Screening of an impurity in a two-dimensional electron gas within the Hartree and the Hartree-Fock approximation in the quantum Hall regime

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We investigate the static nonlinear screening of a single point charge (Coulombic impurity) by a two-dimensional electron gas (2DEG) in a strong perpendicular magnetic field at low temperature. The electron-electron interactions are treated in the Hartree-Fock approximation (HFA). The results are compared to earlier results for Hartree interacting electrons showing quite different screening properties due to the enhancement of the spin splitting of the Landau levels within the HFA. The possibility of different occupation of the spin levels of the impurity and the surrounding 2DEG is discussed in light of experiments.

I. INTRODUCTION

The screening of impurities by a two-dimensional electron gas (2DEG) has been studied in strictly 2D models in zero magnetic field B, showing clearly the differences between screening in two and three dimensions.[1] The impurity screening has also been investigated in quasi two-dimensional electron systems where the influence of the surrounding heterostructure is accounted for.[2] Measurements of the electrical conductivity of a 2DEG and the broadening of the Landau levels in the quantum Hall regime have spurred an interest in the effects of randomly distributed impurities on the properties of the 2DEG.[3–7]

The effects of the position of impurities in quantum wells and the influence of the width of the wells on their ionization energy has been studied systematically with far infrared spectroscopy.[8,9] Many researchers[10–13] have followed in the footsteps of Bastard,[14] using variational methods to study the dependence of the impurity spectra on the location of the impurity within the quantum well. The model has been extended to account for the band structure and further details of the heterostructure. A similar model has also been investigated in the presence of a perpendicular magnetic field.[15]

How the energy spectrum of an impurity in a lightly doped quantum well is influenced by the magnetic field and the density $\bar{n}_s$ of the two-dimensional electron gas has not been measured to the best of our knowledge. These nonlinear screening effects have been studied within the Hartree approximation for the electron-electron interaction, yielding impurity spectra that oscillate with the occupation of the Landau levels of the surrounding 2DEG.[16–18] Analytical results have also been achieved in the limit of a strong magnetic field and few electrons.[19]

The spin of the electrons has been neglected in these Hartree approximations, but on the other hand there is experimental evidence that the spin and the enhancement of the spin splitting may be very important in lightly doped quantum wells.[20] Here, we shall study the effects of the 2DEG on the impurity spectra both in the Hartree (HA) and the Hartree-Fock approximation (HFA). We will thereby show the importance of the exchange interaction between the electrons, which is responsible for the drastic difference in the screening behavior for the two approximations. In GaAs the effective Landé g factor is so small ($g = -0.44$) that the HA results in almost spin degenerate Landau bands. In contrast, the HFA yields a strong spin splitting of the Landau bands, which has been observed in experiments of the quantum Hall effect, when an odd number of spin Landau bands is occupied. This spin splitting causes the density of states (DOS) at the chemical potential μ to be very different for the two models around values of the magnetic field or the electron density that lead to the occupation of an odd number of spin Landau bands. A high density of states around the chemical potential means the 2DEG has many states over which to redistribute itself in order to effectively screen any external potential, but a low DOS at μ impairs the ability of the 2DEG to screen.[5,6,21–23]

II. MODEL

The model consists of a single Coulomb potential of a point charge

$$V_{\rm imp}(r) = \sigma \frac{e^2}{\kappa r} \tag{1}$$

representing a simple donor ($\sigma = +1$) or an acceptor ($\sigma = -1$) impurity situated in the plane of a 2DEG and a homogeneous positive background charge n_b. κ is the dielectric constant of the surrounding medium. Here we consider a strictly two-dimensional electron system to model qualitatively a real heterostructure where the 2DEG is confined to the lowest electrical subband. To facilitate a numerical approach to the problem we confine the 2DEG to a finite system by cutting off the neutralizing background charge at a radius R, that is considerably larger than both the effective Bohr radius $a_0^* = (\hbar^2\kappa/m^*e^2)$ and the cyclotron radius $l = (\hbar c/eB)^{\frac{1}{2}}$.

In addition the electrons are confined by a potential step $V_{\rm conf}(r)$ at the same radius R. Thus, the average electron density in the system is $\bar{n}_s = N_s/(\pi R^2)$, where N_s is the total number of electrons present in the system. In the Hartree-Fock approximation the state of each electron is described by a single-electron Schrödinger equation,

$$\{H^0 + V_H(r) + V_{\rm imp}(r) + V_{\rm conf}\}\psi_\alpha(\vec{r}) - \int d^2r'\,\Delta(\vec{r},\vec{r}\,')\psi_\alpha(\vec{r}\,') = \epsilon_\alpha\psi_\alpha(\vec{r}) \quad (2)$$

for an electron moving in a Hartree potential

$$V_H(r) = \frac{e^2}{\kappa}\int d^2r'\frac{n_s(r') - n_b(r')}{|\vec{r} - \vec{r}\,'|} \quad (3)$$

and a nonlocal Fock potential with

$$\Delta(\vec{r},\vec{r}\,') = \frac{e^2}{\kappa}\sum_\beta f(\epsilon_\beta - \mu)\frac{\psi^*_\beta(\vec{r}\,')\psi_\beta(\vec{r})}{|\vec{r} - \vec{r}\,'|}, \quad (4)$$

which is neglected in the Hartree approximation. Here $f(\epsilon_\beta - \mu)$ is the Fermi distribution at the finite temperature T. $n_s(r)$ is the electron density

$$n_s(r) = \sum_\alpha |\psi_\alpha(\vec{r})|^2 f(\epsilon_\alpha - \mu), \quad (5)$$

