throughout the Brillouin zone. g_{k_z} is a gap function since it represents the difference between the energy of the two quasiparticle states that exist in the HAFM phase, as one can see by differentiating Eq. (19) with respect to the corresponding occupation numbers f_{1k_z} and f_{2k_z}, respectively:

$$E_{1,2}(k_z) = \tfrac{1}{2}\left[\tilde{\epsilon}_{A,k_z,\downarrow} + \tilde{\epsilon}_{S,k_z,\uparrow} \mp \sqrt{\left(\tilde{\epsilon}_{A,k_z,\downarrow} - \tilde{\epsilon}_{S,k_z,\uparrow}\right)^2 + g_{k_z}^2}\right]. \tag{23}$$

When the single-particle energies, written in the HF approximation, in the opposite spin minibands become degenerate, $\tilde{\epsilon}_{A,k_z,\downarrow} = \tilde{\epsilon}_{S,k_z,\uparrow}$, the two quasiparticle energies differ by g_{k_z}. The stability condition for the SDW phase is $\partial^2\langle H\rangle_{HF}/\partial\theta_{k_z}^2 0$, which is always realized when a solution to the gap equation is found since

$$\frac{\partial^2\langle H\rangle_{\rm HF}}{\partial\theta_{k_z}^2} = \sqrt{\left(\tilde{\epsilon}_{A,k_z+Q_z,\downarrow} - \tilde{\epsilon}_{S,k_z,\uparrow}\right)^2 + g_{k_z}^2}. \tag{24}$$

When the expression of the Coulomb interaction is considered from Eqs. (13), along with the form factors from Eq. (15), the energies involved in the gap equation, Eq. (21), are

$$g_{k_z} = \frac{e^2}{b}\int_{-\pi}^{\pi}\frac{d(k_z'b)}{2\pi}\int_0^\infty d(qb)e^{-\frac{(ql)^2}{2}}\sin 2\theta(k_z'a) \times F_{AS}(k_z,k_z'-k_z), \tag{25}$$

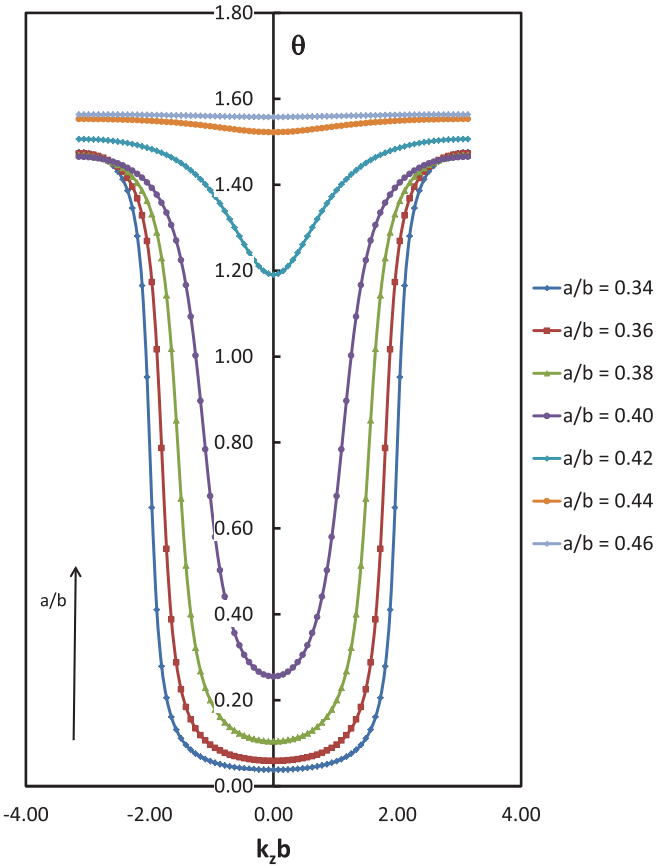

FIG. 4. (Color online) The inclination angle in the first Brillouin zone for as a function of a/b for the same value of the tunneling probability $e^{-\kappa b} = 0.1$. The ratio a/b increases in the direction of the arrow.

