Skyrmion Physics Beyond the Lowest Landau Level Approximation

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The effects of Landau level mixing and finite thickness of the two-dimensional electron gas on the relative stability of skyrmion and single spin-flip excitations at Landau level filling factor $\nu = 1$ have been investigated. Landau level mixing is studied by fixed-phase diffusion Monte Carlo and finite thickness is included by modifying the effective Coulomb interaction. Both Landau level mixing and finite thickness lower skyrmion excitation energies and favor skyrmions with fewer spin flips. However, the two effects do not work ‘coherently’. When finite thickness is included the effect of Landau level mixing is strongly suppressed.

In a seminal paper Sondhi et al.\textsuperscript{4} predicted that if the ratio of the Zeeman energy to the exchange energy is sufficiently small the quasiparticle excitations of the $\nu = 1$ integer quantum Hall state should be charged ‘skyrmions’ with topologically nontrivial spin textures.\textsuperscript{5} The existence of these exotic excitations is now well confirmed in typical experiments the number of reversed spins per skyrmion is

$$\hbar = \frac{1}{2m} \sum_{i=1}^{N} \left( \hat{r}_{i} \times \left( \frac{\hbar}{i} \nabla_{i} + \frac{e}{c} A_{i} \right) \right)^{2} + V_{C} + H_{Z}. \quad (1)$$

Here $V_{C} = \sum_{i<j} V(r_{ij})$ is the Coulomb interaction where $r_{ij}$ is the chord distance between electrons $i$ and $j$ and $H_{Z} = -\mu_{B} \sum_{i} S_{i} \cdot B$ is the Zeeman interaction. We work in the Wu-Yang gauge in which the vector potential is $A = e_{0} \hbar c N_{\phi}(1 - \cos \theta) / (2eR \sin \theta)$. The softening of the short-range part of the Coulomb interaction due to finite thickness of the lowest subband wave function of the 2DEG is included through the modified interaction

$$V(r) = \frac{e^{2}}{\epsilon \sqrt{r^{2} + \beta^{2}}}$$

where $\beta$ is a parameter characterizing the thickness.\textsuperscript{6}

For the $\nu = 1$ ground state the electron spins are fully polarized and the lowest Landau level is completely full. On the sphere this occurs when $N = N_{\phi} + 1$ and the corresponding wave function is a Slater determinant of lowest Landau level wave functions. If the electron positions are given in terms of the complex coordinate $z = \tan(\theta/2) \exp(-i\phi)$, where $\theta$ and $\phi$ are the usual spherical angles, then, exploiting the Vandermonde form of the Slater determinant, the ground state wave function can be written

$$\psi_{gs} = U^{N_{\phi}/2} \prod_{i<j} (z_{i} - z_{j}) \otimes (\uparrow_{1} \uparrow_{2} \cdots \uparrow_{N}) \quad (2)$$

where $U = \prod_{k}(1 + |z_{k}|^{2})^{-1}$.

Single spin-flip excitations of the system are constructed by removing a spin up electron from the ground state, flipping its spin, and reintroducing it into the lowest spin-down Landau level. Letting $K$ denote the number of reversed spins associated with a given quasiparticle excitation this procedure produces a $K = 0$ quasihole with charge $+e$ and a $K = 1$ quasielectron with charge $-e$. The transport gap which determines the activated temperature dependence of the longitudinal resistivity at $\nu = 1$ is set by the excitation energy for creating a quasielectron and quasihole with infinite separation. On the
energies. The variational result for the Coulomb contribution to the energy gaps computed using these states in which the kinetic energy is completely quenched with up to 100 electrons. For \( \beta = 0 \) our results agree with previous calculations of \( \delta(K) \).

\[ \psi_{sf} = A U^{N_A/2} \prod_{i<j, i \neq 1} (z_i - z_j) \otimes (\downarrow_1 \uparrow_2 \cdots \uparrow_N) \]  

where the operator \( A \) antisymmetrizes the wave function under the exchange of all pairs of electrons.