with the chemical potential μ. The label α represents the radial quantum number n_r, the angular quantum number M, and the spin quantum number $s = \pm\frac{1}{2}$. H^0 is the single particle Hamiltonian for one electron with spin in a constant perpendicular external magnetic field.[24,17] A Landau band index n can be constructed from the quantum numbers n_r and M as $n = (|M| - M)/2 + n_r$, whereby the values of M are limited to the range $-n \leq M < \infty$ within the nth Landau band. The Landau levels of H^0 with energy $E_{n,M,s} = \hbar\omega_c(n + \frac{1}{2}) + sg^*(\mu_B/\hbar)B$ are degenerate with respect to M with the degeneracy $n_0 = (2\pi l^2)^{-1}$ per spin orientation. μ_B is the Bohr magneton $(e\hbar/2mc)$. The filling factor of Landau levels is defined by $\nu = n_s/n_0 = 2\pi l^2\bar{n}_s$. It assumes even integer values when an even number of spin Landau levels is filled. The cyclotron frequency is given by $\omega_c = eB/(mc)$. The neutralizing background charge is a smooth function of r,

$$n_b(r) = \left(\bar{n}_s - \frac{\sigma}{\pi R^2}\right)\left[\exp\left(\frac{r - R}{\Delta r}\right) + 1\right]^{-1}, \quad (6)$$

and the confinement potential step is

$$V_{\rm conf}(r) = U_0\left[\exp\left(\frac{R - r}{4\Delta r}\right) + 1\right]^{-1}, \quad (7)$$

where $\Delta r = 22$ Å. The calculations are carried out with GaAs parameters: $m^* = 0.067m_e$, $\kappa = 12.4$, and $g^* = -0.44$. Then the effective Bohr radius is $a_0^* \approx 97.9$ Å and the effective Rydberg energy is $E^*_{\rm Ryd} \approx 5.92$ meV. For the magnetic field $B = 3$ T the cyclotron radius is $l \approx 148$ Å and $\hbar\omega_c \approx 5.2$ meV. A sufficient height of the potential step is then $U_0 = 60$ meV. The system radius R is selected large enough to prevent influence of the finite size on the energy spectrum of the impurity, so we set $R \leq 1000$ Å.

The Hartree-Fock energy spectrum ϵ_α and the corresponding wave functions are now found by solving (2)–(7) iteratively in the basis[16,17,25] of H^0. The Hartree interaction V_H does not mix states of the basis with different M quantum numbers. The matrix elements of the interacting Hamiltonian are thus diagonal with respect to M. It has, therefore, only to be diagonalized with respect to n_r and s within each iteration step. The "kernels" of the interaction, $n_s(r)$ and $\Delta(\vec{r},\vec{r}\,')$, carry the effects of all the other M states on a certain M state.

The chemical potential μ is recalculated in each iteration in order to preserve the total number of electrons N_s. The number of basis functions used in the diagonalization is chosen such that a further increase of the subset results in an unchanged density $n_s(r)$.

III. RESULTS

In order to vary the occupation of the Landau bands the magnetic field is held at $B = 3.0$ T while the elec-

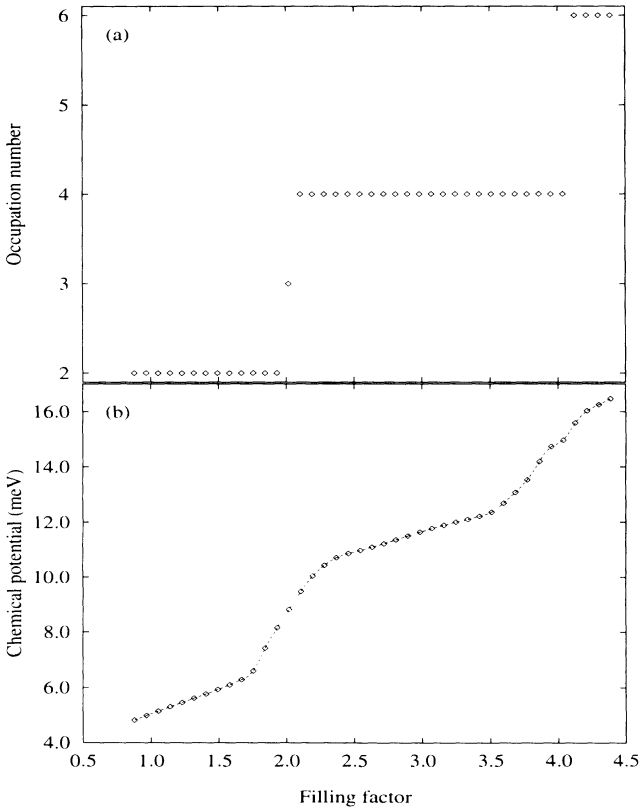

FIG. 1. (a) The occupation of the $M = 0$ states and (b) the chemical potential μ as functions of the average filling factor ν of the Landau bands for the model with a donorlike impurity ($\sigma = +1$) within the Hartree approximation at $T = 1.0$ K. $R = 1000$ Å, $U_0 = 60$ meV, and $B = 3.0$ T. GaAs bulk parameters: $m^* = 0.067m_0$, $\kappa = 12.4$, $g^* = -0.44$.

