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## LETTER TO THE EDITOR

# Spin-dependent fractional QHE states in the $N=0$ Landau level 

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#### Abstract

Spin assignments of fractional QHE states in the $N=0$ Landau level are determined from finite-size calculations of the Coulomb energy. There is a spin-unpolarised ground state at $\frac{2}{3}$ filling, with partial polarisation at $\frac{3}{5}$ filling and full polarisation at $1 / q$ filling with $q$ odd. This is explained in terms of competition between Coulomb repulsion, exchange and interaction of unlike spins. The experimental consequences are briefly discussed.


At high magnetic fields the FQHE in the $N=0$ Landau level is caused by the Laughlin/ Haldane spin-polarised electron liquid [1, 2]; however, as first noted by Halperin [3], spin reversal is favourable in GaAs at low fields. Following pioneering work by Chakraborty and Zhang [4], spin effects at particular filling factors, $\nu$, have been widely studied with attention focused on the unpolarised state [5] at $\nu=\frac{2}{5}$ and spin-reversed excitations [6,7] at $\nu=\frac{1}{3}$. This Letter reports a systematic theoretical study of all accessible fractions, and unifies earlier results in a new picture. $\dagger$ It is found that, in the absence of the Zeeman energy, the preferred spins at important fractions $\nu<1$ are: $\frac{1}{3}, \uparrow \uparrow ; \frac{2}{3}, \uparrow \downarrow ; \frac{2}{5}, \uparrow \downarrow ; \frac{3}{5}, \uparrow$, where $\uparrow \uparrow, \uparrow$ and $\uparrow \downarrow$ denote full, part and unpolarised. Corresponding results for $2>\nu>1$ follow from electron-hole symmetry: $\frac{5}{3}, \uparrow \uparrow$; $\frac{4}{3}, \uparrow \downarrow ; \frac{8}{5}, \uparrow \downarrow$; and $\frac{7}{5}, \uparrow$. The contrasting behaviour at $\nu=\frac{1}{3}$ and $\nu=\frac{2}{3}$ is remarkable. It occurs because a selection rule regulates the competition between Coulomb repulsion, exchange and a 'resonant' interaction between unlike spins. This is illustrated with computations of the cyclotron orbit centre correlation-a measurable function. Tilted field experiments [8] are consistent with the results reported here.

The total energy of $n$ ideal 2D interacting electrons consists of a Coulomb term, $E_{\mathrm{C}}$, and a Zeeman term: $E=E_{\mathrm{c}}(s, B \cos \theta)+g^{*} \mu_{\mathrm{B}} B s_{z}$. $E_{\mathrm{C}}$ depends on the spin quantum number $s$ ( $\operatorname{spin}$ squared $=\hbar^{2} s(s+1)$ ) and the component of magnetic field $B$, normal to the 2DEG. When $g^{*}>0$ the Zeeman energy is lowest when the $z$ component of spin, $s_{z}=-s$. A fully spin-polarised state corresponds to the maximum value of $s, s_{\max }$, which is $n / 2$ when $\nu \leqslant 1$ and $n\left(1 / \nu-\frac{1}{2}\right)$ when $2>\nu>1$. The minimum value of $s, 0$ for $n$ even and $\frac{1}{2}$ for $n$ odd, corresponds to an unpolarised state. Each $s$ has a ground state (GS) but the absolute ground state (AGS) occurs at the spin $s^{*}$, which minimises $E$. If $s^{*}=s_{\max }$ the AGS is fully polarised for all $B$. However if $s^{*}<s_{\max }$ a fully polarised aGs is not favoured when $B$ is sufficiently small. Instead it is partly polarised or unpolarised, depending on the value of $s^{*}$. The spins $s^{*}$ are determined here by finite-size calculations of $E_{c}$.

+ Preliminary results were presented at the 1988 Würzburg conference [16].


Figure 1. Spin dependence of $E_{\mathrm{c}}$ for finitesize systems. (a) $n=6, \nu=\frac{2}{3} ;(b) n=6$, $\nu=\frac{3}{3} ;(c) n=5, \nu=\frac{1}{3} ;(d) n=4, \nu=\frac{2}{5}$.