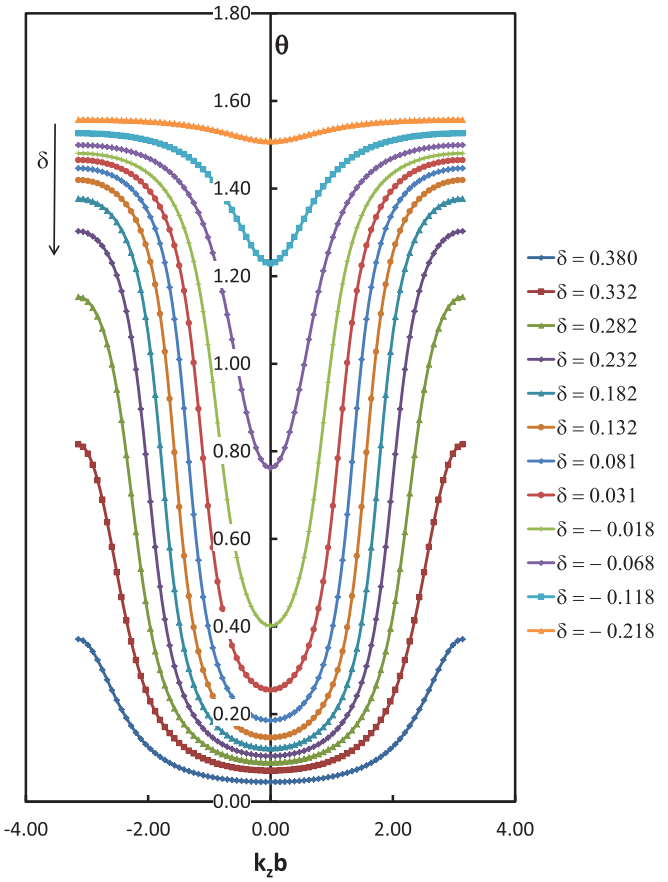

FIG. 5. (Color online) The inclination angle in the first Brillouin zone of a SL plotted for different values of δ (measured in units of $e^2/\varepsilon l$). $\delta = 0.382e^2/\varepsilon l$ generates a paramagnetic ground state. The arrow shows the increase in δ.

$$\tilde{\epsilon}_{S,k_z,\uparrow} = \epsilon_{S,k_z,\uparrow} - \frac{e^2}{b}\int_{-\pi}^{\pi}\frac{d(k_z'b)}{2\pi}\int_0^{\infty} d(qb)e^{-\frac{(ql)^2}{2}} \times \cos^2\theta(k_z'b)\tilde{F}_{SS}(k_z,k_z'-k_z), \tag{26}$$

$$\tilde{\epsilon}_{A,k_z,\downarrow} = \epsilon_{A,k_z,\downarrow} - \frac{e^2}{b}\int_{-\pi}^{\pi}\frac{d(k_z'b)}{2\pi}\int_0^{\infty} d(qb)e^{-\frac{(ql)^2}{2}} \times \sin^2\theta(k_z'b)\tilde{F}_{AA}(k_z,k_z'-k_z,0) - \frac{e^2}{b}\int_{-\pi}^{\pi}\frac{d(k_z'b)}{2\pi}\int_0^{\infty} d(qb)e^{-\frac{(ql)^2}{2}}\tilde{F}_{AS}(k_z,k_z'-k_z,0), \tag{27}$$

V. RESULTS AND DISCUSSION

Equation (22) is solved self-consistently, for each value of k_z within the first Brillouin zone $(-\frac{\pi}{b},\frac{\pi}{b})$, as a function of interunit cell tunneling probability $t = e^{-\kappa b}$ for different values of the independent system parameters Δ, a/b, and magnetic field present both in the definition of δ in Eq. (7) and the magnetic length l. The latter is fixed by its ratio to the SL constant, such that $l/b = 10^{-2}$.