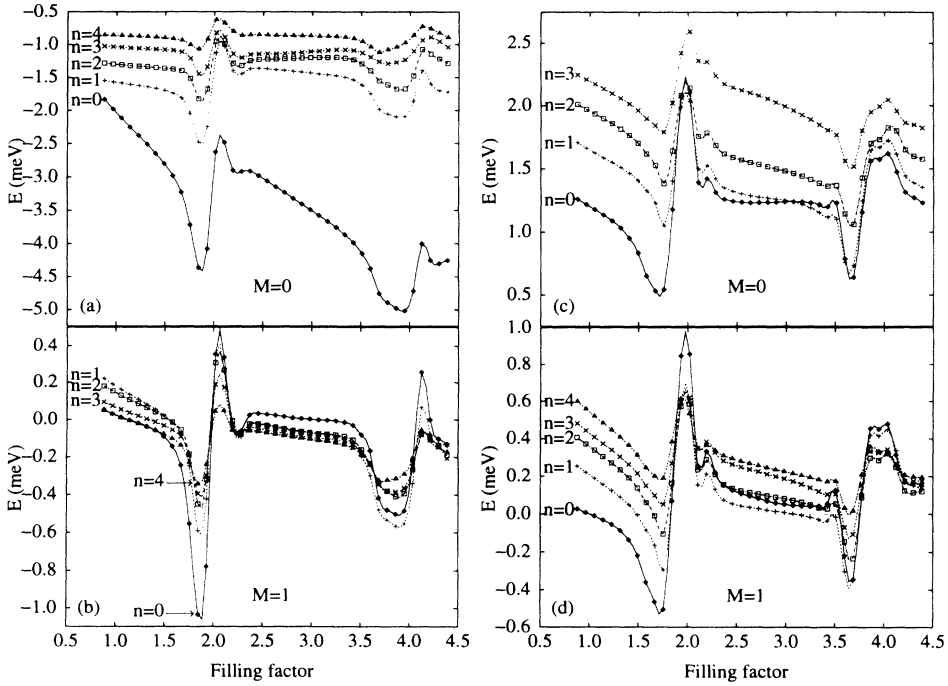

FIG. 2. Energy shift in the Hartree approximation of (a) the $M = 0$ and (b) the $M = 1$ states as a function of ν for a donorlike impurity ($\sigma = +1$) present in the system. Energy shift in the Hartree approximation of (c) the $M = 0$ and (d) the $M = 1$ states as a function of ν for an acceptorlike impurity ($\sigma = -1$) present in the system. The Landau band index n is indicated in the figure. $T = 1.0$ K. Other parameters are as in Fig. 1.

tron number N_s [or the average electron density $\bar{n}_s = N_s/(\pi R^2)$] is varied. In the Hartree approximation the Landau bands will be almost degenerate inside a system without an impurity, thus closely approaching flat Landau levels. It is therefore possible to use the average filling factor $\nu = 2\pi l^2 \bar{n}_s$ to describe the occupation of the lower bands in the interior of the system. For $B = 3.0$ T and $g^* = -0.44$ the spin splitting of the Landau bands $(g^*\mu_B/\hbar)B \approx 0.076$ meV corresponding to k_BT at the temperature $T \approx 0.88$ K is much smaller than their separation $\hbar\omega_c \approx 5.2$ meV corresponding to k_BT at $T \approx 60$K. In previous publications[16,17] the properties of the model

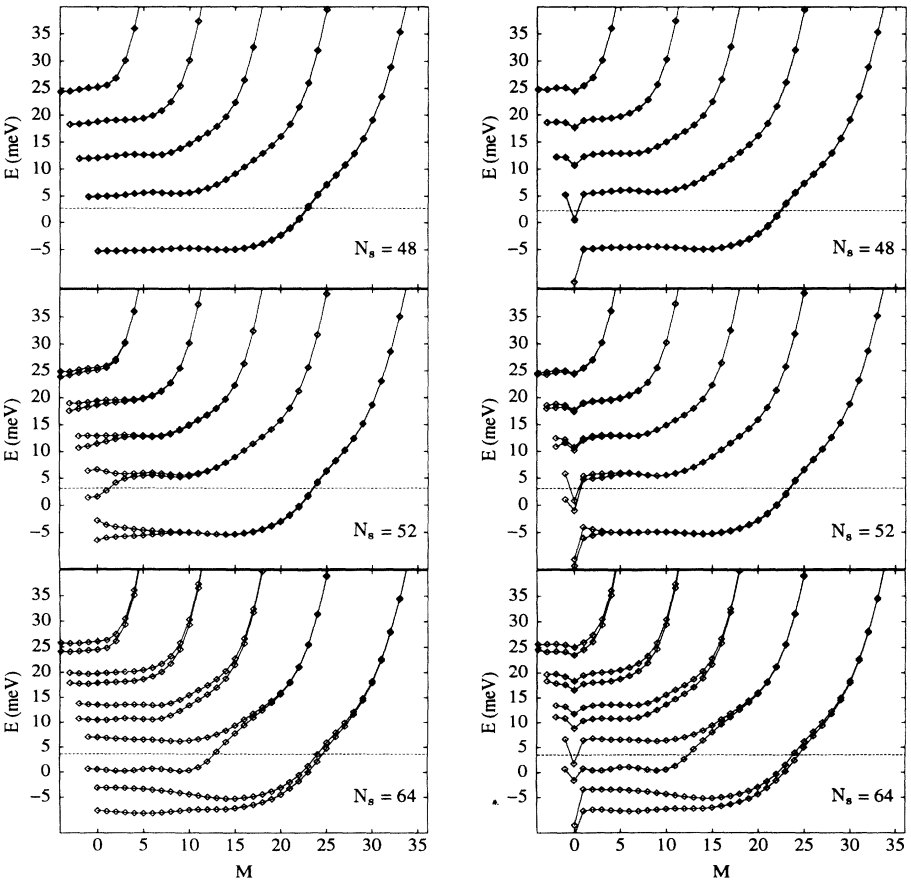

FIG. 3. Energy spectra and chemical potential μ (dashed line). The total number of electrons N_s is indicated in each subfigure. The left figures are for the system without an impurity ($\sigma = 0$) and the right figures show the system with one donorlike impurity ($\sigma = +1$). Other parameters are as in Fig. 1.