The calculations are done in the well known toroidal geometry which has the electrons in a rectangular, periodic cell of width $a$, height $b$. The starting point is the Hamiltonian given by Yoshioka [9] but modified to deal with spin [4]. As the aim is to study the physics, corrections for finite thickness and Landau level mixing are not included. Each eigenstate is found as a linear combination of Slater determinants that represent configurations of occupied Landau orbitals. However, this is harder than in the spin polarised case because the Hamiltonian matrix is larger. To mitigate this, basis states are constructed to be eigenstates of $\hat{S}^{2}$ and $\hat{S}_{z}$ which transform according to the magnetic translational $[10,11]$ and twofold rotational symmetry of the spatial part of the Hamiltonian. The program used was verified against the results of Zhang and Chakraborty [4].

Results for spin dependence of $E_{\mathrm{c}}$ are given in figure 1. This shows the energies per electron, measured in units of $e^{2} / 4 \pi \varepsilon_{0}(2 \pi / A)^{1 / 2}$ where $A$ is the area of the periodic cell. Each set of levels represents the lowest part of the energy spectrum for electrons in a rectangular cell with aspect ratio $R \equiv b / a=0.8$. This $R$-value lifts the degeneracies that occur for electrons in a square cell, while ensuring that exchange matrix elements are not unrealistically small. Only levels for $\nu<1$ are shown. Energies for $2>\nu>1$ can be obtained by electron-hole symmetry: in the absence of Landau level mixing, the spectrum at $2-\nu$ differs from the spectrum at $\nu(<1)$ merely by a constant offset [7]. Figure 1 confirms the spin assignments sitated earlier. Perhaps significantly, the value $s^{*}=1$ at $\nu=\frac{3}{5}$ corresponds to partial fillings of $\nu \downarrow=\frac{2}{5}, \nu \uparrow=\frac{1}{5}$ for the two spin components. The same partial fillings and $s^{*}$ appear to follow from the hierarchical model [2] if it is

Table 1. Spins $s^{*}$ deduced from finite-size results.

| $n\rangle^{m}$ |  | 5 | 6 | 7 | 8 | 9 | 10 |  | 12 | 13 | 14 | 15 | 16 | 17 | 18 |  |  | 20 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 4 | 2 | 2 | 0 | 1 | 0 | 1 | 0 | 1 | 2 | 1 | 0 | 1 | 2 | 1 | 0 |  | 1 | 2 |
| 5 |  | $\frac{3}{2}$ | $\frac{5}{2}$ | $\frac{1}{\frac{1}{2}}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{3}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{3}{2}$ | - | $\frac{3}{2}$ | 1 |  |  |  |  |
| 6 |  |  | 3 | 3 | 0 | 0 |  | 1 | 1 | 1 |  |  |  |  |  |  |  |  |

assumed that spin reversal occurs at each stage. Figure 1 also shows that gaps for $\Delta s=$ $\pm 1$ transitions are smaller than for $\Delta s=0$. This is consistent with existing ideas about spin-reversed excitations [6, 7] and may well explain recent observations [8] of Zeemandominated gaps at low $B$. Table 1 details $s^{*}$ for a complete range of $\nu$, expressed as $\nu=n / m$ where $m$ is the number of magnetic flux quanta through $A$. Most fractions, particularly $\nu=\frac{1}{2}$, have part or unpolarised AGS (unpolarised AGS at $\nu=\frac{5}{2}$ are discussed in [12]). With the exception of $\frac{4}{16}$ (where $E_{\mathrm{c}}$ differences are $<0.1 \%$ ) the trend is that fully polarised AGS are only favoured at $\nu=1 / q$ with $q$ odd.

To understand the physics of this the eigenstates have been examined in detail. The feature common to part and unpolarised AGS is a strong tendency for double occupation of Landau orbitals. This is quantified by the pair sum, $N_{\mathrm{p}}$, defined as the expectation value of $\Sigma_{j} n_{j \uparrow} n_{j \downarrow}$. Here the $n$ are number operators and $j$ labels the centre coordinate of the Landau orbitals. (In a periodic cell the $x$-components of the orbit centres are at $X_{j}=$ $j \delta X$, where $\delta X=2 \pi l^{2} / b$ and $l^{2}=\hbar / e B$.) Figure 2 shows how $N_{\mathrm{p}}$ for unpolarised GS depends on $m$. Clearly there are minima at $\nu=1 / q$ with $q$ odd and maxima in between. The maxima do not always coincide with $1 / q$ at $q$ even. However, as explained later, there are good reasons for believing that minima always occur at $\nu=1 / q$ with $q$ odd.