We present numerical results for a GaAs-type SL, whose parameters are chosen such that we can illustrate the first-order phase transitions from ferromagnetic into HAFM into paramagnetic order.

In Fig. 2 we plot the spin coupling angle within the first Brillouin zone as a function of the tunneling probability $t = e^{-\kappa b}$ that determines the bandwidths Δ_{SAS} and Δ for a ratio $a/b = 0.4$. The Zeeman splitting between the minibands is fixed at $0.1e^2/\varepsilon l$ in Fig. 2(a) and at $0.05e^2/\varepsilon l$ in Fig. 2(b). At extremely low values of the tunneling, the system is found in a ferromagnetic ground state that corresponds to $|k_z, S, \downarrow\rangle$ and $|k_z, A, \downarrow\rangle$ being occupied. This behavior mirrors the phenomenology exhibited by a single double layer[12,17] and a multilayer system in the approach of Ref. 14. As the tunneling increases, the widening of the bandwidth compensates the Zeeman splitting between the opposite spin minibands, allowing for the coupling potential g to increase. The result is the formation of a HAFM phase, whereby the coupling angle between the opposite spins that interact decreases from $\pi/2$ and assumes a variable behavior within the first Brillouin zone. The decrease in the angle value is sharper in the center of the Brillouin zone since in that region the difference between the S and A minibands is maximum. By increasing the tunneling even further, the minibandwidth spread overcomes

the Zeeman splitting and paramagnetic order, which corresponds to $\theta \sim 0$ minimizes the energy of the system, as the system assumes a band structure similar to the one depicted in Fig. 1.

The sequence described above is closely reproduced by the behavior of the gap function g_{k_z}, given in Eq. (22), which is plotted inside the first Brillouin zone as a function of t in Fig. 3 for the same SL parameters. The gap function is almost zero for both ends of the tunneling probability range of values, signaling the presence of the ferromagnetic (at low tunneling) and paramagnetic ordering (at high tunneling). The gap opens up for those values of the tunneling probability where the difference between the minibandwidth and the Zeeman splitting is of the order of magnitude of the Coulomb interaction. Thus, it is the latter that stabilizes the HAFM phase, where the gap distinguishes among the two types of quasiparticles that can be created.

The same behavior is observed if the tunneling probability between the wells, and consequently the bandwidth, are modified by changing the ratio of the two characteristic lengths of the SL, a/b. Stronger intraunit cell tunneling realized for smaller values of a is leading to an increase in Δ_{SAS} that drives the system from its ferromagnetic configuration into a HAFM ordering, into a paramagnetic state, as shown in Fig. 4.

Next, in Fig. 5 we present the variation of the coupling angle θ within the first Brillouin zone as a function of the energy difference δ. We consider a system whose bandwidth is large enough such that in the presence of a Zeeman splitting the lowest two occupied minibands are, as depicted in Fig. 1, $|k_z, S, \downarrow\rangle$ and $|k_z, S, \uparrow\rangle$. Numerically, this situation is described by $\delta = 0.382e^2/\varepsilon l$ and $a/b = 0.4$. As the value of δ decreases, the inclination angle starts to increase, signaling the presence of spin-flip transitions performed on account of the Coulomb interaction contribution. This trend continues monotonically with the decrease in δ. For small but positive values of δ, the Coulomb interaction stabilizes the spin-flip transitions into a long-range magnetic order that corresponds to an antiferromagnetic coupling of the electron spins, rotated from the $\hat{z}$ direction by an angle θ that varies continuously within the first Brillouin zone, between $[0,\pi/2]$. As the value of δ decreases further, the system continuously transitions into a ferromagnetic order that corresponds to a constant value of the inclination angle of $\pi/2$.