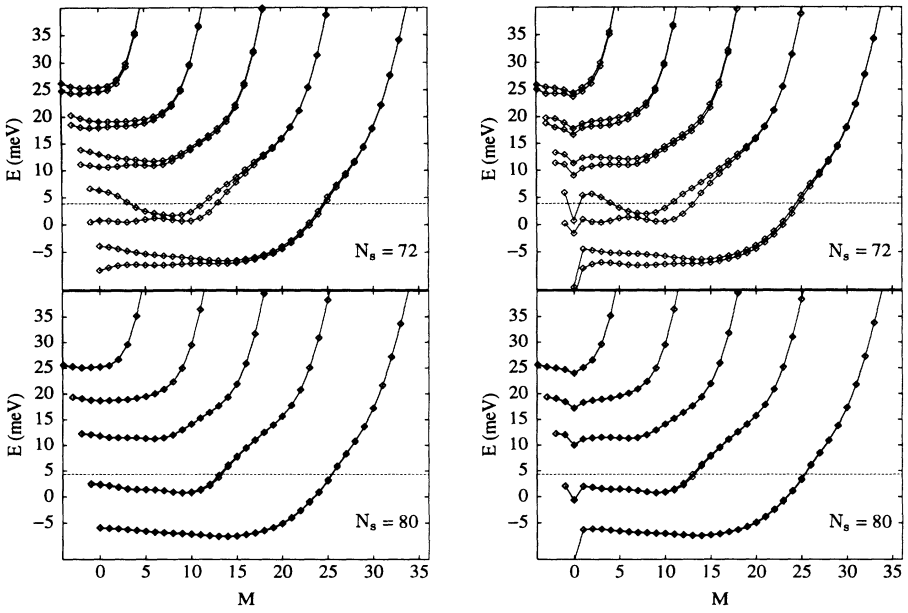

FIG. 4. Energy spectra and chemical potential μ (dashed line). The total number of electrons N_s is indicated in each subfigure. The left figures are for the system without an impurity ($\sigma = 0$) and the right figures show the system with one donorlike impurity ($\sigma = +1$). Other parameters are as in Fig. 1.

within the HA have been detailed when ν has been varied by keeping $\bar{n}_s$ constant but changing B and neglecting the spin degree of freedom. Here we will shortly discuss the results of the HA in the present model, mainly in order to be able to compare to the different results of the HFA in the same model.

A. The Hartree approximation

In Figs. 1(a) and 1(b) the occupation of a donorlike impurity and the chemical potential μ are seen, respectively, as functions of the filling factor ν at the temper-

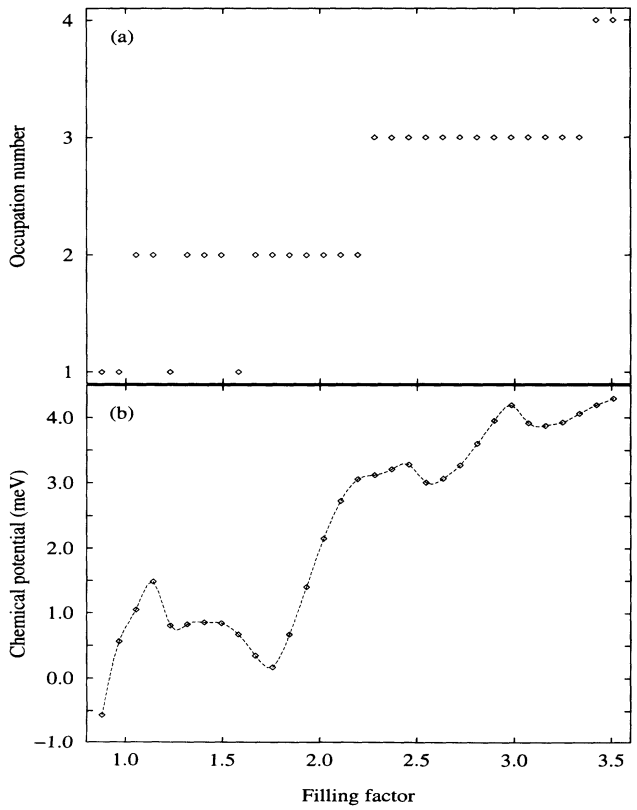

FIG. 5. (a) The occupation of the $M = 0$ states and (b) the chemical potential μ as functions of the average filling factor ν of the Landau bands for the model without an impurity ($\sigma = 0$) within the Hartree-Fock approximation at $T = 10.0$K. Other parameters are as in Fig. 1.

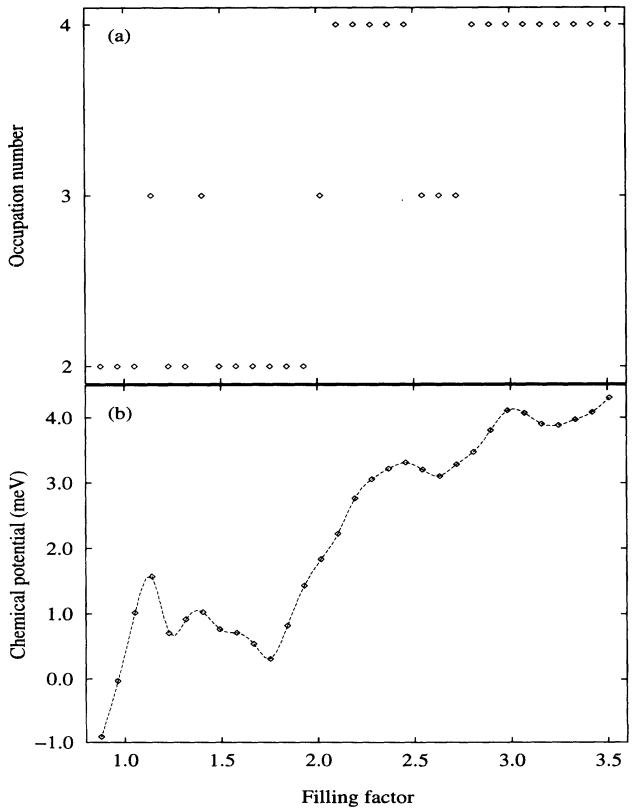

FIG. 6. (a) The occupation of the $M = 0$ states and (b) the chemical potential μ as functions of the average filling factor ν of the Landau bands for the model with a donorlike impurity ($\sigma = +1$) within the Hartree-Fock approximation at $T = 10.0$ K. Other parameters are as in Fig. 1.

ature $T = 1.0$ K. As expected, there are steps in μ at even integer filling factors, when it "jumps" between almost spin degenerate Landau bands. The jumps are not abrupt because of the existence of edge states in the gap between bulk Landau levels.[16,17] When $\nu > 2$ the $M = 0$ states are occupied by two electrons of opposite spin orientations, or in other words, the impurity "binds" two electrons. The occupation of the impurity (or the $M = 0$ states) changes whenever ν becomes larger than an even integer. For the largest part of the ν range the impurity is not spin polarized, since the two spin states are almost degenerate in energy.

