Landau Level Mixing and Skyrmion Stability in Quantum Hall Ferromagnets

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We present a Hartree-Fock study that incorporates the effects of Landau level mixing and screening due to filled levels into the computation of energies and states of quasiparticles in quantum Hall ferromagnets. We use it to construct a phase diagram for skyrmion stability as a function of magnetic field and Zeeman coupling strengths. We find that Landau level mixing tends to favor spin-polarized quasiparticles, while finite thickness corrections favor skyrmions. Our studies show that skyrmion stability in high Landau levels is very sensitive to the way in which electron-electron interactions are modified by finite thickness, and indicate that it is crucial to use models with realistic short distance behavior to get qualitatively correct results. We find that recent experimental evidence for skyrmions in higher Landau levels cannot be explained within our model.

I. INTRODUCTION

It has been recognized that exotic magnetic excitations known as skyrmions may exist in a two-dimensional electron gas in a strong homogeneous magnetic field (quantum Hall system) near spin-polarized groundstates. These are excitations of a two-dimensional spontaneous ferromagnet, the physics of which is relevant to this system (despite the presence of a strong magnetic field), because of the small Landé g-factor in GaAs systems (where most experiments take place), which makes the Zeeman coupling very small compared to other energy scales (Coulomb interaction, cyclotron energy) in the problem. Skyrmions are spin configurations with a non-trivial winding number (Pontryagin index). They were first discussed in the context of four-dimensional field theories and were later recognized as states occurring in the non-linear sigma model description of two-dimensional ferromagnets. For filling factors $\nu \equiv N/N_0$ close to one ($N$ is the number of electrons and $N_0$ is the number of magnetic flux quanta penetrating the system), these turn out to be the lowest energy quasiparticles under typical experimental circumstances. Skyrmions can thus be introduced into the groundstate by adding or removing charge from the system.

Experimentally, the case for the existence of skyrmions in a system close to $\nu = 1$ is quite strong. NMR experiments show a degrading of the spin polarization with deviation of filling factor from one that is in remarkably good agreement with Hartree-Fock theory. The quasiparticle spin measured in transport experiments are also reasonably well accounted for by Hartree-Fock calculations. Electromagnetic absorption experiments further support that doping away from $\nu = 1$ injects skyrmions into the system.

In weaker magnetic fields, near filling factor $\nu = 3$, early experiments suggested that spin-polarized quasiparticles are lower in energy than skyrmions, so the effects seen near $\nu = 1$ would not be present at higher filling. This is consistent with calculations of skyrmion energies near $\nu = 3$ that include finite thickness corrections, which indicate that skyrmions will be present only at much smaller Zeeman couplings than realized in typical experiments. The size of the skyrmion may be quantified by a number $K$, the difference in the spin component $S_z$ between the skyrmion and the spin-polarized quasiparticle. Because of the necessarily small Zeeman coupling, stable skyrmions close to $\nu = 3$ have large values of $K$. They also become unstable with respect to spin-polarized quasiparticles at a finite value of $K$. (For $\nu = 1$, $K \to 0$ as the Zeeman coupling reaches the maximum value for which the system supports skyrmions; i.e., the skyrmion state smoothly goes into the spin-polarized quasiparticle state.) For a two-dimensional electron gas (2DEG) with width of about $2\ell$, where $\ell = \sqrt{\hbar/eB}$ is the magnetic length, the minimum $K$ expected is approximately 4.

Recently, however, NMR experiments have uncovered evidence that some anomalous degrading of spin polarization does occur as one dopes away from $\nu = 3$ at relatively high Zeeman couplings. These experiments further indicate that the number of overturned spins per quasiparticle is quite small, $K \sim 1$. The simple models usually considered are inconsistent with this, and one is naturally led to inquire as to what other ingredients might change the critical Zeeman coupling and smallest $K$ observable near $\nu = 3$. Two possible answers are Landau level mixing and screening by filled Landau levels. It should be noted that these are not distinct effects: screening by filled Landau levels occurs because they may admix high (unoccupied) Landau levels to smooth fluctuations due to external potentials and/or inhomogeneous electron densities in partially filled levels. Conversely, the states which may be used for Landau level mixing in a partially filled level are limited to those that are not occupied by electrons in other levels, due to Pauli exclusion. Thus, a correct treatment of either screening or Landau level mixing near $\nu = 3$ must include both these effects.

In this work, we present a method by which these may be incorporated into the Hartree-Fock description.
of skyrmion states.

