Hartree-Fock theory of Skyrmions in quantum Hall ferromagnets

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We report on a study of the charged-Skyrmion or spin-texture excitations which occur in quantum Hall ferromagnets near odd Landau-level filling factors. Particle-hole symmetry is used to relate the spin-quantum numbers of charged particle and hole excitations and neutral particle-hole pair excitations. Hartree-Fock theory is used to provide quantitative estimates of the energies of these excitations and their dependence on Zeeman coupling strength, Landau-level quantum numbers, and the thicknesses of the two-dimensional electron layers. For the case of ν near three we suggest the possibility of first-order phase transitions with increasing Zeeman coupling strength from a many-Skyrmion state to one with many maximally spin-polarized quasiparticles. [S0163-1829(97)08016-8]

I. INTRODUCTION

In the limit of strong magnetic fields where all electrons are confined to a single orbital Landau level, interacting two-dimensional electron systems (2DES's) exhibit a rich variety of unusual properties. The quantum Hall effect, which occurs when the chemical potential of the 2DES has a discontinuity at a density n^* which depends on magnetic-field strength,[1] is a prominent example. In the quantum Hall effect the incompressible ground state at density n^* can be a strong ferromagnet, i.e., its total spin quantum number S can equal $N/2$, so that electronic spins are completely aligned by infinitesimal Zeeman coupling. Surprisingly, in light of the strong magnetic fields, the physics associated with *spontaneous* magnetization in these systems is experimentally accessible because the Zeeman coupling is typically quite weak compared to other characteristic energy scales and can even be tuned to zero, for example, by the application of hydrostatic pressure to the host semiconductor. Recently there has been considerable interest in charged excitations of the incompressible ground state at $\nu=1$ which has total spin quantum number $S=N/2$. As first noticed in numerical exact diagonalization calculations,[2] and demonstrated in recent experiments,[3,4] the spin polarization in these systems is strongly reduced away from $\nu=1$, where the ground state must incorporate the charged excitations of the $\nu=1$ state. This behavior can be understood,[5,6] quantitatively in the limit of very weak Zeeman coupling, by identifying the elementary charged excitations with the topological solitons (Skyrmions) of the $O(3)$ nonlinear sigma ($NL\sigma$) model in two spatial dimensions.[7] With an appropriate kinetic term,[8] the latter describes the long-wavelength $T=0$ dynamics of any Heisenberg ferromagnet in two dimensions. Two features distinguish the quantum Hall case. First, the Skyrmions carry electrical charge as a consequence of their topological charge,[9,5,10] and hence have a stable finite size for small but nonzero Zeeman coupling. Second, they are present in the ground state near (but not precisely at) $\nu=1$, and as a consequence have an obvious influence on observable properties.

In this article we discuss the elementary charged excitations of quantum Hall ferromagnets using a Hartree-Fock approximation approach.[6,11] The Hartree-Fock approximation can describe charged excitations which are sufficiently localized in space to invalidate the gradient expansion that underlies the $NL\sigma$ model description. A weakness of both the Hartree-Fock and $NL\sigma$ model calculations, which we will discuss further below, is the failure to respect the quantization[12–14] of total electronic spin. This paper is organized as follows. In Sec. II we make some general remarks on the implications of particle-hole symmetry for relationships between the energies and spin quantum numbers of

positively and negatively charged excitations of quantum Hall ferromagnets and for the neutral decoupled particle-hole pair excitations which are important in activated transport experiments.[15] The considerations in this section do not depend on the Hartree-Fock approximation. In Sec. III we explain some formal aspects of the Hartree-Fock approximation calculations we perform in order to explore the elementary charged excitations, and how their energetic ordering depends on Zeeman coupling strength. Section IV presents and discusses our numerical results. We comment on the importance of the orbital Landau-level index[16] and on the thickness of two-dimensional electron layers. We conclude with a brief summary in Sec. V. An Appendix discusses the spectral transfer in the presence of the Skyrmion, analogous to that underlying midgap states in solitons in one-dimensional systems.

We close this section with a remark on the terminology used in this paper. In $NL\sigma$ models the energy of a ferromagnet is expressed in terms of a function which specifies the direction of the local ordered moment as a function of the two-dimensional spatial coordinate. The energy functional in the ''pure'' $NL\sigma$ model invoked in discussions of broken symmetry states contains only a gradient term and the topological solitons of this model can be determined exactly.[7] As the gradient term is scale invariant in two dimensions, the energy of these solutions is independent of their size. The $NL\sigma$ model appropriate for quantum Hall ferromagnets with a small Zeeman coupling has two additional terms which compete: a Zeeman coupling which favors small Skyrmions, and a Coulomb interaction which favors large Skyrmions; together these determine the size and energy of the Skyrmion and also its precise profile which differs from those of the pure $NL\sigma$ model solutions.[17] In a microscopic quantum treatment[13,2] a spin multiplet of elementary charged excitations with total spin $S=N/2-K$ exists for each non-negative integer K. At large values of K, the correlations of the quantum states are well described by the classical soliton solutions; presumably, a treatment of the fluctuations about them, along the lines of soliton quantization in other problems,[7] would reproduce the exact states. However, frequently the lowest-energy charged excitations occur at relatively small integer values of K, where both the symmetry-restoring quantum fluctuations and the neglected higher gradient terms are large, and the field-theoretic description is no longer accurate. While, strictly speaking, one might wish to reserve the term ''Skyrmion'' for excitations that are well described by the $NL\sigma$ model solitons, in this paper we take the liberty of referring to all elementary charged excitations of quantum Hall ferromagnets as Skyrmions.

II. PARTICLE-HOLE SYMMETRY

When the spin degree of freedom is included, the particle-hole symmetry of the Hamiltonian[1] for interacting electrons in the lowest Landau-level relates electronic states at Landau level filling factors ν and $2-\nu$. Here $\nu \equiv N/N_\phi$, where N is the number of electrons, and $N_\phi = AB/\Phi_0 \equiv A/(2\pi\ell^2)$ is the orbital degeneracy of the Landau level. (B is the magnetic-field strength, $\Phi_0 = hc/e$ is the electronic magnetic flux quantum, and ℓ is the magnetic length.) The particle-hole symmetry of this system occurs because, apart from the constant quantized kinetic energy which is conventionally chosen as the zero of energy, the Hamiltonian contains only the term describing interactions of electrons within a degenerate Landau level. In the occupation number representation, many-particle states can be specified either by the set of single-particle states within the Landau level which are occupied or by specifying the set which are empty, i.e., by specifying the states occupied by holes in the Landau levels. It is convenient to combine the particle-hole transformation with a spin reversal, so that the creation operators for spin-up particles are mapped to annihilation operators for spin-down holes, and creation operators for spin-down particles are mapped to annihilation operators for spin-up holes. Under this mapping

$$N_\uparrow \to N_\phi - N_\downarrow \equiv N'_\uparrow ,$$

$$N_\downarrow \to N_\phi - N_\uparrow \equiv N'_\downarrow . \tag{1}$$

It follows that $N = N_\uparrow + N_\downarrow \to N' = 2N_\phi - N$ and $S_z = (N_\uparrow - N_\downarrow)/2 \to S'_z = S_z$, where S_z is the $\hat{z}$ component of the total spin. The Hamiltonian H changes by a constant[18]

$$H = H' + 2(N - N_\phi)\epsilon_0 = H' + 2(N_\phi - N')\epsilon_0 , \tag{2}$$

where H' is normal ordered in terms of hole creation and annihilation operators and is identical to H except for the replacement of electron operators by hole operators, and ϵ_0 is the energy per electron in the ground state at $\nu = 1$ which is readily calculated for any specified model electron-electron interaction. For 2D electron systems with a uniform neutralizing positive background charge,

$$\epsilon_0 = -\tfrac{1}{2}\int \frac{d^2\vec{q}}{(2\pi)^2} \exp(-|q|^2\ell^2/2) v(q), \tag{3}$$

where $v(q)$ is the Fourier transform of the effective electron-electron interaction.