When an impurity represented by the potential $V_{\rm imp}$ in (1) is added to the system the main change in the energy spectrum is a shift of the states around $M = 0$ up or down depending on the sign σ of the charge of the impurity. The influence is largest for the $M = 0$ states since only the wave functions for these states do not vanish for $r = 0$, in the neighborhood of which the potential $V_{\rm imp}$ is strongest. Figures 2(a) and 2(b) show this energy shift for the $M = 0$ and the $M = 1$ states due to the presence of a donorlike impurity ($\sigma = +1$) in the system. For the $M = 0$ states [Fig. 2(a)] the shift is always negative and peaks for even values of ν (when μ is situated between Landau bands), reflecting the poor screening of $V_{\rm imp}$ when few states are available around μ for the electrons to redistribute themselves. On the other hand the screening is strong for other values of ν where the 2DEG has enough states available within k_BT from μ to redistribute itself. The screening at even integer values of ν does not vanish due to the nonlinear screening properties of the model.[22,21,26] The $M \neq 0$ states are not necessarily shifted in the same direction as the $M = 0$ states due to the characteristic overscreening in two-dimensional electron systems.[16,18] The corresponding energy shifts for an acceptorlike impurity ($\sigma = -1$) are presented in Figs. 2(c) and 2(d).

B. The Hartree-Fock approximation

The energy spectra for the 2DEG with and without a donorlike impurity at the center are shown in Figs. 3 and 4 for $T = 10.0$ K in the Hartree-Fock approximation. The discontinuity in the slope of a Landau band where it crosses μ is a well known property of the Hartree-Fock approximation for an electron gas where the electrons interact through the Coulomb interaction. For $N_s = 48$ or $\nu \approx 2.1$ in Fig. 3 we see that μ is in between almost spin degenerate flat Landau bands (LB's). For $N_s = 52$ or $\nu \approx 2.3$, μ is approaching the second LB, the states with $s = +1/2$ and $M = -1, 0, 1$ are occupied. This partial spin polarization of the second LB causes the self-energy of the electrons to be spin dependent due to the exchange potential. This in turn, causes the spin splitting of the LB's to be strongly enhanced.[27,25] The spin splitting has attained its maximum around $N_s = 64$ or $\nu \approx 2.8$ and decreases with increasing N_s until it vanishes completely for $N_s = 80$ or $\nu \approx 3.5$. The occupation of the $M = 0$ states and μ as functions of ν in the HFA without an

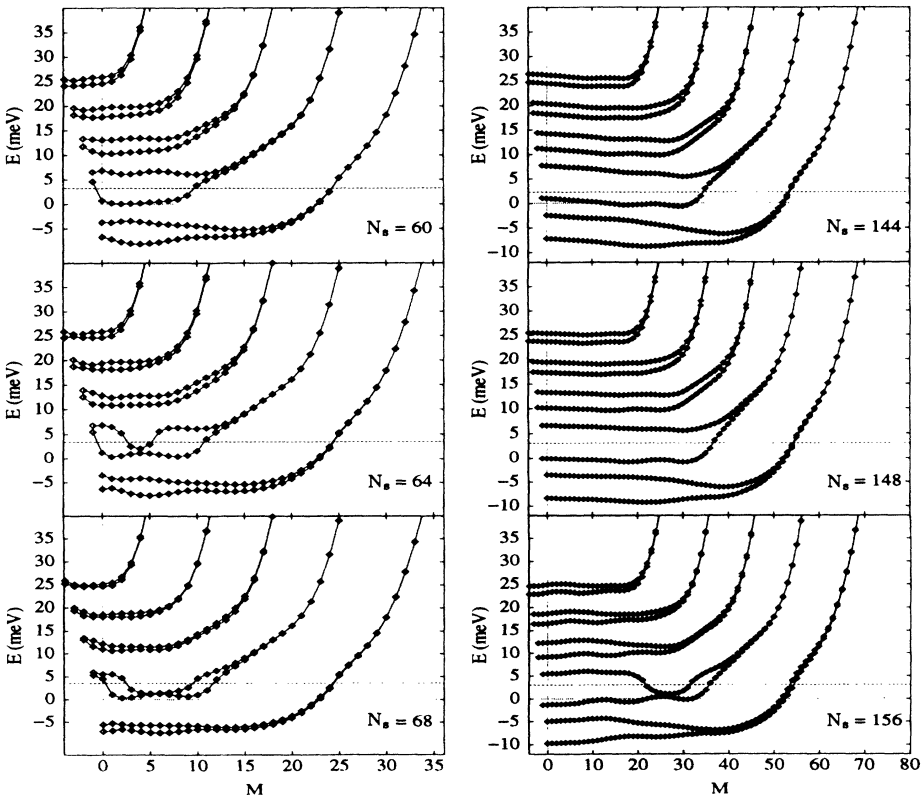

FIG. 7. Energy spectra and chemical potential μ (dashed line) in the Hartree-Fock approximation for $T = 1.0$ K for a system without an impurity. R=1000 Å for the *left* hand figure and R=1500 Å for the *right* hand figure. The total number of electrons N_s is indicated in each subfigure. Other parameters are as in Fig. 1.