Our principal conclusions may be summarized as follows: (i) For skyrmions near \( \nu = 1 \), Landau level mixing tends to lower the quasiparticle energy, although not enough to quantitatively explain the activation energies seen in experiment. Introduction of a finite width of one magnetic length lowers the energy of the skyrmion by approximately 40\%, and inclusion of Landau level mixing lowers the energy by approximately another 20\% for \( \hbar \omega_c/(e^2/\kappa l) \approx 0.6 \), where \( \omega_c = eB/\hbar c \) is the cyclotron frequency of the electrons, and \( \kappa \) is the dielectric constant of the host crystal. The resulting quasiparticle gap is approximately a factor of 2 larger than what is found in experiment. This result agrees qualitatively with that of another study of Landau level mixing effects on \( \nu = 1 \) skyrmions. (ii) For \( \nu = 1 \), Landau level mixing tends to suppress quasi-hole-like skyrmions (i.e., lowering the maximum Zeeman coupling for which they are stable), while enhancing the stability of quasielectron (anti-)skyrmions. (iii) For \( \nu = 3 \) and higher, we find that a sufficiently realistic model of the effective electron-electron interaction, as modified by the finite thickness of the electronic wavefunctions, is necessary to obtain reliable results. Use of a simple potential due to Zhang and Das Sarma grossly overestimates the stability of \( \nu = 3 \) skyrmions; more realistic potentials allow skyrmions only for very small Zeeman couplings. (iv) Screening and Landau level mixing for \( \nu = 3 \) and \( \nu = 5 \) tend to lower the energy of spin-polarized quasiparticles more than that of skyrmions, making the latter even less stable. (v) The results of Ref. cannot be understood solely on the basis of Hartree-Fock states for skyrmions.

The remainder of this article is organized as follows. In Section II below, we discuss the method used to allow screening and Landau level mixing to be included in our calculations. Section III gives details of our results, and we conclude with a summary of our findings in Section IV.

II. HARTREE-FOCK METHOD WITH LANDAU LEVEL MIXING

Most previous Hartree-Fock studies of skyrmions have relied on Landau level representation of the single particle states. We choose instead to construct the wavefunctions in real space. This enables us to include in the model Landau level mixing occurring in weak magnetic fields, without having to expand over the large number of Landau levels necessary in the former approach. We thus trade the calculational convenience of working with the functions given in closed analytic form (Landau levels) for a closer description of the single-particle states by representing them on a real-space grid.

In this calculation we aim to model all the participating particles, including the ones in the filled levels. Our Hartree-Fock wavefunction is a Slater determinant composed of single-particle states which have \( L_z \pm S_z \) as a good quantum number but whose radial form is to be determined self-consistently:

\[
|\Psi_{\text{skyrmion}}\rangle = \prod_{i,m} \gamma_{im}^\dagger |0\rangle
\]

\[
\langle \vec{r}, \sigma | \gamma_{im}^\dagger |0\rangle = \left[ \frac{f_{im}(r)}{g_{im}(r)e^{\pm \theta}} \right] e^{i m \theta}.
\]

Here \( r \) and \( \theta \) are polar coordinates, \( m \) is the angular momentum quantum number, and \( i \) labels different states of the same \( m \). The sign \( \pm \) corresponds to two families of solutions, + for antiskyrmion (or quasielectron spin structured solution) and – for skyrmion (quasihole).

In very strong magnetic fields, the functions \( f(r) \) and \( g(r) \) take the form expected for Landau level states. When the strength of the magnetic field is lowered to bring the ratio of cyclotron and Coulomb energy scales close to 1, the form of the radial part relaxes toward some modified form, as dictated by the interactions in the system.

Using the trial form of the wavefunction, the many-body Schrödinger equation with the Hamiltonian

\[
H = \frac{1}{2m} \int d^2r \sum \sigma \Psi_\sigma^\dagger \vec{r} \frac{\hbar}{i} \vec{\nabla} - \frac{e}{c} \vec{A}(\vec{r}) \Psi_\sigma(\vec{r}) + \frac{1}{2} g_\mu B \int d^2r [\Psi_\uparrow^\dagger(\vec{r}) \Psi_\uparrow(\vec{r}) - \Psi_\downarrow^\dagger(\vec{r}) \Psi_\downarrow(\vec{r})] + \frac{1}{2} \sum_{\sigma \sigma'} \int d^2r d^2r' \Psi_{\sigma'}^\dagger(\vec{r}) \Psi_\sigma(\vec{r}) \nu(\vec{r} - \vec{r}') \Psi_{\sigma'}(\vec{r}') \Psi_{\sigma}(\vec{r}')
\]

(2)

