Exchange-enhanced spin splitting in a two-dimensional electron system with lateral modulation

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The effective spin splitting of the Landau bands produced by an external unidirectional periodic-modulation potential is studied in the thermodynamic Hartree-Fock (HF) approximation. The HF energies, which depend on three quantum numbers, the center coordinates of the wave functions, and the discrete Landau and spin quantum numbers, and also the thermodynamic density of states (TDOS), which is experimentally accessible by magnetocapacitance measurements, are calculated numerically for representative values of wavelength and strength of the modulation potential. For GaAs at low temperatures, the exchange enhancement can yield an effective spin gap comparable with the cyclotron energy. The spin gaps occur in strips, in which the center coordinates correspond to HF energies near the Fermi energy. The width of these strips depends on the steepness of the modulation potential and, in an intricate manner, on temperature and screening effects. Screening effects may lead to broad peaks in the TDOS, while van Hove singularities due to the one-dimensional Landau bands lead to sharp peaks in the TDOS. The conditions, under which such structures should be resolved in experiments, are discussed.

I. INTRODUCTION

Equilibrium and transport properties of a two-dimensional electron system (2DES) in a lateral superlattice and subjected to a perpendicular magnetic field have been investigated by several experimental and theoretical groups, and recent reviews are available.[1,2] Characteristic oscillatory effects have been discovered in the opposite limits of weakly modulated systems with a 1D or a 2D superlattice,[1,2] and of strongly modulated "antidot" systems where the electrons are expelled from a periodic array of forbidden regions.[1,3] In both cases, the interesting effects were found in magnetoresistance measurements at low magnetic fields where, in the language of quantum mechanics, many Landau levels are occupied and a classical or semiclassical explanation seems appropriate. The characteristic features of these effects have been explained convincingly within the noninteracting electron picture,[1,2,4,5] and are apparently independent of the electron spin.

On the other hand, magnetoresistance anomalies observed on a 2DES with unidirectional periodic modulations of intermediate strength at higher magnetic fields[6,7] seem to depend sensitively on electron-electron interaction effects, such as screening and exchange enhancement of the g factor, and are not well understood at present. In experiments on the 2DES in a $Al_xGa_{1-x}As$-GaAs heterostructure, with a lateral superlattice produced by holographic illumination, an internal structure of the Shubnikov-de Haas peak with Landau quantum number $n = 1$, i.e., for filling factors $4 \geq \nu \geq 2$, was observed, which became more pronounced with increasing modulation strength (realized by an applied gate voltage) whereas the mobility decreased simultaneously. Although the structure looked similar to the usual spin splitting of the Shubnikov–de Haas peak, this was ruled out, since spin splitting was hardly resolved already in the limit of weak modulation, where the mobility was much higher and, therefore, the collision broadening was much smaller.[6] More recent experiments on samples with higher mobility show that the usual spin splitting, which is observed for small or zero modulation strength, levels out with increasing modulation strength. At stronger modulation, again, a double peak structure occurs, although with a slightly different appearance. At an intermediate modulation strength a three-maxima internal structure of the $n = 1$ peak is observed at $T = 4.2$ K, which sharpens with decreasing temperature. Finally, at $T = 1.1$ K the peak at the lowest magnetic field value develops a shoulder, indicative of a fourfold internal structure of the Landau band with $n = 1$.[7]

We take these experimental results as evidence for a complicated and interesting interplay between, on one hand, the effect of the 1D modulation, which tends to introduce a double-peak structure into the DOS contribution of each Landau band due to the van Hove singularities of the quasi-one-dimensional band structure, and, on the other hand, the effect of the Coulomb interaction between the electrons, which tends to increase the effective spin splitting (exchange-enhanced g factor) (Ref. 8) and to screen the modulation potential.[9–11]

For the case of a *homogeneous* 2DES, it is well known[8] that the exchange term of the Coulomb interaction can lead to a drastic enhancement of the spin splitting. In the

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Hartree-Fock approximation (HFA) each of the highly degenerate Landau energy levels $E_{n\sigma}$ ($n = 0, 1, ...$, $\sigma = \uparrow, \downarrow$ or, equivalently, $+, -$) is lowered by the exchange energy, which depends on the filling factors $\nu_{n'\sigma}$ of the Landau levels $n'\sigma$ with the same spin.[8] Therefore, the effective Zeeman splitting depends on the position of the Fermi level, as well as on the temperature and, eventually, on a collision broadening of the Landau levels due to interaction of the 2D electrons with randomly distributed impurities,

$$E_{n\downarrow} - E_{n\uparrow} = \gamma\hbar\omega_c + \frac{e^2}{\kappa l}\sum_{n'} c_{nn'}(\nu_{n'\uparrow} - \nu_{n'\downarrow}) \equiv \gamma_{\rm eff}\hbar\omega_c, \tag{1.1}$$

where $\hbar\omega_c$ is the cyclotron energy and l is the magnetic length, $\gamma\hbar\omega_c$ is the bare Zeeman splitting, proportional to the bare g factor, κ the dielectric constant of the semiconductor and $c_{nn'}$ a numerical constant ($c_{00} = \sqrt{\pi/2}$). In GaAs ($g \approx -0.4$), $\gamma = 0.013$ is very small, but $\gamma_{\rm eff}$ can be up to two orders of magnitude greater, so that the effective spin gap can be of the order of the cyclotron energy. Consequently, the spin splitting of the Landau levels is well observable in the experiments, despite the small value of γ.

Whereas in the *homogeneous* 2DES the direct Hartree term of the Coulomb interaction, which describes the interaction of an electron with the electrostatic potential produced by the charge density distribution of the 2DES, leads to an irrelevant energy shift (which is usually compensated by the interaction of that electron with a uniform positive background charge) so that the exchange effect is the most relevant contribution of the interaction, in a *laterally modulated* 2DES the Hartree term leads to screening of the modulation potential. The Hartree approximation has been used to study screening effects in the quantum Hall regime,[10,11] while spin and collision broadening effects were neglected. Screening was found to be very nonlinear with a tendency to favor, for sufficiently smooth external potential, the pinning of Landau bands at the Fermi energy.[10] If the potential varies only slowly on the scale of the magnetic length, the Hartree approximation reduces to the local, nonlinear Thomas-Fermi approximation in which, at sufficiently low temperatures, the 2DES decomposes into alternating "compressible" and "incompressible" regions.[12–14] In the compressible regions a Landau band is pinned at the Fermi level, so that there the Landau energy together with the effective potential is constant (perfect screening). In an incompressible region the Fermi energy falls in the gap between adjacent Landau bands, and the electron density is constant. Electrostatics, i.e., the Hartree approximation, favors the formation of compressible regions with perfect screening, in which the states at the Fermi energy are only partly occupied.[13,14] Apparently this is in competition with the tendency of the exchange interaction to minimize the energy by the enhancement of the effective spin gap around the Fermi energy, which becomes maximum if states with one spin direction are completely occupied while those with opposite spin are empty. Due to this competition one expects a modification of the Hartree picture of screening with its incompressible and compressible regions. In particular, it is not obvious, whether a lateral modulation of the 2DES can coexist with an exchange-enhanced spin splitting, and under which conditions peak structures due to one or the other should be resolved in experiments. Previously published theoretical[15–18] and experimental[19–22] work related to these questions does also not provide a clear picture of the situation, although recent experiments indicate the existence of spin-split edge states in the quantum Hall regime.[20–22]