impurity present in the system is shown in Fig. 5. The spin splitting of the second LB ($n = 1$) when ν assumes values in a range around $\nu \approx 3$ is evident as the $M = 0$ states are occupied by three electrons in this range. The chemical potential μ has a large step around $\nu = 2.0$ and smaller ones around $\nu = 1$ and 3. The structure of μ is generally more complicated in the HFA than in the HA (Fig. 1). The occupation of the $M = 0$ states in a system with a donorlike impurity (the occupation of the impurity) and μ as functions of ν are seen in Fig. 6. Here μ has the same qualitative features as in a system without an impurity (Fig. 5) but the occupation of the $M = 0$ state is different due to the downward shift of its energy. Further details of Fig. 5 and Fig. 6 will be discussed below.

In Fig. 4 for $N_s = 72$ we see that when μ is moving away from a position in between the LB's with $n = 1$ and of opposite spin orientations, with increasing N_s, then the spin splitting first reduces for a limited range of M values, around $M \approx 4$. In order to confirm that this is not due to the limited number of LB's in the numerical calculations we checked that this happens exactly in the same manner when more LB's are included in the model. The left hand side of Fig. 7 shows the "closing down" of the spin splitting for the same LB, but lower temperature $T = 1.0$K. The initial reduction happens for slightly lower values of the quantum number M and, in addition, the reduction occurs concurrently for $M = 0$. The closing down of the spin splitting for the same LB but a larger system ($R = 1500$ Å) is shown in the right hand side of Fig. 7, where clearly the reduction first appears for much higher values of M, representing states close to the edge of the system. The particular manner of how the spin splitting closes down when μ moves away from LB's with the same n but opposite spin orientations is thus dependent on the size of the system and the temperature.

The total energy of the system is reduced by forming regions of different spin polarization (and charge

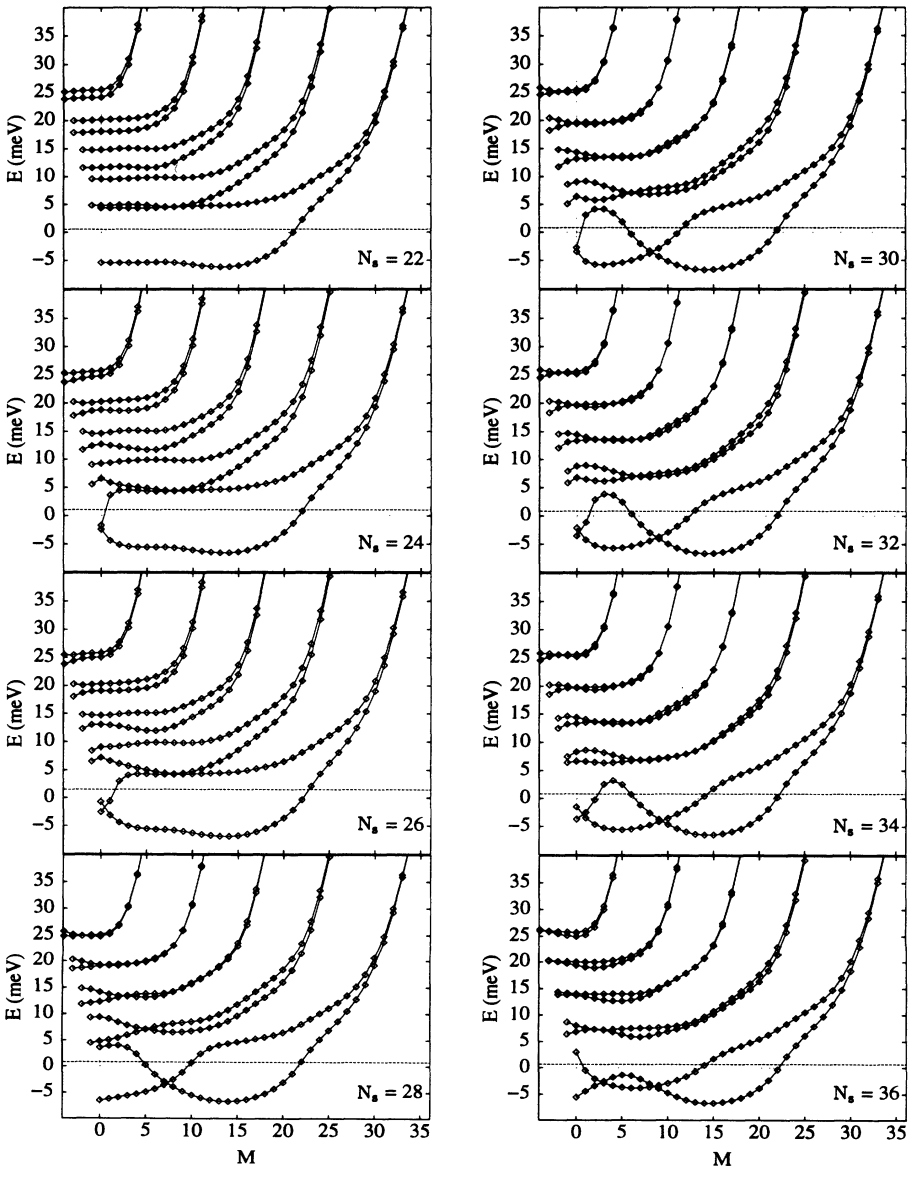

FIG. 8. Energy spectra and chemical potential μ (dashed line) in the Hartree-Fock approximation for $T = 10.0$ K for a system without an impurity. The total number of electrons N_s is indicated in each subfigure. Other parameters are as in Fig. 1.