In the following sections we will evaluate the energy change in the system when a single electron is removed from the system at a fixed magnetic field. As mentioned above and shown in Ref. 13, the set of elementary charged excitations at $N = N_\phi - 1$ is composed of a single spin multiplet with $S = N/2 - K$ for each non-negative integer K. With finite Zeeman coupling, the lowest-energy state in each multiplet has $S_z = S = N/2 - K = N_\phi/2 - (K + 1/2)$, and the energy of this state relative to the $\nu = 1$ ground state of the quantum Hall ferromagnet may be written as

$$\epsilon_K^- = U_K + g^* \mu_B B (K + \tfrac{1}{2}). \tag{4}$$

Here g^* is the g factor of the host semiconductor, and U_K may be interpreted as the interaction contribution to the internal energy of the quasihole. It follows from the particle-hole transformation [Eq. (1)] that the corresponding elementary charged excitations at $N = N_\phi + 1$ have $S_z = S = N'/2 - K = N_\phi/2 - (K + \frac{1}{2})$, and an energy relative to the $N = N_\phi$ ground state given by

$$\epsilon_K^+ = U_K + 2\epsilon_0 + g^* \mu_B B (K + \tfrac{1}{2}). \tag{5}$$

For example, the state with $K = 0$ is the single-Slater-determinant elementary excitation which appears in the stan-

dard Hartree-Fock approximation. Note that ϵ_K^- and ϵ_K^+ differ by a constant, so that their minima always occur at the same value of K. For two-dimensional electrons in the lowest Landau level with purely Coulombic interactions, $U_{K=0}=(e^2/\epsilon\ell)(\pi/2)^{1/2}$ and $\epsilon_0=-(e^2/\epsilon\ell)(\pi/8)^{1/2}$, so that $\epsilon_{K=0}^-=U_{K=0}+g^*\mu_B B/2$ and $\epsilon_{K=0}^+=g^*\mu_B B/2$. It follows[5] from the $NL\sigma$ model that $U_{K\to\infty}=\frac{3}{4}U_{K=0}$, so that large-$K$ states will have lower energy if the Zeeman coupling is sufficiently weak. At intermediate values of K, numerical calculations of one sort or another are necessary to estimate U_K. In Sec. III we use a generalized Hartree-Fock approximation to obtain realistic estimates of U_K including effects of the finite thickness of the quasi-two-dimensional electron layers, and to discuss the influence of the Landau-level index for which the quantum Hall ferromagnet occurs.

The value of K at which ϵ_K^- and ϵ_K^+ are minimized has been determined experimentally both by measuring the ground-state spin polarization[3,4] near $\nu=1$, and by measuring[15] the dependence on Zeeman coupling strength of energy required for the creation of free-particle-hole pairs at $\nu=1$. For ν close to 1, interactions between elementary charged excitations can be neglected,[19] so that the partial spin polarization is given for $\nu<1$ by

$$\xi\equiv\frac{N_\uparrow-N_\downarrow}{N_\uparrow+N_\downarrow}=\frac{2S_z}{N}\approx 1-2K(1-\nu)/\nu, \tag{6}$$

and for $\nu>1$ by

$$\xi\equiv\frac{2S_z}{N}\approx 1-2(K+1)(\nu-1)/\nu. \tag{7}$$

Note that $d\xi/d\nu=2K$ just below $\nu=1$ and $-2(K+1)$ just above $\nu=1$. The polarization ξ may be measured in experiments[3,4] that are sensitive to the spin magnetization of the system. Finally, the activation gap Δ measured in transport studies[15] is the energy to make an unbound particle-hole pair,

$$\Delta=\epsilon_K^+ + \epsilon_K^- = 2U_K + 2\epsilon_0 + g^*\mu_B B(2K+1). \tag{8}$$

The derivative of this energy with respect to the strength $(g^*\mu_B B)$ of the Zeeman coupling term is $2K+1$. As we discuss at greater length below, experiments[3,4,15] performed at typical fields in GaAs 2DES's are all consistent with $K=3$, in good agreement with calculations presented in subsequent sections.

III. QUASIPARTICLE ENERGIES AND EXCITATION GAPS

In this section some formal aspects of the Hartree-Fock theory for the charged excitations at $\nu<1$ are briefly discussed. Further technical details are provided in a previous paper on this topic[6] and in the Appendix. (The excitations at $\nu>1$ may be obtained from these by particle-hole symmetry as explained above.) Because of the symmetry of the Skyrmion charged excitations, it is convenient to work in the symmetric gauge where single-particle wave functions in the lowest Landau-level (LLL) have the simple form

$$\phi_m(z)=\frac{z^m\exp(-|z|^2/4\ell^2)}{(2^{m+1}\pi\ell^2 m!)^{1/2}}. \tag{9}$$

Here $m=0,1,\ldots$ is the angular momentum, and $z=x+iy$ expresses the 2D coordinate as a complex number. Note that states with larger m are localized further and further from the origin. We consider single-Slater-determinant states of the form

$$|\Psi\rangle=\prod_{m=0}^{\infty}(u_m a_m^\dagger + v_m b_{m+1}^\dagger)|0\rangle, \tag{10}$$

where $|0\rangle$ is the particle vacuum and $|u_m|^2+|v_m|^2=1$, so that the wave function is normalized. Here $a_m^\dagger$ creates a down-spin electron and $b_m^\dagger$ creates an up-spin electron in the mth angular momentum state.

The form of these wave functions is essentially dictated by the symmetry of the classical Skyrmion solutions which are invariant under the action of $L_z\pm S_z$ for the Skyrmion (anti-Skyrmion). This plus the requirement of LLL occupancy uniquely picks Eq. (10) as the appropriate Hartree-Fock wave functions. It is also easy to demonstrate, using Eq. (10), that the expectation value of the total spin operator in this state describes a spin texture with unit topological charge, provided that u_m varies slowly with m from $u_{m=0}=1$ to $u_{m\to\infty}=0$ ($v_{m=0}=0$ and $v_{m\to\infty}=1$).