The reason why double occupation (henceforth called 'pairing') can be favoured is related to the physical nature of the Landau orbitals. In a periodic cell they are localised in $x$ but delocalised in $y$ : for $N=0$ each orbital occupies a strip of width $\simeq 2 l$, centred on $X_{j}$. Paired electrons interact via a type of 'resonance' where occupations mix in the manner $j \uparrow, j \downarrow \rightleftharpoons j+h \uparrow, j-h \downarrow$. This can be visualised be denoting pairs with $\|$ and single occupations with $\uparrow$ or $\downarrow$, interspaced with dots to represent empty orbitals. For example, the picture is. $\| . \rightleftharpoons \downarrow . \uparrow$ when $h=1$. The resonant mixing (RM) lowers energy by introducing correlation which makes the electrons stay apart along $y$. This can be seen from a simple argument based on the uncertainty principle. The operator identities given in [13] lead to the commutation relation, $[X, y]=i l^{2}$, between the centre coordinate $X$ and the Cartesian coordinate $y$, so $X$ and $y$ obey the uncertainty relation $\Delta X \Delta y \simeq l^{2}$. Now apply this to the motion of two electrons relative to their centre of mass. When they partly occupy the same Landau orbital the resonant interaction between them leads to an uncertainty $\Delta X \simeq h \delta X$ hence $\Delta y \simeq b / 2 \pi h$. In effect, the interaction allows the otherwise delocalised state to develop structure in the $y$ direction on a length scale $\simeq b / h$. This can be understood in detail by examining the correlation function, $g(r)$, that is the expectation value [9] of

$$
A \sum_{i \neq j} \delta\left(\boldsymbol{r}+\boldsymbol{r}_{i}-\boldsymbol{r}_{j}\right) / n(n-1)
$$

In second quantisation

$$
g(r)=\sum_{\substack{s s^{\prime} \\ i j k l}} F(l-i, i-k, r) \delta_{i+j, k+l}^{\prime}\left\langle c_{i s}^{+} c_{j s^{\prime}}^{+} c_{k s^{\prime}} c_{l s}\right\rangle
$$

where the $c$ are the usual fermion operators and the prime on the Kronecker delta means that sums are taken modulo $m$. The function $F$ is related to the Landau orbitals $\Phi$,

$$
\begin{gathered}
F(l-i, i-k, \boldsymbol{r}) \delta_{i+j, k+l}^{\prime}=A \int_{\text {cell }} \mathrm{d} \boldsymbol{r}_{1} \mathrm{~d} \boldsymbol{r}_{2} \Phi_{i}^{*}\left(\boldsymbol{r}_{1}\right) \Phi_{j}^{*}\left(\boldsymbol{r}_{2}\right) \delta\left(\boldsymbol{r}+\boldsymbol{r}_{1}-\boldsymbol{r}_{2}\right) \\
\times \Phi_{k}\left(\boldsymbol{r}_{2}\right) \Phi_{l}\left(\boldsymbol{r}_{1}\right) / n(n-1)
\end{gathered}
$$



Figure 2. Pair sum for finite-size unpolarised states. The points give $N_{\mathrm{p}}$; the lines are to guide the eye. (a) $n=4, s=0 ;(b) n=5, s=\frac{1}{2}$.

The physical content of $g$ is a little clearer when the terms involving number operators are treated separately. After some rearrangement

$$
\begin{equation*}
g(\boldsymbol{r})=\sum_{s s^{\prime} \prime} \rho_{s s^{\prime}}(j) G_{s s^{\prime}}(j, \boldsymbol{r})+\sum_{\substack{s s^{\prime} \\ i j k}}\left\langle c_{i+k s}^{+} c_{i+j s^{\prime}}^{+} c_{i s^{\prime}} c_{i+j+k s}\right\rangle F(j, k, \boldsymbol{r}) \tag{1}
\end{equation*}
$$