For the same system parameters, the variation of the gap function within the first Brillouin zone is plotted as a function of δ in Fig. 6(a). As δ decreases, the gap increases from a very small value, which can be explained on account of the canted antiferromagnetism that exists in the unit

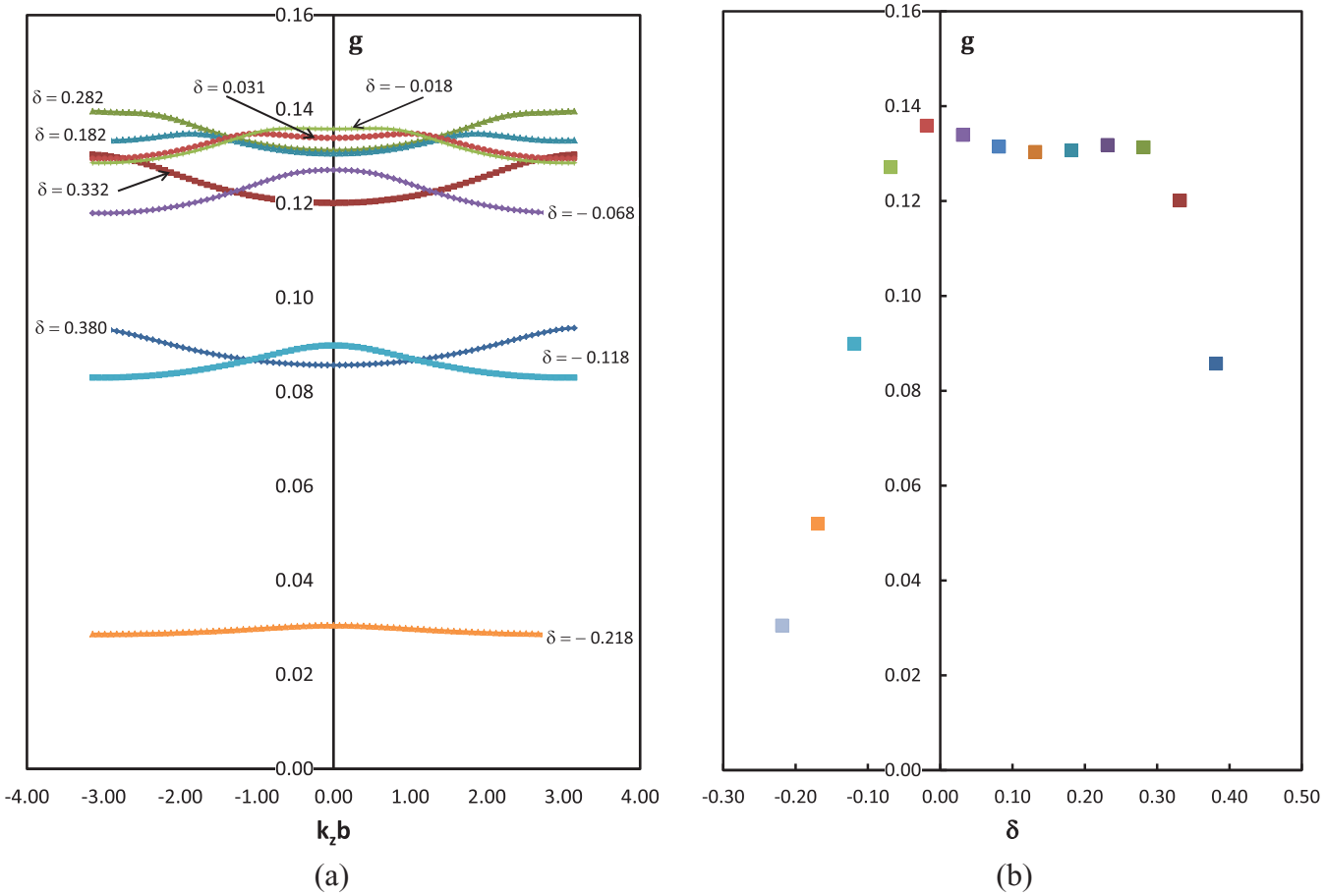

FIG. 6. (Color online) The gap function inside the first Brillouin zone for different values of δ in (a). The most significant values are highlighted. The gap at the center of the Brillouin zone as a function of δ in (b). Both q and δ are expressed in $e^2/\varepsilon l$ units.