This wave function is a generalization of the single-Slater-determinant wave function proposed[11] by Moon *et al.*, for which the expectation value of the vector spin operator gives a spin texture identical with that of the pure $NL\sigma$ model Skyrmion. The additional variational freedom in the wave function of Eq. (10) allows deviations from the pure $NL\sigma$ model, so that microscopically localized charged excitations may be optimized in a way which depends on the details of the 2DES being considered. Far from the origin, this state is locally identical to ferromagnetic ground states, and all spins are aligned with the Zeeman magnetic field which is assumed to point in the ''up'' direction. Near the origin the projection of the total spin along the field direction becomes negative. It is easy to establish that the total decrease in electron charge near the origin compared to the ferromagnetic ground state $(\Pi_{m=0}^\infty b_m^\dagger|0\rangle)$ corresponds to one electron. The total number of reversed spins in this wave function is

$$K=\sum_{m=0}^{\infty}|u_m|^2. \tag{11}$$

The $K=0$ Hartree-Fock hole excitation is obtained by choosing $u_m=0$ for all m. Note that the quantization of the number of reversed spins is not captured by these generalized Hartree-Fock variational wave functions. The quantization is obviously of some importance in the usual experimental circumstance since K is small. In this case better variational wave functions could be obtained, in principle, by projecting[12,13] the Hartree-Fock wave functions onto states with definite numbers of reversed spins. Here we account for quantization when necessary simply by restricting ourselves to solutions where K (the *mean* number of reversed spins) is an integer.[20]

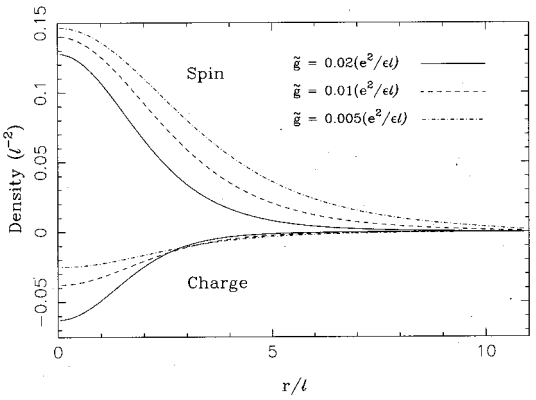

FIG. 1. Charge and spin densities for quasihole Skyrmions in the lowest Landau level for a system of zero thickness, evaluated for different values of $\tilde{g}$. The maximum angular momentum state kept in these computations was $M_{\max}=120$ (see text).

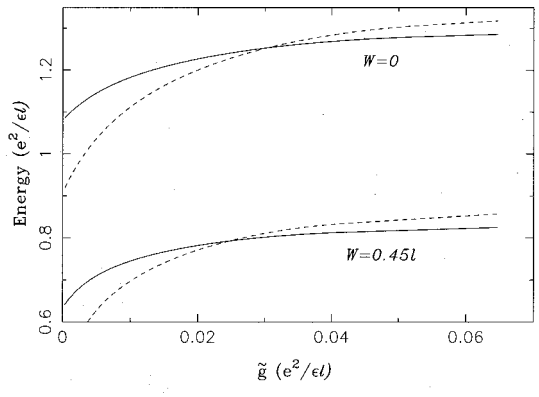

FIG. 2. Minimum hole creation energy (solid line) and transport activation energy (dashed line) in a $\nu=1$ quantum Hall ferromagnet as a function of $\tilde{g}$. All energies are in units of ($e^2/\epsilon\ell$), and results are shown for both strictly 2D and finite-thickness models. The maximum angular momentum state in these calculations was $M_{\max}=120$.

We find optimized Skyrmion wave functions by minimizing $\langle\Psi|H|\Psi\rangle$, where the Hamiltonian includes electron-electron interactions and Zeeman coupling. This procedure gives rise to a set of self-consistent equations listed in Ref. 6 which need to be solved numerically. Some typical results for the spin and charge densities relative to the ground state are illustrated in Fig. 1 for Skyrmions in the lowest Landau level in a sample of vanishingly small thickness, for several values of[21] $\tilde{g}$, where $\tilde{g}\equiv g^*\mu_B B$ is the Zeeman coupling strength.[22] The total energy of this state, relative to the energy of the ferromagnetic ground state, can be separated into interaction energy and Zeeman energy contributions as in Eq. (4):

$$\epsilon^-(K(\tilde{g}))=U(K(\tilde{g}))+\tilde{g}[K+\tfrac{1}{2}]. \tag{12}$$

For each value of $\tilde{g}$ the self-consistent Hartree-Fock (HF) equations determine the value of K which minimizes ϵ and, given K, the shape of the Skyrmion state (specified by the u_m values) which minimizes the interaction energy. For pedagogical purposes and for comparison with the field-theoretical approach it is useful to consider the interaction energy as a function of K rather than $\tilde{g}$. $U(K)$, which is just the Legendre transform of $\epsilon^-(K)$, can be obtained from the $K(\tilde{g})$ and $\epsilon^-(K(\tilde{g}))$ produced by the self-consistent Hartree-Fock calculations using Eq. (12). Formally minimizing Eq. (12) with respect to K, we find that the optimal value of K for a given $\tilde{g}$ is determined by

$$\tilde{g}=-\frac{dU(K)}{dK}. \tag{13}$$

Thus the global relationship between the equilibrium value of K and the Zeeman coupling strength is conveniently summarized in a plot of dU/dK versus K. We will use such plots in Sec. IV to discuss the importance of the finite thickness of two-dimensional electron layers and of the Landau-level index of the ferromagnetic state in determining $K(\tilde{g})$. The naive expectation is that the lowest-energy Skyrmion state should monotonically shrink as $\tilde{g}$ increases; we see from Eq. (13) that this is possible only if $d^2U(K)/d^2K$ is positive definite, which is the usual requirement of convexity needed to obtain a continuous Legendre transform. The maximum value of $-dU(K)/dK$ gives the maximum value of $\tilde{g}$ at which Hartree-Fock Skyrmion states with $K\neq 0$ occur.