In view of this situation, a detailed magnetotransport calculation for modulated 2D electron systems seems desirable, which includes Coulomb effects like screening and g-factor enhancement, and, of course, the effects of collision broadening and finite temperature, which are known to influence the latter crucially. This, however, is a very ambitious project. In the present paper we only want to take a first step towards this aim, and restrict our consideration to equilibrium properties. Furthermore, we will completely neglect collision broadening effects, and we will consider only a simple sinusoidal external modulation potential. Finally, we will restrict our treatment of Coulomb interactions to the Hartree-Fock approximation as the simplest approximation which is able to describe both screening and g-factor enhancement. The HFA should give useful qualitative insight into the physics of the problem, even if a more involved approach[23] should be required for quantitatively reliable results.

Thus, in this paper we investigate, within the thermodynamic Hartree-Fock approximation, the spin splitting of the Landau bands in the presence of a unidirectional external potential. In Sec. II, we describe the self-consistent calculation of the energy spectrum and the particle density. In Sec. III, the resulting Landau bands, with $n = 0, 1, 2$, are presented for some representative values of wavelength and strength of the modulation potential. Since the HF energy spectrum itself is not accessible to the experiment, we focus in Sec. IV on the spin splitting of the "thermodynamic density of states," which can be directly obtained by magnetocapacitance measurements. Our conclusions are presented in Sec. V, and some calculation details concerning the energy bands are given in the Appendix.

II. THE MODEL

We study a two-dimensional electron gas subjected to a strong perpendicular magnetic field and a unidirectional lateral modulation potential $V_{\rm ext} = V\cos(Kx)$ of period $a = 2\pi/K$. The potential is assumed to be of sufficiently small amplitude and large period ($lV/a \ll \hbar\omega_c$), so that it does not lead to a significant coupling of Landau levels. We treat the electron-electron interaction in the Hartree-Fock (HF) approximation and assume that electrical neutrality is ensured by a uniform background of positive charges. We describe the magnetic field B in z direction in the Landau gauge, choosing the vector potential along the y axis. Then the Hamiltonian has translational

symmetry in y direction, and the HF wave functions are of the form $\langle \mathbf{r}|nk\rangle = L_y^{-1/2}\exp(iky)\phi_{n,k}(x)$, with L_y a normalization length and $\mathbf{r} = (x, y)$. They have to be calculated from the HF equations, self-consistently with the corresponding energy levels, which can be written as

$$E_{nk\sigma}^{(HF)} = E_{nk\sigma}^{(0)} + E_{nk}^{(H)} + E_{nk\sigma}^{(F)}, \tag{2.1}$$

where the first term is the energy of a single electron in the presence of the magnetic field and the external modulation potential. If one neglects the electron-electron interaction, the HF states $|nk\rangle$ reduce to the usual Landau states, $\phi_{n,k}^{(0)}(x) = \varphi_n(x - X_0)$, i.e., harmonic oscillator functions with Landau quantum number n and center coordinate $X_0 = -l^2k$, and $E_{nk\sigma}^{(0)}$ describes the Landau bands of a noninteracting electron system, as obtained from the first-order perturbation theory [see Appendix, Eq. (A5)],

$$E_{nk\sigma}^{(0)} = \left(n + \frac{1}{2} - \frac{1}{2}\gamma\sigma\right)\hbar\omega_c + \langle nk \mid V_{\text{ext}} \mid nk\rangle . \tag{2.2}$$

For the interacting system, the direct (Hartree) contribution to the Landau bands is given by

$$E_{nk}^{(H)} = \langle nk \mid \int d\mathbf{r}'\, v(\mathbf{r} - \mathbf{r}')\rho(\mathbf{r}') \mid nk\rangle , \tag{2.3}$$

where $v(\mathbf{r}) = e^2/\kappa|\mathbf{r}|$ is the Coulomb potential with the background dielectric constant κ, and

$$\rho(\mathbf{r}) = \sum_{nk\sigma} \mathcal{F}_{nk\sigma}\,|\langle \mathbf{r} \mid nk\rangle|^2 \tag{2.4}$$

is the electron density. Here the occupation factors are defined as $\mathcal{F}_{nk\sigma} \equiv \mathcal{F}[(E_{nk\sigma}^{(HF)} - \mu)/k_BT]$, with $\mathcal{F}(x) = (e^x + 1)^{-1}$ the Fermi function, T the temperature, and μ the chemical potential, determined by the mean value $\langle\rho\rangle$ of the electron density. The positively charged background cancels the integral of the Coulomb potential $v(\mathbf{r})$ over the whole space, and thus $\langle\rho\rangle$ does not contribute to Eq. (2.3).

The exchange (Fock) energy can be written as[24]

$$E_{nk\sigma}^{(F)} = -\sum_{n'k'} \mathcal{F}_{n'k'\sigma} \int \frac{d^2q}{(2\pi)^2}\, v_{\mathbf{q}} |\langle nk|\, e^{i\mathbf{q}\cdot\mathbf{r}}\, |n'k'\rangle|^2 , \tag{2.5}$$

with $v_q = 2\pi e^2/\kappa|\mathbf{q}|$. As far as only low Landau levels are concerned, the Hartree-Fock wave functions $\langle \mathbf{r}|nk\rangle$ can be expressed as linear combinations of only a few Landau wave functions, being exponentially localized around $X_0 = -l^2k$. Therefore, the exchange matrix element of the Coulomb potential—as a function of X_0'—is concentrated in a strip $\mathcal{S}(X_0)$ of width $\Delta X_0 \approx 4l$ around X_0, and decreases exponentially with increasing $(X_0' - X_0)^2/l^2$, see Eq. (A7). Hence, for sufficiently smooth modulations (small amplitude, large wavelength), the exchange energy of a given state $|nk\sigma\rangle$ is essentially the sum of the occupation factors of the states with the same center of coordinate and spin direction, $\mathcal{F}_{n'k\sigma}$. Consequently, the enhancement of the Zeeman splitting will be given only by the states with energies close to the Fermi level, and will be proportional to the spin polarization. The largest enhancement will occur in the band intersected by the Fermi level, but a comparable spin splitting will be induced in the other bands, through the terms with $n \neq n'$, Eqs. (2.5) and (A7).