where

$$
\rho_{s s^{\prime}}(j)=\sum_{i}\left\langle n_{i s} n_{i+j s^{\prime}}\right\rangle
$$

and $G_{s s^{\prime}}(j, \boldsymbol{r})=F(0, j, \boldsymbol{r})-\delta_{s s^{\prime}} F(j, 0, r)$. Physically, $\rho_{s s^{\prime}}$ is the correlation of cyclotron orbit centres occupied by spins $s s^{\prime}$; its contribution to $g$ is broadened by $G_{s s^{\prime}}$, the correlation function for two non-interacting electrons with orbit centre separation $j \delta X$. In principle, $\rho$ could be deconvolved from measurements of $g$. The remaining term in (1) describes 'hopping' and 'spin flips'. It is strongly affected by RM. Indeed the numerical results, combined with analytic evaluation of the overlap $F$, show that to order $\exp \left(-a^{2} / l^{2}\right)$, RM contributes to $g(0, y)$ in proportion to $-\cos (2 \pi h y / b)$. This is a reduction in correlation when $y$ is small and corresponds to a reduction in Coulomb energy. The importance of RM is confirmed by numerical experiments in which the corresponding matrix elements are set to zero. Then energies of four-electron unpolarised as change by $\simeq 0.1 \%$ at $\nu=\frac{1}{3}$ but $\simeq 6 \%$ at $\nu=\frac{2}{3}$. As a result the $\frac{2}{3}$ AGS reverts to being fully polarised. (Percentages are calculated without the constant Madelung [9] contribution to $E_{\mathrm{c}}$.)

RM competes with Coulomb 'repulsion' and 'exchange' because pairing costs repulsive energy $\dagger$, but the competition is regulated by a selection rule. The gs eigenvector is composed of a mixture of configurations of occupied Landau orbitals. Each configuration has a quantum number [9], $J$, related to the sum of the occupied orbital indices: $J=$ $\sum_{i s} j_{i s} \bmod m$. If $c$ is the highest common factor of $m$ and $n$, only $J \leqslant p$ is relevant because the states occur in degenerate multiplets [11]. Configurations can interact (normally via a chain of intermediates) only if they have the same $J$. The most important configurations have low energy as measured by the sum of repulsive and exchange terms. Table 2 gives examples that occur, with relative probability $P$, in $s=0$ Gs. The lowest-energy configurations consist entirely of singly occupied orbitals, arranged in regularly spaced clusters [14]. The optimum configurations with pairs are regular arrangements when the number of pairs is $n / 2$, but more complicated when the number of pairs is less than $n / 2$. Because of the competition with repulsion and exchange, the system can only benefit $\dagger$ 'Repulsion' and 'exchange' come from the diagonal part of the Hamiltonian but RM comes from the offdiagonal part.

Table 2. Examples of cluster (size 2) and pair configurations in $n=4 s=0 \mathrm{GS}$. Note regular spacing and larger probability of 2-pair configuration at $\nu=\frac{2}{3}$.



Figure 3. Orbit centre correlations versus separation $j=X / \delta X$. The points give $\rho$; the lines are to guide the eye. (a) $\frac{1}{3}$ ground, $n=5 ; s=\frac{5}{2}$; (b) $\frac{1}{3}$ ground, $n=5, s=\frac{1}{2}$; (c) $\frac{1}{3}$ first excited state, $n=5, s=\frac{1}{2} ;(d) \frac{1}{3}$ ground, $n=5, s=\frac{1}{2} ;(e) \frac{2}{3}$ ground, $n=6, s=3 ;(f) \frac{2}{3}$ ground, $n=6, s=0$.
from RM when energetically favourable configurations containing pairs interact with cluster configurations. This does not happen at $\nu=1 / q$ with $q$ odd because optimal arrangements of clusters do not have the same $J$ as optimal arrangements containing pairs. For example, at $\nu=\frac{4}{12}$ the configuration $1 \uparrow, 1 \downarrow, 7 \uparrow, 7 \downarrow$ is optimal and has $J=$ 4 whereas the configuration $1 \uparrow, 2 \uparrow, 7 \downarrow, 8 \downarrow$ is optimal but has $J=2$. In fact the general rule for even $n$ is that at $\nu=\frac{1}{3}$ regular arrangements of $n / 2$ pairs have $J=n$, while regular arrangements of identical clusters have $J=n / 2$ (regardless of cluster size); at $\nu=\frac{2}{3}$ both types of configuration have $J=n / 2$. This is a strong hint that the $J$ selection rule which determines finite-size behaviour is important for larger systems.