IV. HARTREE-FOCK THEORY NUMERICAL RESULTS

A. Lowest Landau level: $n=0$

In Figs. 2 and 3 we show results for $\epsilon(K(\tilde{g}))$, $\Delta(K(\tilde{g}))$ and $K(\tilde{g})$ obtained by solving the Hartree-Fock equations at a series of $\tilde{g}$ values for the case of a strictly 2D electron system and for the case of a quasi-2D electron system with the finite layer thickness modeled to approximate the typical experimental situation. Finite thickness can be introduced into the calculation by assuming all the electrons are in the same confined state $\chi(z)$ of either the inversion layer or quantum well in which they reside. The effective two-dimensional electron-electron interaction may then be written in the form

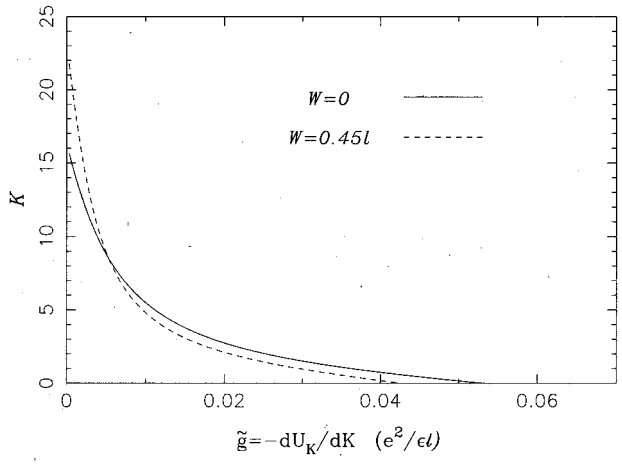

FIG. 3. Number of reversed spins per hole in a $\nu=1$ quantum Hall ferromagnet as a function of $\tilde{g}/(e^2/\epsilon\ell)$. Results are shown for both strictly 2D and finite-thickness models. Note that for self-consistent solutions of the Hartree-Fock equations $\tilde{g}=-dU(K)/dK$. The maximum angular momentum state in these calculations was $M_{\max}=120$.

$$v(\vec{r}) = \int \frac{d^2k}{(2\pi)^2} e^{i\vec{k}\cdot\vec{r}} \int dz_1 dz_2 |\chi(z_1)|^2 |\chi(z_2)|^2 \times \frac{2\pi e^2}{k} e^{-k|z_1 - z_2|},$$

which is softer than the Coulomb interaction at short distances, but at large distances approaches the $1/r$ form. The precise wave function chosen for our calculation is the Fang-Howard[25] form $\chi(z) = [12W^3]^{-1/2} z e^{-z/2W}$, where W may be understood as a measure of the thickness of the two-dimensional layer. Finite-thickness corrections tend to reduce the energy scales of this system; for example, $\epsilon_0 = -0.6267$ for the strictly 2D model, and $\epsilon_0 = -0.3963$ for the quasi-2D finite-thickness model for $W = 0.45\ell$. However, we have found that the optimal values for the total number of flipped spins in the Skyrmion states are not dramatically affected by finite thickness.

In Fig. 2, we see that both ϵ and Δ rise rapidly toward their $K=0$ values as $\tilde{g}/(e^2/\epsilon\ell)$ increases. The rapid increase in the energy with increasing $\tilde{g}$ is associated with the rapid shrinking of the optimal size of the Skyrmion charged excitation, as seen in Fig. 3. For typical experimental systems,[3,4,15] $\tilde{g} \approx 0.015 - 0.020 e^2/\epsilon\ell$ and the measured number of flipped spins $K \approx 3$, in good agreement with the present numerical results. The small Zeeman coupling strength required to reduce Skyrmions to microscopic size is at first sight surprising, and reflects the relatively weak K dependence of $U(K)$. As explained in Sec. III, $U(K=0) - U(K=\infty) = (\pi/32)^{1/2}(e^2/\ell)$ for the Coulomb interaction model. For large K the principal correction to the $NL\sigma$ model $K \to \infty$ value for $U(K)$ is the Coulomb self-interaction of the excess charge. Assuming that the spin and charge structure of the Skyrmion have the same size, this energy is $\sim (e^2/\ell) K^{-1/2}$. From Eq. (13) the optimal value of K implied by this approximation is $\propto \tilde{g}^{-2/3}$, while the change in ϵ is proportional to $\tilde{g}^{1/3}$. A more careful analysis[5] by Sondhi *et al.* replaced $\tilde{g}$ in these estimates by $\tilde{g}|\ln(\tilde{g})|$. The $\tilde{g}^{1/3}$ behavior at small $\tilde{g}$ means that even weak Zeeman coupling compared to the characteristic interaction energy is sufficient to eliminate most of the energy difference between the lowest-energy charged excitation and the $K=0$ Hartree-Fock quasiparticle energy.

As explained in Sec. III we can extract results for $U(K)$, the internal energy of a Skyrmion hole as a function of the number of reversed spins, from Figs. 2 and 3. These results are shown in Fig. 4. Note that $d^2U(K)/dK^2$ is positive definite. The property that $K(\tilde{g})$ is not markedly altered by finite-width corrections to the effective interaction is associated with the weak K dependence of the difference between the two curves in this figure. The results shown here hint at a practical technical difficulty with these Hartree-Fock calculations. In practice we are forced to truncate the set of single-particle angular momenta we include in our wave functions for both the ferromagnetic ground state and for the charged excitation at a finite value of $m = M_{\max}$. Since the single-particle orbital with angular momentum m is localized near a ring with radius $\ell[2(m+1)^{1/2}]$, this corresponds to working with a finite-size electron disk of radius $R \approx \ell(2M_{\max})^{1/2}$. The energy difference between the ferromagnetic ground state and the state with the charged excitation will be given accurately by our calculation if the tail of the disturbance associated with the charged excitation does not extend to the edge of our system. As the Zeeman coupling weakens and the Skyrmions become larger, finite-size effects become increasingly important. It is for this reason that the $U(K)$ results shown in Fig. 4 do not accurately approach the analytically known $K \to \infty$ asymptote, which for the case of strictly 2D interactions has the value $(9\pi/32)^{1/2}(e^2/\epsilon\ell) \approx 0.94(e^2/\epsilon\ell)$. (It is possible, however, to obtain an accurate value for this limit by regularizing the $\tilde{g}=0$ Skyrmion by placing it on a sphere. This is sketched in the Appendix.) The smaller the value of $\tilde{g}$, the larger the value of $M_{\max}$ required to obtain accurate results. The convergence properties of our calculations with respect to $M_{\max}$ are illustrated in Fig. 5, where K is plotted as a function of $(\tilde{g}|\ln(\tilde{g})|)^{-2/3}$. From the asymptotic analysis[5] we know that for $M_{\max} \to \infty$ this curve will follow a roughly straight line for large K. For each finite $M_{\max}$ the numerical results bend away from this line, underestimating the number of reversed spins in the lowest-energy charged excitation. From Fig. 5 we estimate that calculations performed with $M_{\max} = 120$ are accurate for $\tilde{g} > 0.01(e^2/\ell)$, calculations with $M_{\max} = 480$ are accurate for $\tilde{g} > 0.005(e^2/\ell)$, and calculations with $M_{\max} = 1920$ are accurate for $\tilde{g} > 0.002(e^2/\ell)$. The number of angular momentum states required to obtain good convergence for the total number of

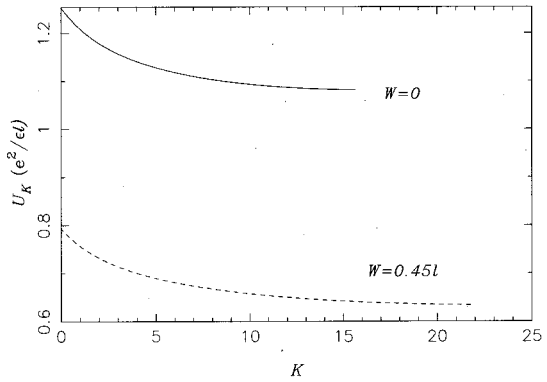

FIG. 4. Internal energy of a Skyrmion hole U as a function of the number of reversed spins K. Results are shown for both strictly 2D and finite-thickness models. The maximum angular momentum state in these calculations was $M_{\max} = 120$.

