RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 52, NUMBER 16 15 OCTOBER 1995-II

Theory of the spin-flip excitations in the $\nu=1$ quantum Hall liquid

Balázs Králik, Andrew M. Rappe, and Steven G. Louie
Department of Physics, University of California at Berkeley, Berkeley, California 94720
and Materials Science Division, Lawrence Berkeley Laboratory, Berkeley, California 94720
(Received 4 August 1995)

We calculated the spin-gap enhancement in the $\nu=1$ quantum Hall liquid using a variational quantum Monte Carlo approach. The approach goes beyond the usual lowest-Landau-level approximation. A significant ($\sim 50\%$ at $r_s=2$) reduction in the single spin-flip gap due to Landau-level mixing is found for typical experimental situations. Final-state effects and the finite thickness of the electron gas are conveniently included in our formalism, and satisfactorily explain recent photoluminescence experiments on δ-doped samples.

The quantum Hall liquids provide an excellent testing ground for the study of cooperative effects in two-dimensional (2D) many-electron systems, since the properties of these systems are dominated by electron correlation effects.[1] In this paper we report calculations on the lowest-lying quasiparticle excitations over a filled Landau level (LL), i.e., at $\nu=nhc/eB=1$. These excitations involve flipping a spin. Despite a decade of work, quantitative agreement between experimental[2–4,6] and theoretical[5–10] determinations of the spin gap has not been achieved. This is mainly due to the fact that although experiments are performed at finite B field, analytical calculations[7] and exact diagonalization studies[11] are only feasible within the lowest Landau level. A perturbative treatment[8] of the Coulomb interaction is similarly only valid when the Coulomb energy $e^2/\epsilon d$ is much smaller than the inter-LL spacing $\hbar\omega_c$. Here d stands for the typical electron-electron separation in the 2D layer. However, the ratio of the Coulomb energy to the kinetic energy, $(e^2/\epsilon d)/(\hbar\omega_c)=\nu r_s/2$, is of order 1 in n-type GaAs quantum wells, and of order 15 in p-type samples. (Here $\pi d^2=1/n=2\pi l_B^2/\nu$, r_s is the electron gas parameter, i.e., d in effective atomic units, and l_B is the magnetic length.) We expect, therefore, that the electron wave functions will mix in higher kinetic energy orbitals, in order to gain correlation energy. This effect becomes increasingly important in more dilute samples. Landau-level mixing lowers both ground and excited state energies, and we find that the spin gap itself is greatly reduced at all values of r_s.

The spin-flip energy ($\Delta_{\rm SG}$) is defined as the discontinuity in the chemical potential $\mu(N)$ at $\nu=1$. This corresponds to the energy of an infinitely separated quasiparticle-quasihole pair, i.e., to the $k\to\infty$ asymptote of the spin waves discussed by Kallin and Halperin.[7] Physically, $\Delta_{\rm SG}$ may be decomposed as

$$\Delta_{\rm SG}=E_Z+|\Sigma_{\uparrow\uparrow}|-|\Sigma_{\uparrow\downarrow}|+\delta_{\rm KE}, \tag{1}$$

where E_Z is the Zeeman energy, the $\Sigma_{ss'}$ are the exchange-correlation self-energies, and $\delta_{\rm KE}$ is the discontinuity $\delta(\partial E_{\rm kin}/\partial N)$ in the first derivative of the kinetic energy. The term $\delta_{\rm KE}$ is required, because LL mixing is of different importance at filling factors $\nu=1$ and $\nu=1+\epsilon$. We define $\Delta_{\rm SG}^{\rm LLmix}=-|\Sigma_{\uparrow\uparrow}^{\rm HF}|+|\Sigma_{\uparrow\uparrow}|-|\Sigma_{\uparrow\downarrow}|+\delta_{\rm KE}$ as the term due to LL mixing. The terms $\Sigma_{\uparrow\downarrow}$ and $\delta_{\rm KE}$ would be 0 in a lowest-LL [Hartree-Fock (HF)] approximation. Comparison of the HF data with the present calculation and with experiment,[2] as seen in Figs. 1 and 2, shows the failure of the lowest-LL theory.

We are able to go beyond the lowest-LL treatment by using a variational quantum Monte Carlo (VQMC) approach to study the quantum Hall system at various filling factors *near* 1. Variational states for $\nu=1$, $\nu=1-\epsilon$ ("quasihole state"), and $\nu=1+\epsilon$ ("quasielectron state") are constructed and optimized, and the spin gap is computed as

$$\Delta_{\rm SG}=E(N+1)+E(N-1)-2E(N), \tag{2}$$

where N stands for the number of electrons that would fill the lowest Landau level. The variational states are not restricted to the lowest LL.