(where \( \sigma \) denotes spin and \( \nu(\vec{r} - \vec{r}') \) the Coulomb interaction), upon variation with respect to the functions \( f \) and \( g \), gives a system of mean-field single-particle equations:

\[
D_m(r) f_{im}(r) = -\frac{1}{2} g_\mu B f_{im}(r) + \int_0^\infty dr' \nu(\vec{r}, \vec{r}') \rho(\vec{r}') - \rho_0 |f_{im}(r')
\]

\[
- \int_0^\infty dr' \sum_{m'} V_{m-m'}^{xx}(\vec{r}, \vec{r}') \rho_{m'}^{\uparrow \uparrow}(\vec{r}', r) f_{im}(r')
\]

\[
- \int_0^\infty dr' \sum_{m'} V_{m-m'}^{xx}(\vec{r}, \vec{r}') \rho_{m'}^{\downarrow \downarrow}(\vec{r}', r) g_{im \pm 1}(r')
\]

\[
e_i f_{im}(r)
\]

(3)

together with the analogous equation for the function \( g(r) \). Here is a dictionary of the notation accompanying Eq. 3 the operator \( D_m \) is given by

\[
D_m = -\frac{\hbar^2}{2m^*} \frac{1}{r} \frac{d}{dr} \frac{d}{dr} - \frac{m^2}{r^2} - \hbar \omega_c \frac{(m^*)^2}{2} \frac{\omega_c^2 r^2}{4m^*}
\]

(4)

with \( \omega_c = eB/m^*e_c \). \( B \) the magnitude of the external magnetic field, and \( m^* \) the effective mass of the electron. \( g \) is the
Landé g-factor, and \( \mu_B \) is the Bohr magneton. \( \rho \)'s denote generalized densities:

\[
\begin{align*}
\rho_{m\nu}^{+1}(r',r) &= f_{m\nu}^+(r')f_{m\nu}(r) \\
\rho_{m\nu}^{-1}(r',r) &= g_{m\nu}^{-1}(r')g_{m\nu}(r) \\
\rho_{m\nu}^{0}(r',r) &= g_{m\nu}^0(r')f_{m\nu}(r) \\
\rho(r) &= \sum_{m'\nu}[\rho_{m\nu}^{+1}(r,r) + \rho_{m\nu}^{-1}(r,r)],
\end{align*}
\]

and \( \rho_0 \) is the uniform background density. \( V^H \) and \( V^{ex} \) are the following integrals of the Coulomb potential over the azimuthal variable:

\[
\begin{align*}
V^H(r,r') &= \int_0^{2\pi} d\theta \int_0^{2\pi} d\theta' v(\vec{r} - \vec{r'}) \\
V^{ex}_{m\nu}(r,r') &= \int_0^{2\pi} d\theta \int_0^{2\pi} d\theta' e^{i(m+m')(\theta-\theta')} v(\vec{r} - \vec{r'}),
\end{align*}
\]

and, finally, \( \epsilon \) stands for the single-particle Hartree-Fock energy.

The finite width of the sample is modeled using the in-plane potential due to Cooper. We replace the Coulomb interaction \( v(\vec{r} - \vec{r'}) \) in the Eq. (6) by

\[
v_C(r) = \int_0^{\infty} dz dz' \frac{e^{-z^2+z'^2}/2w^2}{2\pi w^2} \frac{1}{\sqrt{r^2 + (z-z')^2}}
\]

The symbol \( w \) denotes the width of system in the direction perpendicular do the plane of the system, and \( z, z' \) are coordinates in that direction.

To handle the boundaries of the system, we assume the electron states with angular momentum \( m > m_{\text{max}} \) have the ferromagnetic groundstate form (i.e. Landau levels with well defined spin). The states with \( m \leq m_{\text{max}} \) are explicitly included in the calculation. For \( K \) not too large we find it is sufficient to allow variations of the states with \( m \) of up to 30 for \( \nu = 3 \) and up to 50 for \( \nu = 5 \). In practice, including boundary electrons from the states with \( m \) between 31 and 100 (\( \nu = 3 \)) and between 51 and 120 (\( \nu = 5 \)) describes the effect of the system edge with precision matching the rest of the calculation.

Understanding Eq. (6) as a system of coupled eigenproblems, we look for the self-consistent single particle solutions. (Discretization will turn each eigenvalue into a matrix diagonalization problem which can be handled using standard methods.) The results we thus obtain will be largely presented as comparisons between energies of the spin-polarized quasiparticle and energies of the corresponding skyrmion.

To assess the energy of the skyrmion in the region of parameters where it is not stable, we add to the Hamiltonian a term of the form \( \lambda(S_z - S_0)^2 \), \( S_z \) being the spin operator, and \( \lambda \) a tunable parameter. This term favors a state with total spin \( S_0 \), but is insensitive to the detailed form of the wavefunctions. This allows the variational scheme to pick out the lowest energy Slater determinant of the form given in Eq. (6) within the space of states with the same fixed value of \( K \).