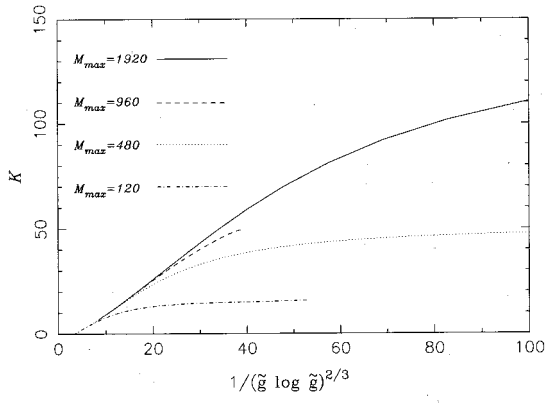

FIG. 5. Number of reversed spins in a Skyrmion hole at weak Zeeman coupling as a function of finite system size.

flipped spins K is much larger than K, despite the fact that the u_m and v_m approach their ground-state values relatively rapidly for $m>K$. As expected from the variational nature of the Hartree-Fock calculations, the energies presented in Fig. 2 and Ref. 6 approach their asymptotic values much more rapidly with increasing $M_{\max}$ than estimates of the optimal value of K. Finally, we note that, except where the contrary is explicitly stated, results reported here and in Ref. 6 were obtained with $M_{\max}=120$. In particular this means that the values of K presented in Fig. 2 below $\tilde{g}=0.01(e^2/\epsilon\ell)$ are slightly underestimated; however, we have found no significant errors in the energies of Fig. 1 for $\tilde{g}>0.002(e^2/\epsilon\ell)$.

In Fig. 4 it is interesting to note that $U(K)$ approaches $K=0$ with a finite slope. This is seen most clearly in Fig. 3 which, using Eq. (13), can be regarded as a plot of K vs $-dU(K)/dK$. The maximum slope of $U(K)$ occurs at $K=0$ and, since $|dU/dK|$ increases monotonically with decreasing K, this slope specifies the largest value of $\tilde{g}$ for which a $K\neq 0$ solution of the Hartree-Fock equations occurs. The property that the Hartree-Fock Skyrmion decreases continuously to zero size with increasing $\tilde{g}$ contrasts with properties which would follow from other forms for $U(K)$. For example if $U(K)$ approached its $K=0$ value from below quadratically, the maximum value of $-dU(K)/d(K)$ would occur at a finite value of K, and the Skyrmion would suddenly collapse to zero size once $\tilde{g}$ exceeded this value. If $U(K)$ approached its $K=0$ value from below as K^s with $s<1$, solutions with finite K would exist at arbitrarily large $\tilde{g}$. Finally, if $U(K)$ was an increasing function of K at small K, reaching a maximum at $K=K^*$, solutions with $K<K^*$ would not exist at any $\tilde{g}$. We will see below that this is precisely the situation which often occurs when the quantum Hall ferromagnet ground state has electrons in $n\neq 0$ Landau levels polarized.

As remarked in Sec. I, it is important to note that our Hartree-Fock approach does not respect the separate quantization of spin and orbital angular momentum in our system, and instead permits only the quantization of the difference of these two quantities. In the Hartree-Fock approximation, as in classical field theories, Skyrmions appear as broken symmetry states of the Hamiltonian. There is a similarity here to the standard BCS treatment of superconductivity, in which particle number is not a good quantum number in the mean-field ground state.[11,12] However, while in the BCS problem there really is a broken symmetry in the thermodynamic limit, in our problem the Skyrmion states only break the symmetry over a finite volume. Hence quantum fluctuations around the mean-field state will, if treated exactly, restore the individual quantization of spin and angular momentum. It is therefore important to address the extent to which these fluctuations influence the results in Fig. 2. In an exact calculation Fig. 2 would take the form of a series of straight-line segments, since the quantum number K can only take on integer values.[13] We expect the Hartree-Fock approach to yield a smooth interpolation of the exact results which is most accurate when its K value is integral. Comparison with exact finite-size calculations[23,24] confirm this expectation. (We note the fortunate feature that the Hartree-Fock treatment is exact both at vanishing $\tilde{g}$, where the infinite Skyrmion *is* a classical object up to trivial global rotations and at large $\tilde{g}$, where it describes the fully polarized quasihole.)

B. First Landau level: $n=1$

Quantum Hall ferromagnets occur at $\nu=1$ and also at larger odd integral filling factors. In the Hartree-Fock approximation, the ground state for $\nu=2n+1$ has all orbitals of both spins with a Landau-level index less than n occupied, and only majority-spin orbitals occupied in the nth Landau level. If Landau-level mixing is ignored, the fully occupied Landau levels play no role and the theory of quantum Hall ferromagnets is altered only by the change in the index of the Landau level onto which the electronic Hilbert space is projected. The Hartree-Fock single-Slater-determinant state is an exact eigenstate of the Hamiltonian just as in the $\nu=1$ case and is expected to be the ground state, at least if n is not too large. The change of Landau-level index may be accounted for without approximation simply by including an additional form factor correction to the effective electron-electron interaction. The Fourier transform of the interaction for electrons projected into the nth Landau level is[26] $v_n(q)=v(q)[L_n(q^2/2)]^2$, where L_n is the nth Laguerre polynomial, and $v(q)$ is the unprojected interaction. As for $\nu=1$, the $K=0$ and $K\to\infty$ limits of the charged excitation energy can[16] be calculated analytically when finite-thickness corrections are neglected. Wu and Sondhi[16] recently pointed out that, for $n\gg 1$, $U_{K\to\infty}>U_{K=0}$ so that Hartree-Fock quasiparticles have lower energy than large spin-texture quasiparticles even when the Zeeman energy is not included. Recent transport experiments[15] seem to imply that, for $\nu=3$, the lowest-energy charged excitations have $K=0$, in contrast with the $n=0$ case and in agreement with theory. In this section we examine the influence of the finite width of the electron layer on the energetics of the quasiparticles.