In the VQMC approach we start with the exact many-electron Hamiltonian

$$H=\sum_i \frac{1}{2m^*}[\mathbf{p}_i+\mathbf{A}(\mathbf{x}_i)]^2+\sum_{i<j} V(|\mathbf{r}_i-\mathbf{r}_j|), \tag{3}$$

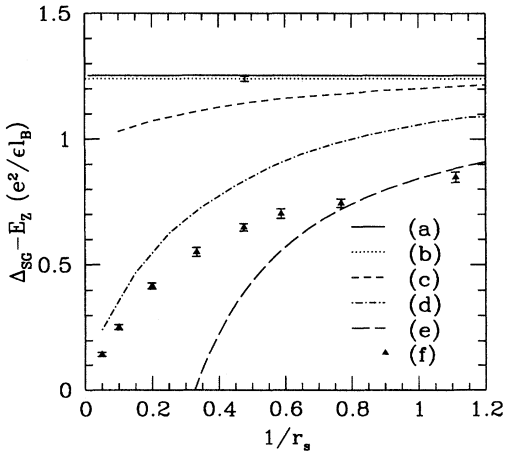

FIG. 1. Various calculations of the spin gap in an idealized 2D electron gas. (*a*) Time-dependent Hartree-Fock from Ref. 7. (*b*) Lowest LL VQMC. (*c*) Skyrmion–anti-Skyrmion pair energy from Ref. 9. (*d*) RPA from Ref. 10. (*e*) Perturbation theory from Ref. 8. (*f*) Correlated-wave function VQMC.

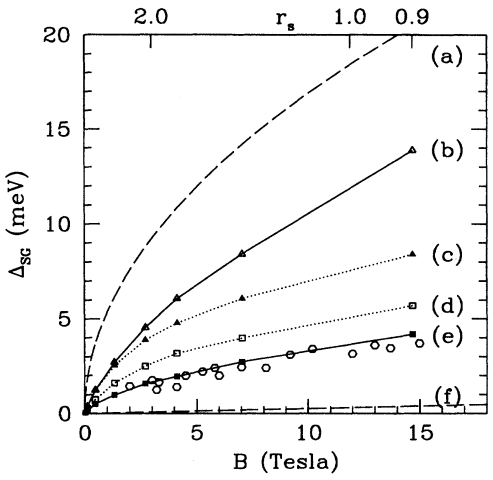

FIG. 2. Experimental corrections: finite thickness (FTC), finite donor distance (FDC), and kinetic energy (KEC). The curves are (*a*) HFA; (*b*) LL mixing VQMC; LL mixing VQMC corrected by (*c*) FTC, (*d*) FTC and KEC, (*e*) FTC, KEC, and FDC; (*f*) Zeeman energy. The empty hexagons are photoluminescence data from Ref. 2. Symbol sizes represent statistical and experimental errors.

where m^* is the effective mass of the GaAs conduction band in atomic units, $\hbar=e=c=1$, and $V(r)$ is the interparticle potential. Both the pure Coulomb and the finite thickness-modified potentials are studied (see below). **A** is the vector potential corresponding to the perpendicular **B** field $B\hat{\mathbf{z}}$ in the Landau gauge with $\mathbf{A}=(-yB,0)$. The calculation consists of stochastically evaluating the variational integral $E_0=\langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle$ to obtain an upper bound for the ground state energy. The properties of infinite systems are simulated by studying up to 100 electrons and imposing generalized periodic boundary conditions in a planar geometry appropriate for a uniform perpendicular magnetic field.[12,13] Long-ranged interaction energies are summed using the Ewald summation technique.[14,15] Calculations with differently sized supercells show that, at $N=50$, the finite size effects are comparable to the statistical errors arising from stochastic integration.

The VQMC method has been shown to be a highly accurate method in studying various condensed matter systems.[13,14,16,17] Since the errors made in evaluating the energies of the "ground," "quasielectron," and "quasihole" states are expected to be similar and small, we expect the value of the spin gap Δ_{SG}, which is formed as a *second difference* of the above variational upper bounds, to be reliable. Ultimately, however, our calculations are justified by accurately matching exact analytical calculations in the appropriate limits. First, entirely neglecting the Jastrow factor in our wave functions corresponds to the time-dependent Hartree-Fock approximation (HFA) carried out by Kallin and Halperin.[7] We find excellent agreement between our lowest-LL result, $\Delta_{SG}^{LLL}=1.24(2)e^2/l_B$, and the energy of a $k\to\infty$ spin wave within the time-dependent HFA, $\Delta_{SG}^{HFA}=1.25e^2/l_B$. Second, our variational spin gap matches the second-order perturbation result of Sondhi[18] in the $r_s\to 0$ limit. Sondhi's expansion in r_s, rigorously exact in this limit, predicts a shift of -0.58 effective Hartree in Δ_{SG} from its HFA value. This shift is in excellent agreement with our variational result at low r_s (see Fig. 1). At high r_s, the perturbation theory fails, diverging from the variational results as expected.