In the following, we will study modulations yielding Landau bands with amplitudes not much larger than the cyclotron energy. In this case, the simple Landau wave functions provide a reasonably good approximation of the Hartree-Fock functions, the equality being achieved in the limit of weak modulations ($V \to 0$ and/or $a \to \infty$). In fact, solving the HF equations is equivalent to minimizing the free energy of the system within a certain class of single-particle wave functions.[25] Here, by fixing the latter, we restrict ourselves to finding a minimum of the energy subjected to additional constraints. However, due to the mentioned reasons, we will call this approximation also Hartree-Fock, even if the energies and the wave functions are not rigorously self-consistent. Quantitatively, this approximation has been tested by comparing the energy bands yielded by the Landau wave functions with variational solutions of the Hartree problem.[26] We have also checked the results by a self-consistent calculation, which describes the HF wave functions as linear combinations of the five lowest Landau functions, and, as a consequence, requires much more computational time. Quantitatively, this leads to a more effective screening, due to a polarization of the wave functions. The width of the totally occupied and of the empty bands becomes somewhat smaller, especially for short-period modulation potentials. Qualitatively, however, there is little change, especially for the bands intersecting the Fermi energy, and the enhancement of spin splitting is very similar to the result of the simple approximation. Since our aim is a *qualitative* understanding of the g-factor enhancement in modulated systems, we use in the following the simple approximation, thus reducing the computational times by more than an order of magnitude.

An analytical solution of the integral equations (2.1)–(2.5) can be found for a weak modulation, in the first order in V.[27] Here we solve them by numerical iterations, starting from the noninteracting solution, see Appendix. We exploit the periodicity of the external potential by expanding in truncated Fourier series the particle density, in the real space, and the single-particle energies together with the occupation factors, in the reciprocal space, and we solve the resulting coupled equations for the Fourier coefficients. The number of included harmonics depends on the particular details of the obtained energy spectra, varying from 15 when the Landau bands are relatively close to a simple cosine form, up to 80 when additional oscillations are present.

The material parameters are chosen here as for GaAs, i.e., $m^* = 0.067m_0$, $\gamma = 0.013$, and $\kappa = 12.4$. The particle density in the absence of the modulation, $n_e = \langle\rho(\mathbf{r})\rangle$, is such that the total filling factor $\nu \equiv 2\pi l^2 n_e = 13/[B]$, $[B]$ being the magnetic field in tesla.

III. ENERGY BANDS

At low temperatures, the enhanced spin splitting of the energy bands due to the exchange energy originates from states with energies in a narrow region around the Fermi level, since only the filling factors of these states depend on the spin orientation. Clearly, with increasing temperature the enhancement vanishes, since the difference of the occupation numbers of states with the same orbital but opposite spin quantum numbers decreases. In modulated systems, where the dispersion of the energy bands can be expressed in terms of a "center coordinate" $X_0 = -l^2 k$, the energy region which is responsible for the exchange enhancement corresponds to a region of X_0 values, i.e., a strip (in each unit cell of the 1D superlattice) in real space. For fixed magnetic field and modulation wavelength, the width of this strip is determined by the modulation amplitude. If the latter is smaller than the enhanced Zeeman energy in the unmodulated homogeneous 2D electron system, the strip of enhanced spin splitting extends over the whole system, as in the homogeneous case. With increasing modulation amplitude the width of this strip shrinks. The magnitude of the exchange energy in a state $|nk\sigma\rangle$ localized at X_0 depends on the range of X_0' values for which the states $|n'k'\sigma\rangle$ contribute to Eq. (2.5), i.e., to Eq. (A7) in our approximation. This is determined by two factors. First, the extent of the (Landau-type) wave functions leads to a kernel with range $\Delta X_0 = \xi l$ of a few magnetic lengths ($\xi \sim 2$), as is seen from Eq. (A7). Second, X_0' values within this range contribute to an enhancement of the spin splitting if the Fermi occupation factors $\mathcal{F}_{n'k'\sigma}$ are different for both spin directions. Maximum enhancement according to Eq. (1.1) would result, if the difference of these Fermi factors had the value 1 over the whole range of the kernel. This means that the variation of the energy eigenvalues in the range of the kernel must be smaller than the effective spin gap, $\Delta X_0 |dE^{\rm HF}_{nk\sigma}/dX_0| < e^2/\kappa l$. If we replace this energy dispersion by the gradient of an effective potential, we may write this condition for the smoothness of the effective potential as

$$\xi a_B^* |dV/dX_0| < \hbar\omega_c \,, \tag{3.1}$$

where $a_B^* = \kappa\hbar^2/me^2$ is the effective Bohr radius (for GaAs $a_B^* \approx 10$ nm). If the potential becomes steeper, only a part of the states $|nk'\sigma\rangle$ in the strip $\mathcal{S}(X_0)$ can contribute to the spin polarization, and the spin gap at X_0 becomes smaller. As a consequence, the exchange enhancement of the spin splitting will be rapidly suppressed if the effective potential becomes so steep that condition (3.1) is violated.

In the examples to be discussed below, the variation of the HF energies on the magnetic length scale is much larger than $k_B T$, and the resulting enhancement of the spin splitting can be comparable with the upper bound resulting from Eq. (1.1), with $\nu_{n\uparrow} = 1, \nu_{n\downarrow} = 0$. The steeper the energy dispersion curve is, the smaller is the resulting enhancement. In the following we will distinguish between modulations with short and with long wavelengths. We consider the wavelength of the external cosine potential as short if, for the magnetic field strengths of interest ($B \sim 5$ T), the spin polarization vanishes when the amplitude of the modulation potential reaches the order of magnitude of the cyclotron energy. In our model this means wavelengths below 100 nm. For such short-wavelength modulations the width (and phase) of the Landau bands $n = 0, 1, 2$ in the absence of Coulomb interaction effects depends on the Laguerre polynomial factors, see Eq. (A5), whereas for the long-wavelength modulations to be considered below ($a \geq 300$ nm) these Landau bands would be parallel in the non-interacting electron approximation. Moreover, screening effects are expected to be much more important in modulated systems with a long wavelength than in those with a short one.