The nature of the quasiparticle excitations at \( \nu = 1 \) depends on the relative size of the Zeeman energy and the exchange energy characterized by the dimensionless ratio \( \tilde{g} = g \mu_B B/(e^2/\varepsilon_l) \). In the limit of large \( \tilde{g} \) the transport gap for the \( \nu = 1 \) integer quantum Hall state is set by the single spin-flip excitation described above. However, as \( \tilde{g} \) is lowered below a critical value the single spin flip becomes unstable to the formation of a neutral skyrmion pair, i.e. a well separated charge +e and charge \(-e\) skyrmion pair, involving more than one flipped spin. A microscopic wave function description of the charge +e skyrmion excitations was developed by MacDonald, Fertig, and Brey who showed that for a model Hamiltonian with a hard-core delta-function repulsion the states

\[ \psi_{sk}(K) = A U^{(N_A+1)/2} \prod_{i<j} (z_i - z_j) \times z_{K+1} z_{K+2} \cdots z_N \otimes (\downarrow_{1} \cdots \downarrow_{K+1} \uparrow_{K+1} \cdots \uparrow_{N}) \]  

are exact eigenstates of \( H \) with charge \( e \) and \( K \) reversed spins.

The wave functions \( \psi_{gs}, \psi_{sf} \) and \( \psi_{sk}(K) \) describe states in which the kinetic energy is completely quenched and there is no Landau level mixing. Therefore the only contributions to the energy gaps computed using these wave functions will come from the Coulomb and Zeeman energies. The variational result for the Coulomb contribution to the single spin-flip energy gap is

\[ \Delta_{sf} = \langle \psi_{sf}|V_C|\psi_{sf} \rangle - \langle \psi_{gs}|V_C|\psi_{gs} \rangle. \]  

In the absence of Landau level mixing an exact particle-hole symmetry in the lowest Landau level transforms a charge +e skyrmion with \( K \) reversed spins into a charge \(-e\) skyrmion with \( K + 1 \) reversed spins. It is therefore possible to compute the energy gap for creating a neutral skyrmion pair by first computing \( \Delta_{sf} \) and then computing the change in Coulomb energy of the charge +e skyrmion as the number of reversed spins is increased,

\[ \delta(K) = \langle \psi_{sk}(K)|V_C|\psi_{sk}(K) \rangle - \langle \psi_{sk}(0)|V_C|\psi_{sk}(0) \rangle. \]

As pointed out by Abolfath et al. the wave functions involve power-law tails which lead to strong finite-size effects. In our variational calculations we have computed \( \delta(K) \) for \( \beta = 0 \) and \( \beta = \ell_0 \) by doing a careful extrapolation to the thermodynamic limit, considering systems with up to 100 electrons. For \( \beta = 0 \) our results agree with previous calculations of \( \delta(K) \).

\[ \Delta_{gs}(\tilde{g}) = \Delta_{sf} + 2\delta(K) + S \tilde{g} \frac{\varepsilon^2}{\varepsilon_l}. \]  

These gaps are plotted vs. \( \tilde{g} \) in Fig. 1 for \( S = 1, 3, 5 \) and 7 and for \( \beta = 0 \) and \( \beta = \ell_0 \). In contrast to Hartree-Fock calculations which describe continuously varying spin textures, our results show the quantum nature of the skyrmion. As \( \tilde{g} \) decreases the energy gap undergoes level crossings in which the total number of reversed spins of the neutral skyrmion pair jumps by two. Note that although we have extended the \( S = 7 \) line down to \( \tilde{g} = 0.01 \) we expect that as \( \tilde{g} \) decreases the density of level crossings will increase until the energy gap becomes, effectively, a smooth function of \( \tilde{g} \).

Increasing the thickness of the 2DEG is seen to lower the skyrmion energy gaps and favors excitations with fewer spin flips. This effect can be understood qualitatively by noting that as the number of reversed spins \( K \) increases the charge of the skyrmion spreads out resulting in a lowering of its Coulomb energy. When the thickness is increased, and consequently the short-range part of the electron-electron repulsion is decreased, the excitation energies of the larger skyrmions will decrease less than those of the smaller skyrmions.