### III. RESULTS

Based on the calculation described in the previous section, we present some of the results the method allows us to obtain; we focus mainly on the singly charged excitations in the first three Landau levels. Consideration of higher Landau levels is also possible, but computation of the potential lookup tables becomes prohibitively expensive, and, as the results so far indicate, leads to no new insight. In the following we shall take the unit of energy to be \( e^2/\kappa \ell \), and the unitless Zeeman splitting to be \( \tilde{g} = \frac{2\mu_B}{e^2/\kappa \ell} \), where \( e \) is the electron charge, \( \kappa \) is the dielectric constant of the host material, \( \ell \) is the magnetic length in the field \( B \) and \( \mu_B \) is the Bohr magneton.

#### A. Skyrmion vs. polarized quasiparticle

In Fig. [1] we show the energy difference between the spin-polarized quasiparticle and the skyrmion of size \( K \), \( V_K - V_{K=0} \). This quantity is a pure interaction energy (i.e. Zeeman energy is not included), and represents the energy gained or lost in deforming a spin-polarized quasiparticle into a skyrmion when Zeeman coupling is absent. Of particular importance is the slope (negative slopes indicate that skyrmion is stable for some value of \( g \)) and the curvature (concave curves will support small-sized skyrmions). For concave curves the largest Zeeman splitting that supports skyrmions is the negative of the initial slope of the curve.

For large cyclotron energies our results are essentially identical to those obtained using the single Landau level method. Note the quasielectron and quasi-hole excitations are precisely degenerate in this case, due to particle-hole symmetry. For smaller values of \( \hbar \omega_c \), the two curves split; surprisingly, the quasihole skyrmion is suppressed by Landau level mixing, whereas the quasielectron skyrmion is enhanced. (The former result is in agreement with Ref. [3].)
FIG. 1. Energy difference between skyrmion and polarized quasihole at $\nu = 1$, for well width of $1.73\ell$ and with $\tilde{g} \to 0$. The full lines correspond to the quasihole and the dashed ones to the quasielectron case. For high cyclotron energies ($100.0e^2/\kappa\ell$; the lower full curve) the results for the two types of excitations overlap. For low cyclotron energies ($0.8e^2/\kappa\ell$; upper full line and non-overlapping dashed line) there is significant difference in the behavior of the two, which reflects itself in the phase diagram, Fig. 8.

The energy gaps (Fig. 2) which result from creation of skyrmion-antiskyrmion pairs when Landau level mixing and finite thickness corrections are included are considerably smaller than what is found for two-dimensional layers and no mixing. However, the resulting energies are still almost a factor of two larger than what is found in experiment. The discrepancy is likely to be due to disorder.

Figs. 3 and 4 present analogous results for $\nu = 3$ and $\nu = 5$. Note the considerably smaller energy scales in these figures, indicating that skyrmions can only be stable (if ever) for small values of $\tilde{g}$. It is apparent that the introduction of Landau level mixing and screening destabilizes the skyrmion. Evidently, spin-polarized particles are better able to take advantage of the admixture of higher Landau levels than skyrmions.

Figs. (3) and (4) present analogous results for $\nu = 3$ and $\nu = 5$. Note the considerably smaller energy scales in these figures, indicating that skyrmions can only be stable (if ever) for small values of $\tilde{g}$. It is apparent that the introduction of Landau level mixing and screening destabilizes the skyrmion. Evidently, spin-polarized particles are better able to take advantage of the admixture of higher Landau levels than skyrmions.

FIG. 2. Skyrmion-antiskyrmion pair excitation gap for two different well widths: $1.73\ell$ (full line) and $1.0\ell$ (dashed line). Upper lines correspond to the cyclotron energy of $100.0e^2/\kappa\ell$ and lower ones to $0.8e^2/\kappa\ell$.

FIG. 3. Energy difference between skyrmion and polarized quasihole at $\nu = 3$; the well width is $1.73\ell$; $\tilde{g} \to 0$. The full lines correspond to the quasihole and the dashed ones to the quasielectron case. The cyclotron energy range is between $100.0e^2/\kappa\ell$ for the lowest line and $0.8e^2/\kappa\ell$ for the uppermost, each cyclotron energy being 50% smaller than the previous higher one.