The orbit centre correlation provides further insight into clustering and pairing. Instead of correlations of specific spins as defined in (1) it is more useful to consider the total correlation $\rho=\Sigma_{s s^{\prime}} \rho_{s s^{\prime}}$ and the unlike spin correlation $\rho_{\uparrow \downarrow}+\rho_{\downarrow \uparrow}$ (figure 3). When normalised, these functions give probability distributions of orbit centre separations. Both functions are symmetric about $j=m / 2$ (because of periodic boundary conditions) and $\rho=n$ when $j=0$, while $\rho_{s s^{\prime}}(0)=N_{\mathrm{p}}$ when $s \neq s^{\prime}$. To understand their meaning first consider a single configuration. A helpful example is $\downarrow \downarrow \ldots \ldots \downarrow \downarrow \ldots \downarrow \ldots$ because it and other configurations with the same $\rho$ dominate the $n=5, \nu=\frac{1}{3}$ AGS. The example has two separations of one unit of $\delta X$ (see clusters) hence $\rho(1)=2$. Similarly, $\rho$ is 0 at $j=2,3$ and has its peak value, 3 , at $j=5$. Now examine the $\rho$ for the exact $s=\frac{5}{2} \mathrm{AGS}$ at $\nu=\frac{1}{3}$ (figure $3(a)$ ). It resembles $\rho$ for the dominant configuration: large at $j=1$ and


Figure 4. Pair correlation functions for polarised (broken curves) and unpolarised (full curves) GS at $\nu=\frac{1}{3}$ and $\frac{2}{3}$. The lower sets of curves give various contributions to the full $g$ (upper curves) as defined in the text. (a) $n=5, \nu=\frac{1}{3}$; (b) $n=6, \nu=\frac{2}{3}$.
small at $j=2$ (reflecting the cluster size 2 ) with peaks at $j=5,10$ (reflecting the cluster spacing). However, the peaks are broader than for the dominant configuration due to mixing with other configurations. (Mixing breaks clusters: . $\downarrow \downarrow . \rightleftharpoons \downarrow \ldots \downarrow$ which reduces energy like RM. Cluster sizes other than 2 also occur but are less important.) Next compare the $\rho$ for the five-electron AGS at $s=\frac{5}{2}$ (figure $3(a)$ ) and the GS at $s=\frac{1}{2}$ (figure $3(b)$ ). They are remarkably similar. This suggests that the physical nature of the $\frac{1}{3} \mathrm{GS}$ is very insensitive to spin. The correlation of unlike spins for five electrons at $v=\frac{1}{3}$ is shown in the centre of figure 3 . For the as at $s=\frac{1}{2}$, which is unaffected by pairing (figure $3(d)$ ), there is very little short-range correlation. However, the situation is different for the first excited state at $s=\frac{1}{2}$ (figure $3(c)$ ). This has the relatively large pair sum of 0.5003 and its unlike spin correlation has peaks at $j=0,2$ with a minimum at $j=$ 1. This is the signature of RM (electrons in a resonant pair cannot have a separation of 1). Finally, examine $\rho$ for the $\frac{2}{3}$ GS. In contrast to $\nu=\frac{1}{3}$, the $\rho$ at $s=0$ (figure $3(f)$ ) and $s=3$ (figure $3(e)$ ) are clearly different. $\rho$ for the $s=0$ AGS has a minimum at $j=1$ and is large at $j=2$ because RM is important. The structured form of $\rho$ is consistent with liquid GS because the $\rho$-contribution to $g$ is modified according to (1): $\rho$ explicitly gives physical information which is hidden in $g$.