The competition between Hartree-Fock and charged spin-texture quasiparticles can be understood in terms of the analytically known expressions for the Hartree-Fock exchange energy per electron for a full Landau level [ϵ_0 in Eq. (3)] and for the spin stiffness[5,11]

$$\rho_s=\frac{1}{16\pi}\int\frac{d^2q}{(2\pi)^2}q^2v_n(q)e^{-q^2/2}. \tag{14}$$

Since $U_{K=0}=-2\epsilon_0$ and $U_{K\to\infty}=-\epsilon_0+4\pi\rho_s$, the difference is

$$\Delta U\equiv U(K=0)-U(K=\infty)$$
$$=-\epsilon_0-4\pi\rho_s=\tfrac{1}{4}\int\frac{d^2q}{(2\pi)^2}[2-q^2]v_n(q)e^{-q^2/2}. \tag{15}$$

For the Coulomb interaction model[16] $\Delta U=-\frac{1}{16}(\pi/2)^{1/2}(e^2/\epsilon\ell)$ in the $n=1$ ($\nu=3$) Landau level, and has a larger negative value for the $n=2$ ($\nu=5$) case. The $[L_1(q^2)]^2$ form factor for electrons in the $n=1$ Landau level strengthens the effective interaction at large q, which has more importance in ρ_s than in ϵ_0 because of the q^2 factor in its integrand. When finite-thickness form factors are also included in the effective interaction, the importance of large q in these integrals will diminish. For sufficiently wide quantum wells it is clear that the sign of ΔU will be positive, and charge spin textures will also occur in the $n=1$ Landau level. The objective of the calculations reported on below is

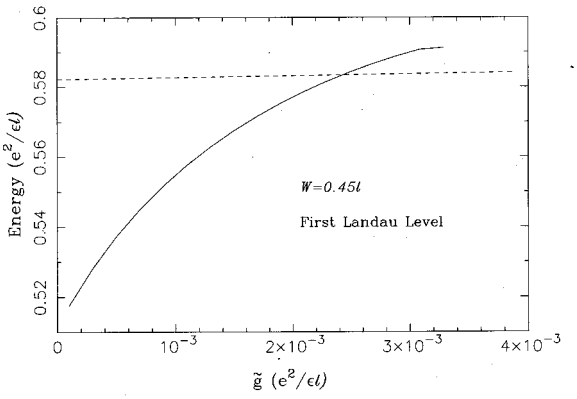

FIG. 6. Energy ϵ_K^- of the $K=0$ quasiparticle (dotted line) and the HF $K>0$ Skyrmion (solid line) as a function of $\tilde{g}$ for $\nu=3$ ($n=1$) and a 2DES with thickness parameter $W=0.45\ell$. The system size used for this calculation was $M_{\max}=480$. All energies are in units of $e^2/\epsilon\ell$.

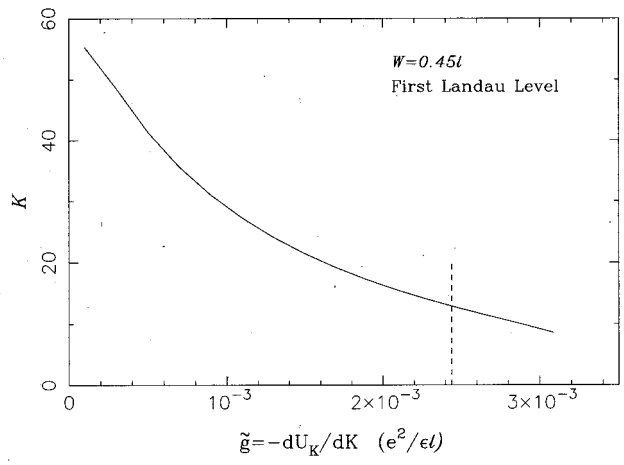

FIG. 7. Number of flipped spins K of the HF $K>0$ Skyrmion as a function of $\tilde{g}$, for $\nu=3$ ($n=1$) and a 2DES with thickness $W=0.45\ell$. Note that for self-consistent solutions of the Hartree-Fock equations, $\tilde{g}=-dU(K)/dK$. The system size used for this calculation was $M_{\max}=480$. All energies are in units of $e^2/\epsilon\ell$. The vertical dashed line indicates the value of $\tilde{g}$ above which the Skyrmion is unstable against the untextured quasihole.

to quantify the stability properties of Skyrmions in $n=1$ quantum Hall ferromagnets with finite width electron layers. We find that Skyrmions in the first Landau level can be stabilized by finite-thickness corrections, although for realistic widths the maximum $\tilde{g}$ for which they are the lowest-energy quasiparticles is roughly an order of magnitude smaller than for the $n=0$ case. Thus the observation of Skyrmions in the first Landau level would require specialized samples or experimental techniques to access this very low Zeeman energy limit.

Figure 6 illustrates the energy ϵ_K^- for both the $K=0$ quasiparticle (dotted line) and the optimal $K>0$ Skyrmion (solid line) as a function of $\tilde{g}$ for a typical experimental sample width, $W=0.45\ell$. The Skyrmion excitation is lower in energy for $\tilde{g}<2.4\times10^{-3}e^2/\epsilon\ell$. The results in Fig. 6 suggest that for filling factors close to, but slightly away from, $\nu=3$, a strong first-order phase transition should take place as $\tilde{g}$ is increased from zero, in which the spin polarization changes very abruptly. That this transition should involve a very large number of flipped spins can be seen by noting that the optimal values of K of the Skyrmions for small values $\tilde{g}$ is extremely large, as illustrated in Fig. 7. Unlike the $n=0$ case, Skyrmion solutions of the Hartree-Fock equations become unstable at a finite value of K (≈9 for $W=0.45\ell$) at which $\tilde{g}=-dU(K)/dK$ reaches its maximum value ($\approx0.003e^2/\epsilon\ell$ for $W=0.45\ell$). For $\tilde{g}$ larger than this value there are no $K\neq0$ solutions of the Hartree-Fock equations.

We estimate the number of flipped spins in the Skyrmion state for $W=0.45\ell$ at the critical value of $\tilde{g}$ to be approximately $K=14$, using our Hartree-Fock approach with a system size of $M_{\max}=480$. It should be noted that at finite Skyrmion concentrations, especially for such large Skyrmions, a calculation[19] including interactions among the Skyrmions would give a more reliable estimate for the jump in the spin polarization at the transition. We expect that such interactions would most likely somewhat reduce the magnitude of this jump. (Related finite-size studies have been carried out by Jain and Wu.[16])

In general, the stability of $K>0$ Skyrmions is most easily assessed by considering the internal energy U_K. As in Sec. III, U_K may be computed numerically by finding ϵ_K^- using the Hartree-Fock method, and then subtracting off the Zeeman contribution to the energy, as in Eq. (4). The results of such a calculation are illustrated in Fig. 8 for several values of the layer thickness W. These results confirm that Skyrmions are the lowest-energy charged excitations for large enough layer thickness, but become higher in energy than the $K=0$ quasiparticle as the system approaches the two-dimensional limit. For $n=1$, U_K may have local minima both at $K=0$ and $K\to\infty$. For this reason it is possible for the Hartree-Fock equations to have two separate solutions for the same values of $\tilde{g}$, as shown in Fig. 6. (In the $NL\sigma$ model calculation,[16] the energy of the Skyrmion branch *increases*