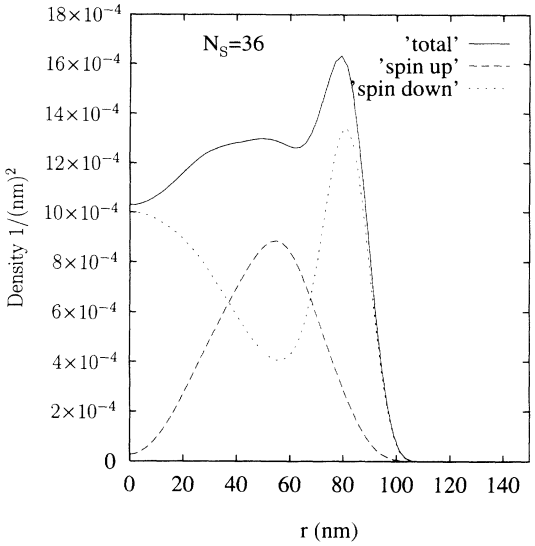

FIG. 9. Total electron density and the electron density for each spin direction as functions of the radius r of the system (Hartree-Fock approximation). $N_s = 36, T = 10.0$ K. Other parameters are as in Fig. 1.

density[28]), a kind of a "spin-density wave."[29] This wave is not the well known charge-density wave, with a constant wavelength, caused by an instability of the homogeneous state in the HFA at a low temperature.[30] The wavelength and character of this spin- or charge-density wave is determined by the size of the confined system. Thus, we are observing a confined spin-density wave in the system.

The situation becomes even more interesting when the closing down of the spin splitting of the lowest LB ($n = 0$) is observed. At low temperature, $T = 1.0$ K, the reduction of the spin splitting starts at certain values of M just as in the next higher LB for the two temperatures we have discussed above ($T = 1.0$ K or 10 K).

The situation for $T = 10.0$ K is presented in Fig. 8. Here the LB's ($n = 0$, $s = -1/2$) and ($n = 0$, $s = +1/2$) do not simply approach one another with increasing N_s but they actually cross forming regions of different spin polarization of the 2DEG as is confirmed in Fig. 9. The effective g factor is not only enhanced, or oscillates as a function of ν, or is modulated inside the system, but it also changes sign within the system.

The reason why this crossing of LB's occurs at higher values of T is connected with the fact that the occupation of states with opposite spin orientations is almost the same, such that small perturbations to the Landau levels can change this occupation ratio differently in different regions of the 2DEG and thus cause the exchange potential to vary strongly with location.[29] For a still higher temperature, when k_BT approaches the inter-Landau-band separation, the occupation difference of the two spin orientations completely vanishes together with the enhancement of the spin splitting.

In the HFA the shift of the ($n = 0, M = 0, s = \pm\frac{1}{2}$) states seen in Fig. 10 due to the addition of an impurity is much more complex than the corresponding shift in the HA (seen in Fig. 2). The enhancement of the spin splitting of the LB's prevents the density of states from becoming high around μ as can happen in the HA. The screening in the HFA therefore does not oscillate as strongly with ν as in the HA. Oscillations in the energy shift of the ($n = 0, M = 0, s = \pm\frac{1}{2}$) states due to oscillations in the screening properties of the 2DEG are thus overwhelmed by oscillations of the enhancement of the spin splitting. In Fig. 10(a) we see that the spin splitting is largest when μ is between the states of the first LB ($n = 0$), i.e., around $\nu \approx 1$. The splitting is smaller when all the states with low M of the first LB are occupied and μ is amongst the states of the second LB. This reflects the general fact seen in many of the energy spectra

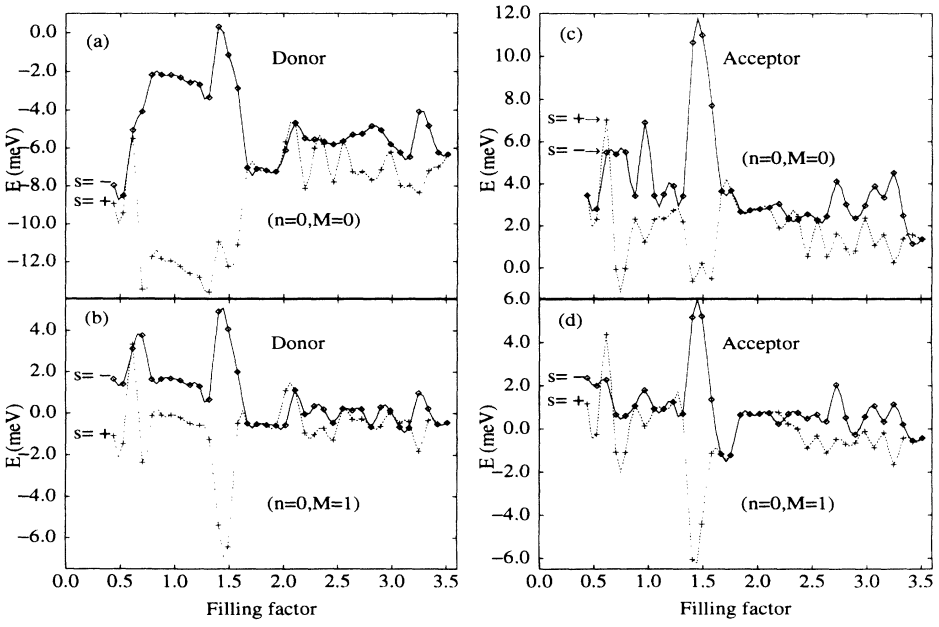

FIG. 10. Energy shift in the Hartree-Fock approximation of (a) the $n = 0, M = 0, s = \pm\frac{1}{2}$ and (b) the $n = 0, M = 1, s = \pm\frac{1}{2}$ states as a function of ν for a donorlike impurity ($\sigma = +1$) present in the system. Energy shift in the Hartree-Fock approximation of (c) the $n = 0, M = 0, s = \pm\frac{1}{2}$ and (d) the $n = 0, M = 1, s = \pm\frac{1}{2}$ states as a function of ν for an acceptorlike impurity ($\sigma = +1$) present in the system. $T = 1.0$ K. Other parameters are as in Fig. 1.