We now turn to the effect of Landau level mixing on the skyrmion energy gaps. The importance of Landau level mixing in a given system is characterized by the electron gas parameter \( r_s = 1/(a_B \sqrt{n}) \), where \( n \) is the carrier density and \( a_B = \hbar^2/2m_e \) is the effective Bohr radius. It is straightforward to show that \( r_s = (\nu/2)^{1/2}(e^2/\varepsilon_l)/\hbar \omega_c \) where \( \hbar \omega_c = \hbar e B/mc \) is the
coulomb energy so that, at fixed $\nu$, in the limit $r_s \to 0$ the coulomb energy is much larger than the Coulomb energy and there is no Landau level mixing. However, in typical experiments $r_s$ is of order 1 or higher and Landau level mixing cannot be ignored.

To study Landau level mixing we have used the fixed-phase diffusion Monte Carlo method,\(^{10}\) which has proven to be a useful tool for studying the effect of Landau level mixing on quantum Hall states.\(^{11}\) All of the wave functions considered here have been given in the form

$$ \psi = A \psi_{\text{space}}(r_1, \cdots, r_N) \otimes (\downarrow_1 \cdots \downarrow_K \uparrow_{K+1} \cdots \uparrow_N) \quad (8) $$

where $\psi_{\text{space}}$ is completely antisymmetric under the exchange of any pair of electrons $i$ and $j$ where either $1 \leq i, j \leq K$ or $K + 1 \leq i, j \leq N$. In a fixed-phase diffusion Monte Carlo simulation these wave functions are used as trial states by first writing the space part of the wave function in the form

$$ \psi_{\text{space}}(r_1, \cdots, r_N) = |\psi_{\text{space}}(r_1, \cdots, r_N)| e^{i\varphi(r_1, \cdots, r_N)} \quad (9) $$

then 'fixing' the trial phase $\varphi$, and finally constructing an effective bosonic Schrödinger equation for the positive definite wave function $|\psi_{\text{space}}|$ and solving that equation using standard diffusion Monte Carlo techniques.\(^{10}\) The result of this procedure is the lowest energy state of the form (8) subject to the constraint that the phase is the same as that of the trial function.

We have implemented this procedure using $\psi_{gs}$, $\psi_f$ and $\psi_{sk}(K)$ as trial wave functions to obtain, respectively, the fixed-phase energies $E_{gs}^{FP}$, $E_{sf}^{FP}$ and $E_{sk}^{FP}(K)$ for a system with 30 electrons. For finite $r_s$ it is no longer possible to transform a charge $+e$ skyrmion into a charge $-e$ skyrmion by particle-hole symmetry. Therefore, in order to calculate a physical quantity, we have computed the energy gaps for creating a charge $+e$ skyrmion with $K$ spin flip and a single spin-flip quasi-electron. As before, letting $\Delta sf = E_{sf}^{FP} - E_{gs}^{FP}$ and $\delta(K) = E_{sk}^{FP}(K) - E_{sk}^{FP}(0)$, the corresponding energy gaps are given by

$$ \Delta_s(\tilde{g}) = \Delta sf + \delta(K) + S\tilde{g} \frac{e^2}{\epsilon l_0} \quad (10) $$

where now $S = K + 1$.

FIG. 3. Spin and charge densities as a function of $r/l_0$ ($r$ is the chord distance on the sphere from the center of the skyrmion) for a charge $+e$ skyrmion with $K = 1$ for $r_s = 0$ and $r_s = 20$. Results are for a 30 electron system.