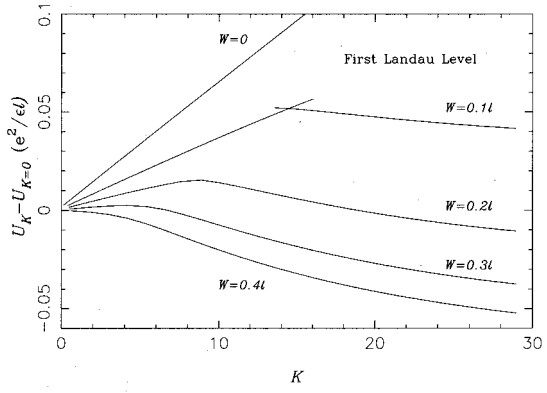

FIG. 8. Internal energy U_K vs K for Skyrmions in the $n=1$ Landau-level systems of varying thicknesses W. Skyrmions are the lowest-energy quasiparticles for sufficiently weak Zeeman coupling if $U_{K\to\infty}<U_{K=0}$. We find two distinct solutions to the Hartree-Fock equations for $W=0.1\ell$ in the vicinity $K=13$, leading to a cusp in U_K; for larger values of W only one solution is found, and the cusp becomes a smooth minimum. Where $d^2U(K)/dK^2<0$, solutions to the Hartree-Fock equations can be found only by adding unphysical terms to the Hamiltonian as discussed in the text. The system size used for these calculations was $M_{\max}=480$. Energies are in units of $e^2/\epsilon\ell$.

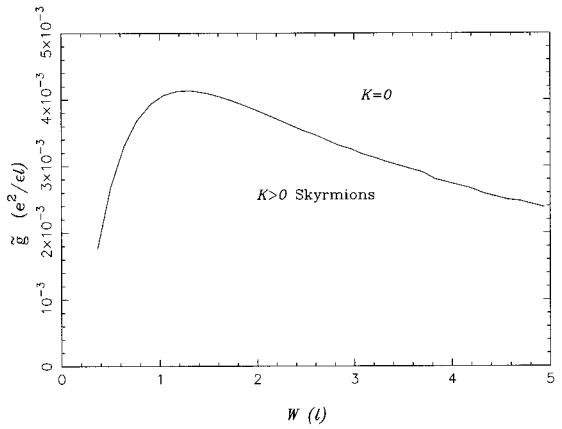

FIG. 9. Phase diagram for the dependence of the globally stable Hartree-Fock quasiparticle at $\nu=3$ ($n=1$) on system parameters $\tilde{g}$ and layer width W. ($\tilde{g}$ is in units of $e^2/\epsilon\ell$ and W is in units of ℓ.) The phase boundary separates parameter values for which the $K=0$ quasiparticle is lowest in energy from parameter values for which $K>0$ Skyrmions are lowest in energy. Systems in which these parameters can be adjusted so as to cross the phase boundary should exhibit a jump in the magnetization. These calculations were performed with $M_{\max}=480$.

from that of the $\tilde{g}=0$ solution in precisely the same fashion as in the LLL case, for there is no distinction between the direct Coulomb interaction in the two Landau levels for Skyrmions of divergent size. From the independent calculation of the lower-energy polarized quasiparticle, it follows that the Skyrmion energy must be nonmonotonic with size and, in the absence of intervening additional extrema, must have minima at both microscopic and infinite sizes.) It is interesting to note that, unlike the case of Skyrmions in the lowest Landau level, the curvature of U_K changes with increasing K (cf. Fig. 4). As mentioned in the discussion following Eq. (13), we do not expect to find stable Skyrmion solutions for the convex regions of the graphs in Fig. 8. Indeed, in order to obtain values for U_K in the small-K limit, it is necessary to add a fictitious term to the Hamiltonian of the form $H_\alpha=\alpha(\hat{S}_z-S_z^0)^2$, where $\hat{S}_z$ is the operator for the total spin angular momentum of the state. Since this term couples only to the total spin of the system, it favors states with $\langle\hat{S}_z\rangle\approx S_z^0$, but does not affect the optimal shape of the spin texture within the subspace of states with this expectation value for the spin. Thus by varying both α and S_z^0 we can obtain states with small values of K, and their intrinsic energy may be obtained by subtracting the expectation value $\langle H_\alpha\rangle$ from the expectation value of the perturbed total Hamiltonian. We note that this procedure produces internal energies that join smoothly onto those obtained for larger values of K where the Skyrmion states are stable for large enough layer thickness.

Our results for this section are summarized in Fig. 9, by a ''phase diagram'' in $\tilde{g}$ and W which shows where the lowest-energy charged excitations are $K=0$ quasiparticles and where they are $K\neq0$ Skyrmion charged spin textures. Even for the most favorable layer thickness, $W\approx1.2\ell$, the maximum value of $\tilde{g}$ for which Skyrmions are stable is outside the accessible range in many typical experimental systems. Nevertheless, we emphasize that if a system with very small effective values of $\tilde{g}$ could be fabricated, for values of ν close to (but not exactly equal to) 3, this line will separate states of maximal polarization ($K=0$) from states with highly degraded polarizations due to the presence of Skyrmion spin textures.

V. SUMMARY

In this work we studied the charged Skyrmion excitations of quantum Hall ferromagnets within the Hartree-Fock approximation. Exact relationships between the energies and spin quantum numbers of quasihole and quasiparticle excitations energies near $\nu=1$ were derived using particle-hole symmetry. An internal energy function $U(K)$ was introduced to describe the relative stability competition between Skyrmion states with different numbers of reversed spins, K. Locally stable Skyrmion states with K flipped spins can occur for any Zeeman coupling strength only if $d^2U(K)/dK^2>0$. In the presence of Zeeman coupling, a stable Skyrmion state must satisfy $dU(K)/dK=-g^*\mu_B B$. Results for the dependence of the K value of the lowest-energy Skyrmion excitations on Zeeman coupling strengths were presented both with and without finite-thickness corrections. Finite-thickness corrections were shown to stabilize Skyrmions in the $n=1$ Landau level, where for zero thickness $K=0$ quasiparticles are lowest in energy at any Zeeman coupling strength. We have proposed that a first-order phase transition between states with relatively large Skyrmions and states with $K=0$ quasiparticles will occur at $\nu=3$ at a critical value of the Zeeman coupling $\tilde{g}$, and be accompanied by a jump in the spin-magnetization of the electron system.

Note added: After the completion of this work, we became aware of a study of finite thickness effects on Skyrmions[28] for electrons on a sphere using an approximate Gaussian form for the confined state $\chi(z)$ of the electrons. Where there is overlap, the results presented there agree reasonably well with our own.