Some energy-band structures for such a situation are shown in Fig. 1 for $a = 80$ nm. The thermal energy is small, of the order of the bare single-particle Zeeman splitting. The exchange energy, larger in the states close to, or below the Fermi level than in the unoccupied states, has a negative sign with respect to the Hartree energy and diminishes the screening effects of the latter. Whereas the Hartree screening tends to decrease the bandwidth, the Fock term tends to lower the lower energies of occupied states (but not the higher energies of unoccupied states) in partly occupied bands, and thus to increase the width of partially occupied bands. An example of this competition is seen in Fig. 1. In the non-

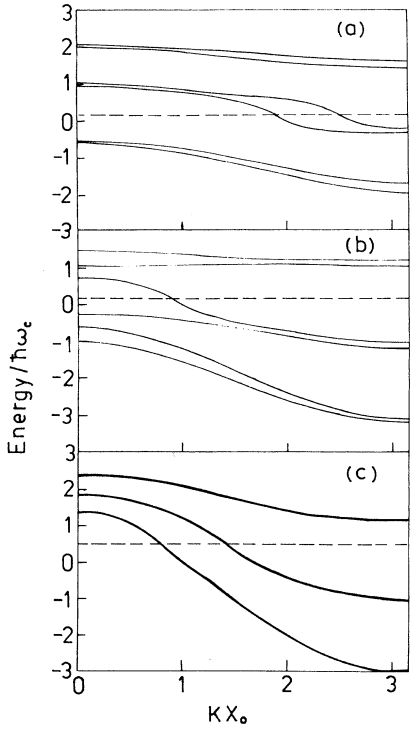

FIG. 1. Landau bands, $n = 0, 1, 2$, for a short modulation, $a = 80$ nm: (a) $V = 10$ meV, $B = 5$ T, (b) $V = 10$ meV, $B = 3.5$ T, (c) $V = 30$ meV, $B = 5$ T. The horizontal dashed lines represent the chemical potential. $T = 1$ K.

interacting approximation the width of the shown bands would decrease with increasing n, becoming very small for $n = 2$, see Eq. (A5). In Fig. 1(a) the range of the wave functions [and that of the kernel in Eq. (A7)] is about one-third of the modulation period ($K\Delta X_0 \sim 2$), so that the electron density varies considerably everywhere, even near the maxima of the modulation potential where, in a broad region of center coordinates X_0, states in the $n = 1$ bands are not occupied. Thus strong screening exists and the Hartree term tends to reduce the band widths. Nevertheless, the exchange enhances the width of the bands crossed by the Fermi level and, due to cross terms with $n \neq n'$ in Eq. (A7), also the width of the adjacent bands. In both Fig. 1(a) and 1(b) an exchange-enhanced spin gap at the Fermi level is obtained in a certain strip of center coordinates. Although $V/\hbar\omega_c$ is larger and, therefore, the average energy dispersion is steeper in Fig. 1(b) than in Fig. 1(a), the enhanced spin splitting is comparable in both cases, since the local energy dispersion near the Fermi level is smaller in Fig. 1(b), in accord with condition (3.1).

For the situation of Fig. 1(c) the external potential modulation is so strong that the energy dispersion near the Fermi level is too large to allow for an exchange enhancement of the spin splitting. The suppression of the g-factor enhancement in this situation is consistent with a prediction by Kinaret and Lee[15] for parabolically confined narrow wires, with a width of the order of the magnetic length: they proved the disappearance of the spin polarization for electron densities exceeding some critical value, which means that the slope of the confinement potential at its intersection with the Fermi energy also exceeds a critical value.

We now consider modulations with a long wavelengths, much larger than the magnetic length. This situation is completely different from that of short wavelengths, and screening effects become much more important.

For a modulation amplitude comparable with $\hbar\omega_c$ and the case of partly occupied bands, we obtain energy bands which show several oscillations within a single period of the applied external periodic potential. These short-period oscillations may be related to the charge-density-wave (CDW) instability of the homogeneous state at low temperatures, which has been predicted within the HFA,[28,29] but never observed experimentally. It has been argued that this CDW instability is possible also in the presence of the impurities, together with negative values for the thermodynamic density of states (TDOS).[30] In recent Hartree-Fock calculations for a rotationally symmetric 2DES an oscillatory dependence of the energy eigenvalues on the angular momentum has been obtained, which may also be related to this CDW instability.[18] Since it is not clear whether this instability is a genuine physical effect or just an artifact of the HFA, we do not want to discuss details which depend critically on such oscillations. We, therefore, focus our attention on typical situations which are not strongly affected by these oscillations.

In Fig. 2, we consider a modulation with wavelength $a = 500$ nm and relatively small amplitude. In Fig. 2(a) the modulation amplitude is nearly twice the cyclotron

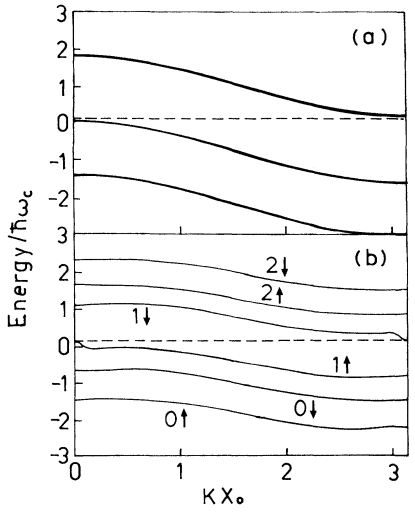

FIG. 2. Landau bands, $n = 0, 1, 2$, for a long modulation, $a = 500$ nm, small amplitude, $V = 5$ meV, and integer filling factors ν [B(tesla)$= 13/\nu$]: (a) $\nu = 4$ ($B = 3.25$ T), (b) $\nu = 3$, ($B = 4.33$ T). The dashed lines: chemical potential. $T = 1$ K.

energy, and the Fermi level is positioned between two Landau bands. Screening is poor, since the two lowest Landau bands ($n = 0$ and 1) are completely occupied and the band with $n = 2$ is empty (filling factor $\nu = 4$). Spin splitting is not resolved on this scale. If we try to interpret the magnetoresistance oscillations of Ref. 6 on the basis of this Fig. 2(a), we would expect that the pronounced double peak structure, which was observed between filling factors $\nu = 4$ and 2, is a consequence of the van Hove singularities of the Landau band $n = 1$, but not of its spin splitting. This interpretation was given in Ref. 6, it is, however, not justified by our calculation for low temperature and zero collision broadening. As we increase the magnetic field, the Fermi level moves into the lower bands and some CDW like oscillations appear. But the most important effect is that, due to the large DOS at the Fermi level, strong screening sets in. Both the large exchange energy and the strong screening at this long wavelengths make the two spin bands with $n = 1$ to separate for filling factor 3, Fig. 2(b). From this result we would conclude that the minimum observed in the magnetoresistance between $\nu = 4$ and 2 is due to the enhanced spin gap at filling factor $\nu = 3$, and *not* due to van Hove singularities. We want to emphasize that this result depends crucially on screening, which is very important for long-wavelength modulations. As the wavelength becomes shorter screening diminishes on one side, and on the other side the bands with $n = 2$ tend to become flat, like in Fig. 1(b). Then the width of the bands with $n = 1$ can become larger than the spin splitting even when the Fermi level intersects them. In this case, one may expect to see in the magnetoresistance experiments effects of the van Hove singularities, but possibly also from the spin splitting. On the other hand, collision broadening effects are important in the experiment,[6] and these will lead to a suppression of screening and g-factor enhancement, so that it is difficult to compare the experimental

results and our present calculations.