FIG. 4. Energy difference between skyrmion and polarized quasihole at $\nu = 5$; the well width is $1.73\ell$; $\tilde{g} \to 0$. The full lines correspond to the quasihole and the dashed ones to the quasielectron case. The cyclotron energies are the same as in Fig. 3.
B. Effect of Finite Well Width

Quasiparticle energies depend on the well width, as illustrated in Figs. 5 and 6. As expected, we find that for narrower wells the difference in energy is less favorable for the skyrmion (Fig. 6). Note that the width used in Fig. 6 is close to an experimentally reported value.

\[ v_{ZdS}(\vec{r} - \vec{r}') = \frac{1}{\sqrt{|\vec{r} - \vec{r}'|^2 + w^2}} \]  

which is commonly used in studying quantum Hall systems (see for example Refs. 13 and 16) gives substantially different results then those presented above (Fig. 3).

\[ v_C(r) \quad \text{and} \quad v_{ZdS}(r) \]

The principal difference between \( v_C(r) \) and \( v_{ZdS}(r) \) is the behavior at small \( r \); the former diverges logarithmically, whereas the latter is regular. Other divergent potentials give results consistent with Figs. 3 and 4; it is likely that the oversimplified behavior at short distances is responsible for the poor performance of \( v_{ZdS}(r) \) in this problem.

C. Phase Diagram

Based on results in Figs. 1, 3, and 6 we can construct the phase diagrams of skyrmion stability for the filling factors of \( \nu = 1, 3, \) and 5. Large \( \omega_c \) and small \( g_c \) is the region favoring the spin structured excitations. We see that the region “shrinks” as one moves to the higher filling factors. Also, according to this calculation the breaking of symmetry between the quasihole and quasielectron excitations upon lowering the cyclotron energy is quite spectacular in the lowest Landau level, whereas it plays no significant role in the higher ones.
FIG. 8. Phase diagram of skyrmion stability. The dashed lines correspond to the the spin structured quasielectron case, whereas the full lines correspond to the quasihole one. Top lines correspond to the case of \( \nu = 1 \), middle to \( \nu = 3 \) and bottom to \( \nu = 5 \). The scale on the abscissa is logarithmic. The width is \( w = 1.73\ell \).

In the paper by Song et al.\(^{14}\) the reported excitation at the parameter values of \( w = 1.73\ell, \omega_c = 0.56, \) and \( g = 1.72 \times 10^{-2} \) falls well outside the boundary expected from the Hartree-Fock calculation.

D. Effect of Impurities

It is tempting to speculate that inclusion of impurity effects can stabilize the skyrmions at values of \( g \) bigger than allowed in a pure sample. To test this idea we can include a simple model of an impurity in our calculation: a point charge (impurity) at a distance \( z_0 \) above the central plane of the system. It is replaced by an effective non-uniform charge density in the plane producing the same potential,

\[
\frac{1}{|\vec{r} - (\vec{r}_0 + \vec{z}_0)|} = \int d^2 r' \rho_{eff}(\vec{r}') \frac{1}{|\vec{r} - \vec{r}'|}.
\]

The effective density can be found to be

\[
\rho_{eff}(\vec{r}) = \frac{1}{2\pi} \frac{z_0}{(z_0^2 + R^2)^{3/2}}
\]

for \( z_0 > 0 \). Results with and without such an impurity are illustrated in Fig. 9. As may be seen, the impurity favors spin-polarized quasiparticle over skyrmion. A similar result is expected for a short-range (e.g. delta-function) impurity potential. Apparently the simplest models of disorder are not likely to explain the results of Ref.\(^{14}\). It is probable that more complicated impurities (e.g. multiply charged or magnetic ones) could stabilize the small-spin skyrmions at \( \nu = 3 \). However, in the absence of data indicating such types of disorder in real samples, an investigation of this phenomenon is left for future work.

FIG. 9. Comparison of skyrmion stability in a system without an impurity (dashed line) and the one with impurity at the distance of 2 magnetic lengths from the sample for \( \nu = 1 \) case. Cyclotron energy is \( 100.0e^2/\kappa\ell \) in both cases.

FIG. 10. The same as Fig. 9 for \( \nu = 3 \) case.

IV. CONCLUSION

In this paper we have presented a real-space method for computing Hartree-Fock states and energies of two-dimensional systems in magnetic fields, appropriate for systems with circular symmetry in which Landau level mixing may be important. The method was applied to compute the effects of Landau level mixing and screening on skyrmion states. It was found that in most cases these tend to destabilize skyrmions, with a notable exception...
occurring for the case of the quasielectron (antiskyrmion) around $\nu = 1$. The calculations indicate that Hartree-Fock states cannot account for the results of Ref. 14 (reporting skyrmions at $\nu = 3$). This is in agreement with earlier studies where Landau level mixing and screening were not included.

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