The variational wave functions we used are of the form

$$\Psi_G=\Psi_J(\mathbf{r}_1,\ldots,\mathbf{r}_N)\mathcal{F}_\uparrow(z_1,\ldots,z_N),$$

$$\Psi_{QE}=\Psi_J(\mathbf{r}_1,\ldots,\mathbf{r}_{N+1})\mathcal{F}_\uparrow(z_1,\ldots,z_N)\mathcal{F}_\downarrow(z_{N+1}), \tag{4}$$

$$\Psi_{QH}=\Psi_J(\mathbf{r}_1,\ldots,\mathbf{r}_{N-1})\mathcal{F}_\uparrow(z_1,\ldots,z_{N-1};\tilde{z}).$$

Apart from the Jastrow factor Ψ_J, these wave functions are Laughlin's ground, quasielectron, and quasihole states in periodic boundary conditions.[12,19] All three wave functions are written for the same magnetic field, and hence represent states with filling factors $\nu=1,\nu=1\pm 1/N$, respectively. The Jastrow factor further correlates the electrons and therefore mixes in higher LL's. Our Jastrow factor Ψ_J is of the form $\Psi_J=\Pi_{i<j}e^{u(r_{ij})}$, where $u(r)$ is a long-ranged two-particle pseudopotential. We use the form $u(r)=-(A/\sqrt{r})[1-\exp(-Fr^{1/2}-F^2r-F^3r^{3/2})]$. At large r, $u(r)\sim 1/\sqrt{r}$ and in the small r limit it satisfies a *cusp condition*[14,15] appropriate for dynamics in a magnetic field. The value of F is fixed by A and the cusp condition, while A is treated as a free variational parameter. We find our results to be insensitive to small changes in A and F, even when varied independently.

Figure 1 shows that the effect of LL mixing (i.e., the Jastrow factor) is dramatic, especially in high r_s samples. In particular, near $r_s=2$ the reduction is approximately 50%. This r_s corresponds to typical experimental electron densities and magnetic fields in GaAs-$Al_xGa_{1-x}As$ heterostructures. The enhancement of the correlation hole is especially significant for the case when the state is not completely spin polarized, and therefore exchange alone does not keep electrons apart.

Sondhi and co-workers suggested[8] that the lowest-energy quasiparticles in the $\nu=1$ quantum Hall system are not perturbatively derived from a single-spin-flipped state, as in our variational state. They suggest that in the parameter range appropriate for GaAs quantum wells with experimentally accessible magnetic fields, the proper quasiparticles are Skyrmions with nontrivial spin order and large total spin. In the small Landé g-factor $g\to 0$ limit, they calculate the Skyrmion–anti-Skyrmion energy to be $\Delta_{SA}=\frac{1}{2}\sqrt{\pi/2}e^2/\epsilon l_B$. Recently a Hartree-Fock calculation of the Skyrmion–anti-Skyrmion energy appropriate for finite g has also been carried out.[9] As seen in Fig. 1, the HF Δ_{SA} energies are significantly larger than our variational Δ_{SG} at all values of r_s. LL mixing effects would lower Δ_{SA}. The comparison shows that LL mixing effects play a dominant role in determining the magnitude of the spin gap, and suggests that single-spin excitations might be better candidates for the lowest-energy excitations for the appropriate experimental conditions.

In addition, Sondhi and co-workers' quantitative estimate for the critical Landé g factor below which Skyrmions might become relevant is based entirely on lowest-LL studies.[11] From a comparison of the energies of variational states with one and more reversed spins, they estimate, for $\nu=1$,

$g_c = 0.054(e^2/\epsilon l_B)/\mu_B B = 1.13 r_s$, which means that at typical values of r_s the actual Landé factor of GaAs is below g_c. However, our results show that a lowest-LL-only treatment significantly overestimates the exchange-correlation energy difference between two electrons of different spin orientation. It follows that LL mixing effects would *lower* g_c.