In Fig. 3, we show results for a modulation with wavelength $a = 500$ nm and a large amplitude, about one order of magnitude larger than the cyclotron energy. For this large amplitude of the external modulation potential depleted strips occur at the potential maxima, where the local filling factor (LFF) $\nu(x) = 2\pi l^2 \rho(x)$ is zero, i.e., the 2D electron system splits into nonoverlapping 1D "wires." In Fig. 3(a), we observe a strong enhancement of the spin splitting in the $n = 1$ Landau band for X_0 values in the center of the wire, and in the $n = 0$ band for X_0 values near the edge. The effective spin splitting of the adjacent bands in the corresponding regions of X_0 values is also relatively strong. The peculiar shape enclosed by the spin splitted bands results from the fact that the relevant spin gap is not constant, but rather opens self-consistently with increasing spin polarization and vanishes as the bands depart from the Fermi level, the bare g factor for GaAs being very small. In the center of the wire the band with $n = 1$, $\sigma = \uparrow$ is nearly pinned at the Fermi energy, an apparent consequence of strong screening.

Obviously, we can take the present calculation for wide nonoverlapping wires as a model for the edge region of a 2D electron gas, similar to previous work in the Hartree[10] and in the Thomas-Fermi[14] approximation. Comparing with the picture of alternating compressible and incompressible strips,[13,14] which arises from the Hartree-type approximation as we mentioned in the Introduction, we observe specific modifications due to the exchange interaction. The concept of incompressible strips remains essentially unchanged: the Fermi energy falls in the gap between (or below) Landau levels and the density is constant. The "compressible" strips, however, change their character. The spin degenerate bands of the Hartree picture, which are pinned at the Fermi level, split in the HFA, and in the interior of these regions the Fermi energy now falls into the large effective spin gap, so that the partial filling factors of both spin directions are there constant, with $\nu_\uparrow(x) - \nu_\downarrow(x) = 1$. Only in relatively narrow strips at the edges of these "compressible" regions the density (of one spin direction) can vary as a function of position. This may become even clearer from Fig. 3(b) and the corresponding plot of the LFF in Fig. 3(c). Here the ratio $V/\hbar\omega_c$ is smaller than in Fig. 3(a), screening is more effective, and the width of the spin-split "compressible" strip is larger. If we extend the concept of incompressible and compressible strips to each spin direction separately, we find only very narrow compressible but wide incompressible strips [see Fig. 3(b) and 3(c)], in contrast to the Hartree picture.[13,14] In the situation of Fig. 3(a) there is a strong overlap of the polarized strips, resulting in a "compressible" strip with strongly varying density, similar to those in the Hartree picture.

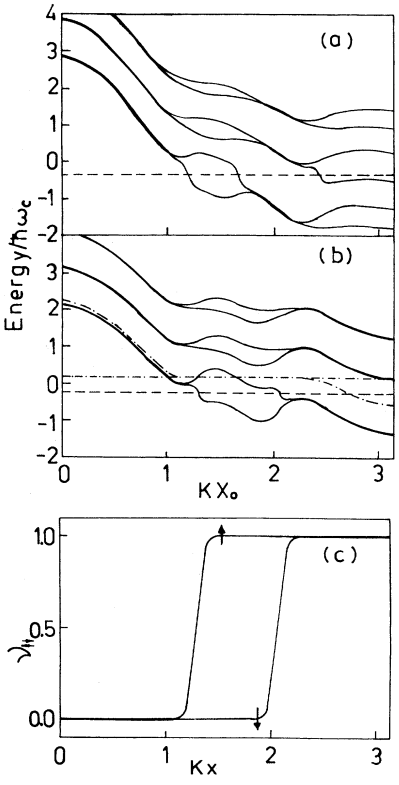

FIG. 3. Landau bands, $n = 0, 1, 2$, for a long modulation, $a = 500$ nm, and large amplitude, $V = 250$ meV: (a) $B = 10$ T, (b) $B = 14$ T, where the dashed-dotted lines show the Hartree approximation (horizontal line: chemical potential); (c) the spin-up and spin-down filling factors for (b). $T = 1$ K.

In Fig. 3(b), we have also indicated by dash-dotted lines the result of the corresponding Hartree calculation for the spin-degenerate $n = 0$ Landau band and the Fermi level (horizontal dash-dotted line). While the Hartree and the HF bands nearly coincide where they are unoccupied, the HF band is clearly lowered in the region of occupied states. It is also clearly seen that the region of exchange-enhanced spin splitting evolves from the compressible region of the Hartree approximation. The fact that the former is somewhat shorter than the latter is consistent with the observation that the exchange term counteracts the Hartree term, which is the origin of the screening and energy-pinning effects.

The shape of the spin splitting of the $n = 0$ Landau band at the edge of the wire obtained in Fig. 3(a) is very similar to a recent result of Dempsey, Gelfand, and Halperin.[17] Using a Ginzburg-Landau-type argument for the edge of a laterally confined 2DES, they have recently shown that the spin splitting of the edge-state energies may be energetically favorable if the energy dispersion of the single-particle states is sufficiently smooth, even if the bare g factor is zero. Our calculations also show that the exchange enhancement of spin splitting can become effective only if the external potential is sufficiently smooth (on the scale of the magnetic length). In accord with previous Hartree results, we see that the width of the "compressible" strips, which in our calculation appear as the spin polarized regions, increases as the "confinement potential" becomes smoother. This is the reason why the width of the spin polarized region in Figs. 3(b) and 3(c) is considerably larger than that obtained in Ref. 17.