These energy gaps are plotted as a function of $\tilde{g}$ in Fig. 3 for $S = 1, 2$ and 3 and for $r_s = 0, 1$ and 5. As $r_s$ is increased the effect of Landau level mixing is seen to be qualitatively similar to that of finite thickness – the skyrmion excitation energies are lowered, with the smaller size skyrmions having their energies lowered the most. This effect can be understood qualitatively by examining the effect of Landau level mixing on the skyrmion spin and charge densities $\rho_s$ and $\rho_c$ defined by

$$ \rho_s(r) = \frac{\langle \psi_{sk}(K) | (\rho_s(r) \mp \rho_c(r)) | \psi_{sk}(K) \rangle}{\langle \psi_{sk}(K) | \psi_{sk}(K) \rangle} \quad (11) $$

where $\rho_s$ is the number density operator for spin $\sigma$ and $\sigma$ is the uniform number density far from the skyrmion. Fig. 3 shows mixed estimates of $\rho_s$ and $\rho_c$ for the $K = 1$ charge $+e$ skyrmion for $r_s = 0$ and $r_s = 20$. For $r_s = 20$ the possibility of mixing in higher Landau levels leads to a spreading out of the charge density of the skyrmion resulting in a lowering of its Coulomb energy at the cost of some kinetic energy. This effect is suppressed as $K$ increases because for larger values of $K$ the charge is already well spread out and there is less energy to be gained by allowing the charge to spread further.
In Fig. 4 the energy gaps are shown for $S = 1$, $2$ and $3$ and $r_s = 0, 1$ and $5$ for thickness parameter $\beta = l_0$. When finite thickness is included the Landau level mixing effect is seen to be much weaker than it is for zero thickness. For example, for $\tilde{g} \simeq 0.06$, when $\beta = 0$ the $r_s = 1$ energy gap is $\sim 25\%$ smaller than its $r_s = 0$ value, and when thickness is included the $r_s = 0$ energy gap drops $\sim 45\%$ for $\beta = l_0$, but the additional reduction of the energy gap due to Landau level mixing is only $\sim 5\%$ when $r_s = 1$.

FIG. 4. Energy gaps for creating neutral excitations consisting of a charge $+e$ single spin-flip quasielectron and a charge $-e$ skyrmion with $K = 0, 1$ and $2$ reversed spins for $r_s = 0, 1$ and $5$ as a function of $\tilde{g}$ for thickness parameter $\beta = l_0$. Each line segment is labelled by the total number of reversed spins $S = K + 1$. Results are for a $30$ electron system.

This weakening of the Landau level mixing effect due to finite thickness can be understood as follows. The thickness correction softens the short-range part of the Coulomb interaction, which in turn reduces the interaction energy the skyrmion stands to gain by delocalizing its charge. It follows that as $\beta$ increases, the quasielectron charge delocalizes less for a given value of $r_s$, and so the reduction of the energy gap decreases. Because of this suppression of the Landau level mixing effect by finite thickness we believe that the experimental observation by Schmeller et al. of skyrmion energy gaps which are significantly smaller than theoretical estimates which ignore Landau level mixing is more likely to be due to disorder effects, which are poorly understood, than Landau level mixing. Note that a similar reduction of the Landau level mixing effect due to finite thickness has been observed for spin-polarized Laughlin quasielectron and quasihole excitations in the fractional quantum Hall effect.

It is apparent from Figs. 2 and 4 that although finite thickness strongly suppresses Landau level mixing, the opposite is not the case. This is consistent with the observations of Králík et al. who performed variational Monte Carlo calculations of the effect of Landau level mixing and finite thickness on the $\nu = 1$ single spin-flip energy gap $\Delta_{sf}$, finding that for $r_s = 1$ the inclusion of finite thickness, of roughly the same size as that considered here, significantly reduced the energy gap. Based on this observation Králík et al. concluded that both finite thickness and Landau level mixing contribute equally to the reduction of the energy gap. However, we believe that if Králík et al. had first included finite thickness and then Landau level mixing they would have observed the same strong suppression of the Landau level mixing effect reported here.

To summarize, using skyrmion trial states recently introduced by MacDonald, Fertig, and Brey, we have performed variational and fixed-phase diffusion Monte Carlo calculations of the effect of finite thickness and Landau level mixing on skyrmion excitations at $\nu = 1$. We find that both effects lower the skyrmion excitation energies and stabilize skyrmions with fewer spin flips. However, we also find that the two effects do not work coherently together — when finite thickness is included the effect of Landau level mixing is strongly suppressed.

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