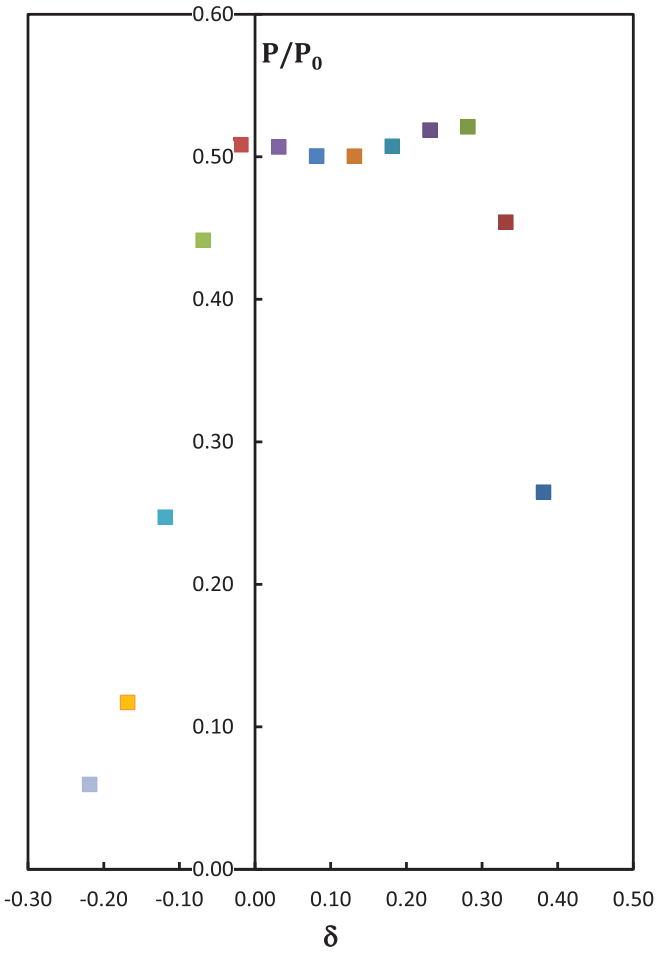

FIG. 7. (Color online) Fractional polarization as a function of δ (expressed in $e^2/\varepsilon l$).

cell,[17] to a value that remains relatively constant, while the magnetization of the system corresponds to a HAFM coupling of the electrons. We represent the variation of g with δ is presented more clearly in Fig. 6(b). We remark that the decrease in δ generates a substantial increase in g, followed by a plateau corresponding to the HAFM phase and a subsequent diminishment that is associated with the ferromagnetic order.

As a measure of the magnetization of the ground state, we consider the fractional polarization, defined as

$$P = \sum_{k_z} \langle c^\dagger_{k_z\uparrow} c_{k_z\uparrow} - c^\dagger_{k_z\downarrow} c_{k_z\downarrow} \rangle_0 = \sum_{k_z} \sin 2\theta_{k_z}. \qquad (28)$$

As depicted in Fig. 7, the fractional polarization peaks within the interval of values of δ for which the HAFM is established and becomes zero at either end, which correspond to ferromagnetic or paramagnetic ordering, respectively.

In conclusion, we have obtained numerical solutions to the gap equation of a superlattice in the presence of a tilted magnetic field at $T = 0$ K that exhibits long-range magnetic ordering characterized by an antiferromagnetic coupling between electrons whose spins are rotated from the $\hat{z}$ axis by a continuously variable angle θ. The existence of a stable HAFM phase is realized when the difference between the opposite spin minibands $|S,k_z,\uparrow\rangle$ and $|A,k_z,\downarrow\rangle$ is of the order of magnitude of the Coulomb interaction between particles. Given the considerable liberty in choosing the system parameters that favor such a behavior in the case of the superlattice, 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.

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