IV. THERMODYNAMIC DENSITY OF STATES

The density of states corresponding to the (temperature dependent) effective-energy spectrum given by the Hartree-Fock approximation has van Hove singularities due to the extrema of the energy dispersion in the center and at the edges of the 1D Brillouin zone. It would be interesting to insert this DOS into a Kubo-type formula to see if the resulting magnetoresistivity[31] could qualitatively reproduce the double-peak curves obtained by Weiss *et al.*,[6] who argued that these structures are due to modulation-induced van Hove singularities while the spin splitting is not resolved. Such a transport calculation is, however, beyond the scope of the present work. Instead, we consider now the thermodynamic density of states (TDOS), an equilibrium quantity which is experimentally accessible via magneto-capacitance measurements.[32]

The TDOS, $D_T \equiv \partial\langle\rho\rangle/\partial\mu$, can be obtained by taking the derivative with respect to μ of the expression

$$\langle\rho\rangle = \int dE\, \mathcal{F}\left(\frac{E-\mu}{k_B T}\right) D(E)\,, \tag{4.1}$$

$D(E)$ being the DOS. For noninteracting electrons $D(E)$ is independent of μ, and the derivative affects only the Fermi occupation factor. While then $D_T = D(\mu)$ at $T = 0$, at finite temperatures the van Hove singularities of the DOS appear as finite peaks in the TDOS.

The relationship between DOS and TDOS becomes much more complicated for interacting electrons, since the DOS itself depends on μ. The TDOS can have even negative values, as has been shown in several experiments, both on Si metal-oxide-semiconductor field-effect transistors (Ref. 33) and on GaAs/$Al_xGa_{1-x}As$ heterostructures,[34,35] and also in Efros' calculations,[36,37] based on an empirical parameterization of sophisticated numerical calculations of the total energy of the homogeneous system as a function of the filling factor.

The Hartree-Fock approximation provides a less sophisticated (and also for pure homogeneous systems at very low temperatures less reliable) approach, but it also yields negative TDOS at low temperatures. This has been shown by a recent model calculation neglecting spin but including disorder effects.[30] Results within our model, neglecting disorder but taking into account the spin effects, are shown in Fig. 4. The Landau levels (dashed lines) are shown together with the chemical potential (solid line) and are plotted in units of the cyclotron energy. If Coulomb effects were neglected, the Landau levels would appear in this plot as spin-degenerate horizontal lines at values $n + 1/2$. In the presence of interaction, the unoccupied Landau levels approach these values in the limit of large magnetic field. In the absence of the modulation the exchange energy (2.5) is a linear combination—with negative coefficients—of the partial filling factors of the occupied Landau levels, and the Hartree energy is zero in Eq. (2.1). As a consequence, in the plot of Fig. 4 the HF energies decrease with decreasing B and, for constant n_e, the chemical potential decreases with increasing filling factor. This results in negative values of the TDOS. In homogeneous GaAs

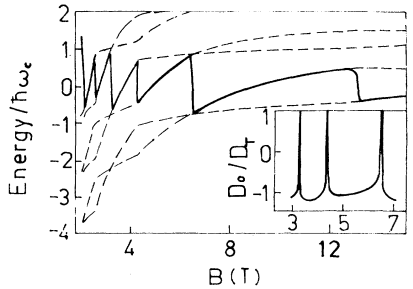

FIG. 4. The chemical potential (solid line) and the Landau levels with $n = 0, 1, 2$ (dashed lines), in magnetic units, versus the magnetic field, for a homogeneous system, in the Hartree-Fock approximation. Inset: the inverse of the TDOS in the $n = 1$ Landau level. $T = 1$ K.

the TDOS in the second Landau level ($n = 1$) ceases to be positive definite for $T < 27$ K. Since the TDOS changes sign with a polelike behavior, we prefer to plot its inverse $1/D_T$, which varies continuously through zero, see inset of Fig. 4.

In Fig. 5 the inverse of the TDOS, in units $D_0 \equiv m_{\rm eff}/(2\pi\hbar^2)$, is shown for a short modulation ($a = 80$ nm) which produces distinct (nonoverlapping) Landau bands.

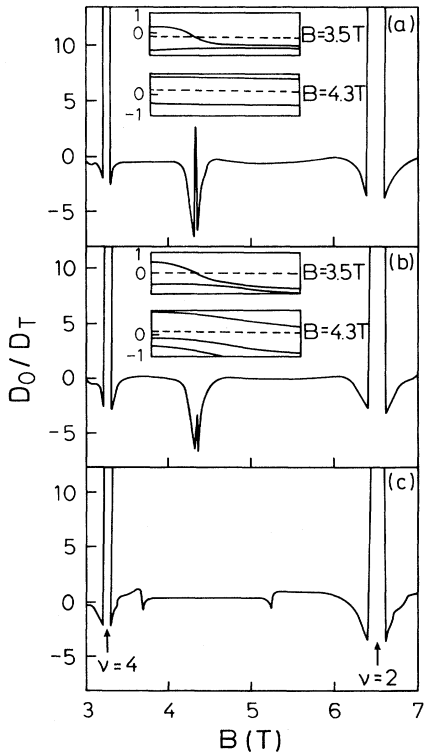

FIG. 5. The inverse of the TDOS in the $n = 1$ Landau level vs the magnetic field, for a modulation with $a = 80$ nm and (a) $V = 0.5$ meV, (b) $V = 5$ meV, (c) $V = 10$ meV. Insets in (a) and (b): Landau bands with $n = 1$ and chemical potential (dashed lines) between van Hove singularities. Two complete band structures for (c) can be seen in Fig. 1(a) and 1(b). $T = 1$ K.

The insets show, for some characteristic values of the magnetic field, the position of the relevant bands (with $n = 1$) relative to the Fermi level. Even for very small amplitudes, $V \ll \hbar\omega_c$, the width of the partially occupied Landau bands can be comparable with the cyclotron energy, due to the strong exchange energy, as discussed in Sec. III. Therefore, the van Hove singularities of the DOS can be well observed even in Fig. 5(a), where they appear as sharp minima of D_0/D_T with negative values. The upper part of the inset of Fig. 5(a) demonstrates the exchange broadening of the partly occupied upper spin band for a filling factor slightly smaller than 4. The lower part demonstrates the well developed spin gap at filling factor $\nu = 3$ ($B = 4.33$ T). At the temperature 1 K chosen in this calculation, this spin gap leads to the sharp upward spike of D_0/D_T at $B = 4.33$ T with positive values near the maximum. The fact that this structure is much narrower that those at $B = 3.25$ T ($\nu = 4$) and $B = 6.50$ T ($\nu = 2$) indicates that the effective spin gap is still much smaller than the effective Landau gaps, which are also enhanced by the exchange. Increasing the modulation amplitude to values comparable with $\hbar\omega_c$, does not change this picture qualitatively as long as the spin-split bands do not yet overlap. As is seen in Fig. 5(b), only the spike structure at $\nu = 3$ is smeared out since the global (indirect) effective spin gap becomes smaller (lower panel of inset). If we increase the modulation amplitude further, we come to a situation depicted in Fig. 5(c). Here, the two spin bands with Landau quantum number $n = 1$ overlap, i.e., there is no global spin gap left for $\nu = 3$, whereas the Landau gaps at filling factors $\nu = 4$ and $\nu = 2$ still remain. The sharp minima in Fig. 5(c) are easily understood from Fig. 1. As the magnetic field is increased above $B = 3.24$ T, the Fermi level moves from above into the upper spin band with $n = 1$ [see Fig. 1(b)] and then, at $B = 3.68$ T through the top of the lower spin band with $n = 1$ into a situation as shown in Fig. 1(a). At $B = 5.24$ T the Fermi level moves through the lower edge of the upper spin band. Between $B = 5.24$ T and $B = 6.5$ T only the lower spin band of the $n = 1$ Landau band is partially occupied. Thus, the minima at 3.3 T and 3.7 T can be interpreted as the spin-split van Hove singularity of the high-energy band edge and those at 5.2 T and 6.4 T as the spin-split van Hove singularity of the low-energy band edge of the $n = 1$ Landau band. The asymmetry of D_T^{-1} has several reasons. First, the temperature and the modulation amplitude are kept constant in absolute units, but in relative units they decrease with increasing magnetic field. Second, the number of states per Landau band increases with increasing B. Finally, for the short-wavelength modulation under consideration, the width of the $n = 1$ Landau band increases with increasing B, see Eq. (A5).