ACKNOWLEDGMENTS

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APPENDIX A: MIDGAP STATES AND THE INFINITE SKYRMION

The most intuitive account of the physics of the Skyrmions relies upon the spin Berry phases generated by adiabatic motion in a textured (effective) magnetic field arising from the magnetic exchange among the electrons themselves. Geometrical considerations show that the Berry phases due to a unit topological charge precisely mimic those of an ad-

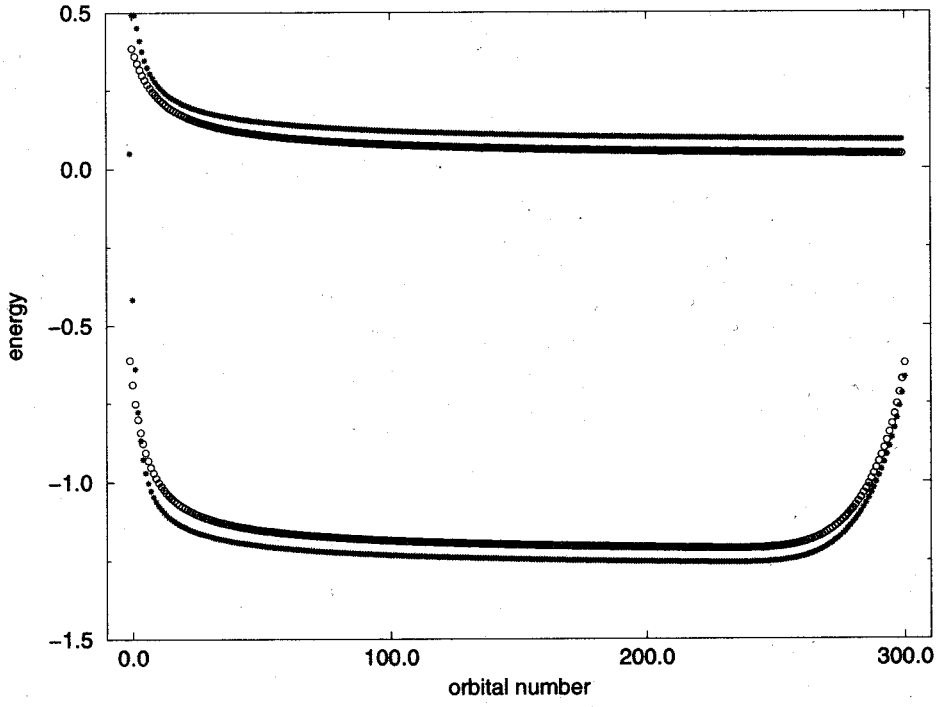

FIG. 10. The Hartree-Fock eigenvalues for Skyrmions in the LLL at $\tilde{g}/(e^2/\epsilon\ell)=0.1$ (stars) and 0.010 (circles). The former is the $K=0$ quasiparticle, and the latter has $K\approx 6$. In both cases there is an extra state in the lower branch. As there are 301 orbitals in the system $M_{\max}=300$, this means that the upper branches have 300 states and lower (occupied) branches have 302 states. Note that the gap is smaller near the origin, which is where the extra charge resides, and near the boundary due to loss of exchange. The shift in the eigenvalues near the origin is due to the Hartree repulsion of the extra charge. Evidently, the eigenvalues are much more uniform for the Skyrmion, but the overall reduction of the gap in its case is a finite-size effect.

ditional quantum of *orbital* flux. The incompressibility of the quantum Hall fluid then implies that an additional electron (or fraction thereof for fractional quantum Hall states) must then be present in the region of the texture which is therefore a (dressed) quasielectron.

A more detailed description of this is to note that ''up'' and ''down'' spins, i.e., the spins that respectively point parallel and antiparallel to the *local* direction of the field in the texture, see oppositely signed fluxes. Consequently while the ''up''-spin (effective) Landau level gains one state the ''down'' Landau level loses one, i.e., the presence of the Skyrmion causes the transfer of one state beween the upper (empty) and lower (filled) bands at $\nu=1$, thus allowing the extra electron to be accommodated in a low-energy state, albeit at the energetic cost of texturing the spins. This is strongly reminiscent of midgap states in one-dimensional systems, i.e., polyacetylene,[27] where a background soliton causes states to appear in a gap, and again there is the cost of creating the soliton which has to be overcome.

Since this description is very much of the one-electron variety, it is instructive to see how it works out in the Hartree-Fock treatment. The situation is clearest for the ''infinite'' Skyrmion, where the texture is arbitrarily slowly varying. It is very useful to regularize this limit by putting the system on a sphere where it takes the form of a purely radial texture, $\mathbf{n}(\theta,\phi)=\hat{\mathbf{r}}$. Again we may deduce the Hartree-Fock description by noting that the classical texture is invariant under the action of $\mathbf{J}=\mathbf{L}+\mathbf{S}$. In the LLL approximation this uniquely picks the wave function and fixes the eigenoperators of the Hartree-Fock Hamiltonian. For a sphere with $2q$ flux quanta threading the surface, the latter are

$$c^\dagger_{j+}=u_j a^\dagger_{j-1/2}+v_j b^\dagger_{j+1/2},\quad |j|\leqslant q+\tfrac{1}{2},$$
$$c^\dagger_{j-}=v_j a^\dagger_{j-1/2}-u_j b^\dagger_{j+1/2},\quad |j|\leqslant q-\tfrac{1}{2}, \tag{A1}$$

where

$$u_j=\left(\frac{q+1/2+j}{2q+1}\right)^{1/2}\text{ and }\quad v_j=\left(\frac{q+1/2-j}{2q+1}\right)^{1/2}. \tag{A2}$$

In this basis the Hamiltonian and wave function are

$$H_{\rm HF}=\sum_{|j|\leqslant q-1/2}\epsilon_- c^\dagger_{j-}c_{j-}-\sum_{|j|\leqslant q+1/2}\epsilon_+ c^\dagger_{j+}c_{j+},$$
$$|\Psi\rangle_{\rm HF}=\prod_{|j|\leqslant q+1/2}c^\dagger_{j+}c_{j+}|0\rangle, \tag{A3}$$

where $|0\rangle$ is the vacuum state. The energies $\epsilon_\pm$ depend upon the details of the interaction and not just on the symmetries of the state. [In the limit of infinite system size these become degenerate with the corresponding up- and down-spin eigenvalues at (exactly) $\nu=1$, as the Skyrmion becomes locally

indistinguishable from the ferromagnetic state.] The form of $H_{\rm HF}$ clearly shows that transfer of one state across the gap. Evidently, all we have used in this is that the states of $H_{\rm HF}$ must be classified only by their eigenvalues under **J** and hence must occur in the multiplets $j+1/2$ and $j-1/2$. This will therefore also survive the perturbative inclusion of Landau-level mixing.

For finite Skyrmions, the picture is (unfortunately) less elegant. The excess charge is now localized in a finite region, and hence affects the Hartree-Fock eigenvalues in the core of the Skyrmion. This can be seen in Fig. 10, where we have plotted the eigenvalues, now on the plane, for Skyrmions at two different values of $\tilde{g}/(e^2/\epsilon\ell)$. While the general scenario of a transferred state between two sets of levels still holds, the individual sets themselves become degenerate only in the large Skyrmion limit.

Finally, we note that putting the infinite Skyrmion on the sphere allows us to compute its energy very accurately, and thus circumvent the problems at small $\tilde{g}$ noted in the text. The only trick here is that we need to subtract the Hartree self-interaction of the Skyrmion charge, $e^2/(2\sqrt{q})$ ($\sqrt{q}$ is the radius of the sphere), which is substantial for small system sizes. This greatly improves convergence and the known infinite system result is recovered to within a few percent already at system sizes with $q \approx 10$.

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