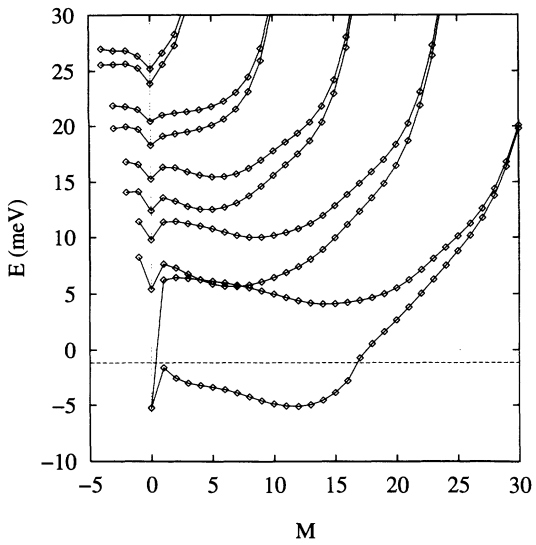

FIG. 11. Energy spectrum in the Hartree-Fock approximation for a system with a donorlike impurity ($\sigma = +1$) present in the system. $T = 1.0$ K, $N_s = 18$. Other parameters are as in Fig. 1.

that the spin splitting is always largest for the LB that is partly occupied.

In the case of an acceptor impurity ($\sigma = -1$) the $M = 0$ states are shifted upward in energy so μ lies between the two spin states [$(n = 0, M = 0, s = -1/2)$ and $(n = 0, M = 0, s = +1/2)$] for a higher N_s than in the case of a donor impurity. This is clearly seen in Fig. 10(c) where the largest spin splitting takes place around $\nu \approx 1.5$, exactly when the state $(n = 0, M = 0, s = +1/2)$ is occupied but the state $(n = 0, M = 0, s = -1/2)$ is not.

The shift in energy of the $M = 0$ states together with spin splitting of the states of a LB can lead to situations where the 2DEG around the impurity can be spin polarized but the impurity itself is not, or the other way around, depending on the type of impurity. In the case of a donor impurity, the impurity levels $(n = 0, M = 0, s = -1/2)$ and $(n = 0, M = 0, s = +1/2)$ are occupied but the surrounding 2DEG is spin polarized as is seen in Fig. 11. This behavior has been reported in experiments by Richter *et al.*[20] Corresponding phenomena can also occur in higher LB's. This difference in occupation of the impurity and the 2DEG can also be seen by comparing Fig. 6 with Fig. 5.

IV. SUMMARY

The energy spectrum of a 2DEG in a quantizing perpendicular magnetic field is quite singular. Inside the finite system the Landau bands become nearly flat as functions of the quantum number for angular momentum M. The density of states reflects this singular behavior and develops strong peaks corresponding to the flat degenerate regions. Between the peaks the relatively few edge states prevent the density of states from vanishing. The screening of an impurity in the center of the 2DEG is governed by this structure when the electron-electron interaction is treated in the Hartree approximation. Mainly the energy of the $M = 0$ states is shifted due to the impurity and the shift strongly depends on the location of the chemical potential with respect to the Landau bands.

In the Hartree-Fock approximation the screening, in general, is weakened by the exchange interaction, but in addition, the spin splitting of the almost flat Landau bands (or levels) within the system is strongly enhanced, thus drastically changing the density of states at the chemical potential. This enhancement of the spin splitting overwhelms the oscillations in the impurity spectra that are caused by the dependence of the screening on the filling factor of the Landau bands. We can expect that the spin splitting would be generally reduced in a system where the Landau bands did not become flat, for example, if the positive charge background of the system was modulated. The closing down of the spin splitting with a higher number of electrons in the system does not happen evenly for the M states, as one observes in infinite systems with a modulated background charge or in systems with a periodically modulated external potential. Instead we see the spin splitting being reduced faster for some values of M than others. The exact behavior is dependent on the size of the system, the temperature, and the location of the chemical potential with respect to the Landau bands. This formation of concentric circular regions of different spin phases only occurs in the case of the closing down of the spin splitting of a certain Landau band. The filling factor is thus approaching an even natural number. In the extreme quantum limit (when $\nu \to 0$) no such phase separation is observed in the Hartree-Fock approximation and only one spin state is occupied. Whether this formation of spin-density waves in the Hartree-Fock approximation for finite systems is physical has to be investigated in higher order approximations. As the Hartree-Fock approximation does not describe the broadening of nearly degenerate Landau levels due to the Coulomb interaction correctly, it can be expected that this approximation overemphasizes the importance of the exchange interaction between the electrons, so one might speculate whether approximations of higher order would decrease the enhancement of the spin splitting and thus increase the oscillations of the impurity spectra with the filling factor ν.

The calculations reported here have been performed for two different temperatures $T = 1$ K and 10 K due to the different behavior of the spin-density waves at these two values of T. The region of N_s or ν over which the spin-density waves form becomes narrower for the lower temperature and also vanishes for much higher temperature than $T = 10$ K, as stated earlier. The calculations are carried out at a finite temperature in order to increase their stability. At $T = 1$ K the bare spin splitting is of the same order as $k_B T$. At a lower temperature than 1 K the spin-density waves form for a narrower region, but the exact behavior at 0 K is outside the range

of the numerical calculations. The present results give an indication what to expect in optical measurements of the properties of a 2DEG in lightly doped quantum wells and heterostructures, but calculations of the cyclotron resonance or the plasmonic structure of the model are necessary in order to compare with experimental data.

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