As a more complicated example we consider in Fig. 6 a long-wavelength modulation, $a = 300$ nm, with a large amplitude, $V = 50$ meV, at a higher temperature than before, $T = 5$ K, so that the CDW-like oscillations are practically suppressed. The Landau bands overlap strongly, and the van Hove singularities can be identified only with the help of the calculated band structures.

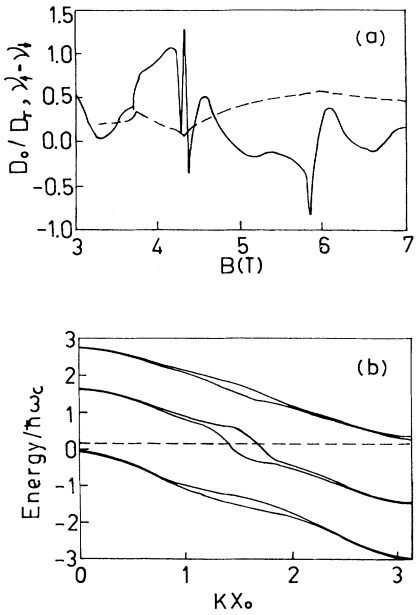

FIG. 6. (a) The inverse of the TDOS (solid line) and the spin polarization (dashed line), for a modulation with $a = 300$ nm and $V = 50$ meV. $T = 5$ K. (b) The corresponding band structure for $B = 4.3$ T.

In Fig. 6(a), they yield four sharp minima of D_T^{-1} arising when the Fermi level crosses maxima (at $X_0 = 0$) or minima (at $X_0 = a/2$) of the spin-split Landau bands. The quantum numbers (n, X_0, σ) of the corresponding HF single-particle states are $(2, a/2, \downarrow)$ for $B \approx 3.7$ T, $(2, a/2, \uparrow)$ for $B \approx 4.3$ T, $(0, 0, \downarrow)$ for $B \approx 4.4$ T and $(1, a/2, \downarrow)$ for $B \approx 5.9$ T [see Fig. 6(b)]. The origin of the additional broad minima of D_T^{-1} is the strong screening of the external modulation. The energy dispersion flattens near the Fermi level, Fig. 3, when the latter moves toward the middle of a Landau band. Consequently, both the DOS and the TDOS increase, and the van Hove peaks may be obscured, if the thermal energy is not sufficiently low in magnetic units, as for $B \approx 3.7$ T.

It is interesting to notice that the fluctuations of the spin polarization are closely related to the van Hove singularities of the DOS. In Fig. 6(a), the extrema of $\nu_\uparrow - \nu_\downarrow$ are associated with the sharp minima of D_T^{-1}. Therefore the interpretation of the oscillations of the TDOS, obtained from magnetocapacitance measurements, might be facilitated by supplementary spin-resonance experiments.

V. SUMMARY AND CONCLUSIONS

The spin splitting of the Landau bands produced by a periodic unidirectional lateral modulation has been studied in the Hartree-Fock approximation. To facilitate the numerical calculations, as an additional approximation the HF wave functions have been replaced by the unperturbed Landau wave functions. This is a reasonably good approximation if the potential is sufficiently smooth on

the scale of the magnetic length, and a sufficient approximation for the present qualitative investigation.

At low temperatures, the self-energy of the state $|n, X_0, \sigma\rangle$ is lowered by the exchange term of the Coulomb interaction. The amount of lowering depends on the extent to which in a certain interval $\mathcal{S}(X_0)$ around X_0, typically a few magnetic length wide, the states $|n', X_0', \sigma\rangle$ with the same spin quantum number σ and with various Landau quantum numbers n' are occupied. The largest contribution to this energy lowering comes from the states $|n, X_0', \sigma\rangle$. The exchange enhanced spin splitting at X_0 is maximum, if in this interval all states $|n, X_0', \uparrow\rangle$ are occupied and all states $|n, X_0', \downarrow\rangle$ are empty. This requirement on the occupation numbers is, in turn, a requirement on the effective spin gap in that interval: it requires that the highest energy of the $|n, X_0', \uparrow\rangle$ states in this interval falls below and the lowest energy of the $|n, X_0', \downarrow\rangle$ states lies above the Fermi energy. Whether this requirement can be satisfied, depends on the steepness of the externally applied potential, which ultimately determines the steepness of the energy dispersion. Apparently the condition for the appearance of a maximum spin gap Δ [$\approx e^2/\kappa l$, see Eq. (1.1)] at X_0 is that the total variation of the Hartree-Fock energy $E^{(HF)}_{nk'\uparrow}$ with $X_0' = -l^2k'$ in the interval $\mathcal{S}(X_0)$ is less than Δ. If the steepness of the external potential $V_{\text{ext}}(x)$ becomes so large that this condition gets violated, only a part of the states in the interval $\mathcal{S}(X_0)$ can contribute to the enhancement of the spin gap at X_0, and the latter will be rapidly suppressed with further increasing steepness of $V_{\text{ext}}(x)$. It is obvious that the condition for maximum enhancement of the spin gap is a local one: if $V_{\text{ext}}(x)$ is sufficiently steep, only a strip of X_0 values (in each unit cell of the periodic external potential) corresponding to HF energies near the Fermi energy will show the enhanced spin gap. With increasing steepness the width of this strip will shrink. With decreasing steepness this strip will become wider, and eventually it may exhaust the whole unit cell of the periodic modulation.