This is illustrated in figure 4 which shows $g(0, y)$ for both polarised and unpolarised GS at $\nu=\frac{1}{3}$ and $\frac{2}{3}$. The upper curves show $g$ and the lower curves two contributions which sum to $g$. The contribution labelled coxc includes the $\rho$-terms from (1) together with the contribution of spin flip processes to the remaining terms, i.e. processes that affect only the distribution of spins (for example $\uparrow . \downarrow \rightarrow \downarrow . \uparrow$ ). When multiplied by $V(r)$ (the Coulomb potential) and integrated this contribution gives the repulsive and exchange contributions to the total energy. The second contribution shown in figure 4 comes from the remaining terms in (1), i.e. hopping processes. At $\nu=\frac{1}{3}$ spin reversal clearly has very little effect on $g(0, y)$ and its effect on $g(x, 0)$ is even smaller. In contrast, there are dramatic effects at $\nu=\frac{2}{3}$. The full $g$ increases at large $y(\approx b / 2)$ and decreases at small $y$. In addition there is a large increase in the coxc contribution at small $y$ which is mostly cancelled by a decrease in the hopping contribution. This change is related partly to RM and partly to changes in exchange effects (a similar but smaller change occurs at $\nu=\frac{1}{3}$ ).

Further, the hopping contribution to $g(0, y)$ is, to a good approximation, proportional to $-\cos (2 \pi y / b)$. As deduced earlier, this is related to RM and leads to the changes in correlation which make the $s=0$ state energetically favourable.

There remains the question of what happens in other geometries. In the toroidal geometry used here the Landau orbitals are simultaneous eigenstates of $X$ ( $x$ component of centre coordinate), $p_{y}$ (momentum: -i $\hbar \partial / \partial y$ ) and energy, with one to one correspondence between eigenvalues of $X$ and $p_{y}$. An alternative is the disc geometry [13] where the orbitals are simultaneous eigenstates of $R^{2}$ (square of radial part of centre coordinate) and $L_{z}$ (angular momentum) as well as energy, with one to one correspondence between eigenvalues of $R^{2}$ and $L_{z}$. In both geometries the orbitals are partly delocalised: when the geometry is toroidal there is delocalisation in $y$ with localisation in $x$ while in the disc geometry there is delocalisation in the polar angle, $\varphi$, with localisation in the radial direction. Double occupation of these orbitals results in mixing of orbitals with different values of $X$ or $R^{2}$ respectively. By analogy with the present results for the toroidal geometry, it is expected that in the disc geometry the mixing will introduce correlations in the $\varphi$ direction. It is plausible that this will reduce the energy of the system but the details need to be verified.

In summary, finite-size results imply the new spin assignments $\frac{2}{3}, \frac{4}{3} \uparrow \downarrow$, $\frac{3}{5}, \frac{7}{5} \uparrow$ together with the expected $[4,5] \frac{1}{3}, \frac{5}{3} \uparrow \uparrow, \frac{2}{5}, \frac{8}{5} \uparrow \downarrow$. The assignments appear to be determined by regulated competition between Coulomb repulsion, exchange and resonant interaction of unlike spins. In practice this has important consequences, particularly for states with small Zeeman energies. Experimental studies of these states [8] are consistent with the predicted spins and spin-reversed excitations [6, 7]. More speculatively, there could be local minima in $E_{\mathrm{c}}(s)$ at favourable partial fillings $\nu \uparrow, \nu \downarrow$ and this could affect the small gaps that occur when the Zeeman component aligns total energies for different $s$. Consequently, there may be interesting, observable structure in the transition $\uparrow \downarrow \rightarrow \downarrow \rightarrow \uparrow \uparrow$. Emergence from the transition may account for threshold effects seen in activation data [15]. In principle, measurements of $g, \rho$ and $s$ would be the ideal way to test the findings reported here.

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Note added in proof. Very recently Clark et al have obtained experimental data which indicate that there is an unpolarised ground state at $\nu=\frac{2}{3}$ [17] in addition to the one already found at $\nu=\frac{4}{3}$ [8]. They observe crossover between polarised and unpolarised behaviour at a field of about 3.1 T when the electron density is $4.5 \times 10^{10} \mathrm{~cm}^{-2}$ and the calculations described here have been extended to estimate this crossover field. When finite thickness effects are included via the Fang-Howard variational wavefunction, crossover for the sixelectron system is found to occur at about 5 T . The agreement with experiment is reasonable in view of uncertainties about finite size corrections, Landau level mixing and the appropriate value of the Fang-Howard variational parameter.

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