It is very difficult to go beyond this qualitative discussion and give simple quantitative criteria which the external periodic potential should meet to guarantee exchange enhancement of spin splitting. The problem is that the simple criterion, which can be formulated for the dispersion of the HF energies, contains already in a complicated manner the effects of nonlinear screening and exchange. In order to present quantitative results, we have therefore illustrated the general trends by numerical calculations for a few typical situations. The calculated energy spectra show strips in which the spin gap is enhanced. The width of these intervals increases with increasing wavelength a and with decreasing amplitude V of the external periodic potential. In GaAs, for $a < 100$ nm the enhancement of the spin-splitting starts to be suppressed when $V \sim \hbar\omega_c$. For long-wavelength modulations, i.e., $a \sim 500$ nm in GaAs, the spin-splitting enhancement is much more stable when V increases, and, due to strong screening, the spin-split electronic states remain pinned in the vicinity of the Fermi level. In this case, the system may be considered locally homogeneous. For the situations we considered, the resulting "compressible" strips are much narrower than the incompressible ones, and for a sufficiently large modulation they may be spin polarized.

In addition to the energy spectra we have calculated the thermodynamic density of states, which is experimentally accessible by magnetocapacitance measurements. At temperatures $\sim$ 1 K, the van Hove singularities of the density of states are reflected in the thermodynamic density of states as sharp peaks. For modulations with short wavelengths and amplitudes preserving the gaps between the Landau bands with different Landau quantum numbers n, we have investigated in some detail the region of the Landau bands with $n = 1$. We obtain an internal four-peak structure in different situations. Due to exchange effects, an enhanced spin gap survives at filling factor $\nu = 3$ up to relatively large modulation amplitudes, see Fig. 5, so that two spin bands with internal van Hove singularities result. At still larger modulation the two spin bands overlap and no global spin gap survives. The locally enhanced spin splitting then leads to spin-split van Hove singularites. At higher temperature or as a consequence of collision broadening effects (which we have not included in our calculations), the spin gap found in the case of weaker modulation may be smeared out, so that an internal three-peak structure might result.

For long modulations, the Landau bands are strongly distorted, due to the screening effects, and the van Hove singularities in the TDOS alternate with broad maxima, due to pinning of Landau bands at the Fermi level, which eventually might even hide the former. However, even in this situation the top and the bottom of the Landau bands can in principle still be identified in the oscillations of the spin polarization.

In conclusion, the interplay of screening, exchange, and lateral modulation leads to a rather complicated Landau band structure, which may depend drastically on the filling factor. One would expect that, at finite temperature and collision broadening, Shubnikov–de Haas peaks in the magnetoresistance or the corresponding peaks in the magnetocapacitance should show a complicated internal structure, depending on whether the enhanced spin splitting or the van Hove singularities, or both, are resolved. In the case of long-wavelength modulation, screening effects (pinning) may even lead to additional structure. This emphasizes that for a proper understanding of the magnetotransport measurements[6] a realistic transport calculation including the modulation potential, the Coulomb interactions, and the collision broadening is inevitable.

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APPENDIX A: FOURIER EXPANSION OF THE LANDAU BANDS

The symmetries of the external potential, being independent of y and periodic in x with period $a = 2\pi/K$,

are reflected in the particle density, which we expand in a Fourier series of the form

$$\rho(\mathbf{r}) = \sum_{m\geq 0} \rho_m \cos(mKx) \ . \tag{A1}$$

Since the HF energy eigenvalues are periodic in the center coordinate $X_0 = -kl^2$, similar Fourier expansions can be adopted in the reciprocal space, i.e., for the occupation factors,

$$\mathcal{F}_{nk\sigma} = \sum_{m\geq 0} f_{nm\sigma} \cos(mKl^2k), \tag{A2}$$

where, obviously, $f_{n0\sigma}$ is the filling factor of the band

$$E^{(HF)}_{nk\sigma} = \sum_{m\geq 0} \epsilon_{nm\sigma} \cos(mKl^2k). \tag{A3}$$

We replace the HF wave functions by the unperturbed Landau wave functions. Then, using Eqs. (2.4) and (A2), we obtain

$$\rho_m = \frac{1}{2\pi l^2} \sum_{n\sigma} f_{nm\sigma} A_n(mlK) \cos(mKx) \ , \tag{A4}$$

where we have explicitly exploited the properties of the Landau wave function, and introduced the notation $A_n(x) = \exp(-x^2/4)L_n(x^2/2)$, L_n being the Laguerre polynomials.[38] Furthermore, the noninteracting terms of the energy bands, Eq. (2.2) with the Landau wave functions, contribute in Eq. (A3) only in the first two terms, with $m = 0, 1$:

$$E^{(0)}_{nk\sigma} = (n + \tfrac{1}{2} - \tfrac{1}{2}\gamma\sigma)\hbar\omega_c + V\cos(Kl^2k)A_n(lK). \tag{A5}$$

The Hartree term, Eq. (2.3), has the expansion

$$E^{(H)}_{nk} = \frac{2\pi}{K}\frac{e^2}{\kappa} \sum_{m\geq 1} \frac{\rho_m}{m} \cos(mKl^2k) A_n(mlK), \tag{A6}$$

the term with $m = 0$ being absent due to the neutrality condition.

The Fourier coefficients of the exchange energies will be determined by those of the Fermi functions, since the former can be written as sums of convolution products of the latter with some combinations of modified Bessel functions K_0 and K_1:[38]

$$E^{(F)}_{nk\sigma} = -\frac{e^2}{2\pi\kappa} \sum_{n'} \int dk' \, \mathcal{F}_{n'k'\sigma} \, e^{-l^2(k-k')^2/4} \times \mathcal{J}_{nn'}[l^2(k-k')^2/4], \tag{A7}$$

where, e.g., for the first two Landau levels,

$$\mathcal{J}_{00}(x) = K_0(x) \tag{A8}$$

and

$$\mathcal{J}_{10}(x) = \mathcal{J}_{01}(x) = x[K_0(x) + K_1(x)],$$
$$\mathcal{J}_{11}(x) = (1 - 2x + 2x^2)K_0(x) - (x - 2x^2)K_1(x). \tag{A9}$$

In the absence of the modulation $\mathcal{F}_{n'k'\sigma} \equiv \nu_{n'\sigma}$ and Eq. (A7) leads to Eq. (1.1). The maximum spin-splitting enhancement occurs in the lowest Landau band, $c_{00} = \sqrt{\pi/2}$, while for the second band $c_{11} = 3c_{00}/4$, and $c_{10} = c_{01} = c_{00}/2$.

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