It is our view that both the Skyrmionic and LL mixing pictures try to capture similar physics, as far as energetics is concerned. In the ground state, at any filling factor, electrons will try to avoid each other by deepening the exchange-correlation hole that surrounds them. In the Skyrmionic picture (see Fig. 3 in Ref. 8) the exchange-correlation hole is enhanced through *exchange* via the introduction of nontrivial spin order, whereas in our treatment the hole is enhanced via changes in the electronic pair correlation function. The correct quasiparticle state will likely contain *both* nontrivial spin order, and enhanced correlations through LL mixing. Further study is warranted on the relative strengths of these two effects.

Smith, MacDonald, and Gumbs[10] have performed random-phase approximation (RPA) calculations to estimate the effect of Landau-level mixing. Their results for the parameters of interest in this paper are also plotted in Fig. 1. Since RPA tends to underestimate correlations, the fact that the RPA gaps are higher than ours is not surprising.

In addition to determining the correct quasiparticle energies in the idealized 2D case, a realistic comparison to experimental measurements such as the photoluminescence results[2] requires calculating various corrections that arise from the practical realization of the 2D electron gas (2DEG). First, the 2D electron liquid has a nonzero thickness which we model via a modified Coulomb interaction of the form $V(r) = 1/\sqrt{r^2+t^2}$. We estimate the appropriate value of the thickness parameter t as the expectation value $\langle z \rangle$ evaluated in the self-consistent triangular well approximation.[20] For the GaAs-$Al_xGa_{1-x}As$ interface at $\nu = 1$, this approximation yields $\langle z \rangle = 1.4$ for $B = 2$ T and $\langle z \rangle = 1.0$ for $B = 15$ T. In Fig. 2, for each of our data points, we took t to be the value appropriate for the particular magnetic field and electron density dictated by the $\nu = 1$ condition. We observe that the usual rule of thumb 40% "phenomenological" finite thickness correction (FTC) to Δ_{SG} [the difference between curves (b) and (c)] is only appropriate at $B \sim 12$ T, i.e., in $r_s \sim 1$ samples. As expected, for large electron-electron separations ($r_s \sim 20$) the effect of finite thickness is greatly reduced.

As first described by Apalkov and Rashba,[21] within the lowest-Landau-level sudden approximation, the first moment $\hbar\bar{\omega}$ of the photoluminescence line from a sample with impurities δ doped away from the electron gas is related to the spin gap by

$$\Delta_{SG} = \frac{N}{2}\left(\delta \frac{\partial \hbar\bar{\omega}}{\partial N} + \int d^2 r V(|\vec{r}_I - \vec{r}|) n(\vec{r}) \delta \frac{\partial h}{\partial N}(\vec{r}_0 - \vec{r}) \right). \tag{5}$$

Here N is the number of electrons in the 2D layer, n is the density, h is the pair correlation function; $\vec{r}_I$ and $\vec{r}_0$ are the position of the impurity and its projection to the 2D layer, i.e., $\vec{r}_I - \vec{r}_0 = z_0 \hat{z}$. z_0 is the distance of the impurity from the 2DEG. We refer to the second term in this expression as the "finite distance correction" (FDC). Note that z_0 is *not* the same as the distance of the impurity from the interface, because the 2DEG extends considerably into the GaAs layer.

The inclusion of Landau-level mixing introduces an additional "kinetic energy correction" (KEC) term into the relationship between the total energy per particle $TE(N)$ in the 2DEG and the photoluminescence line first moment $\hbar\bar{\omega}$. Removing one particle from the layer results in an energy change $\Delta E = 2EE(N) + KE(N) = TE(N) + EE(N)$, where $EE(N)$, $KE(N)$, and $TE(N)$ are the per particle potential, kinetic, and total energies in the 2DEG, respectively. The extra $EE(N)$ term comes from the fact that the Coulomb interaction is a pair interaction. Following the arguments in Ref. 21, we conclude that

$$\Delta_{SG} = \frac{N}{2}\left(\delta \frac{\partial \hbar\bar{\omega}}{\partial N} + \int d^2 r V(|\vec{r}_I - \vec{r}|) n(\vec{r}) \delta \frac{\partial h}{\partial N}(\vec{r}_0 - \vec{r}) + \delta \frac{\partial KE(N)}{\partial N} \right). \tag{6}$$

The third term is the additional KEC, which arises because of the difference between $TE(N)$ and ΔE and because of the fact that there are different amounts of Landau-level mixing in quasielectron, quasihole, and ground states. The KEC vanishes in the lowest-Landau-level approximation, where $KE(N) = \hbar\omega_c/2$ has no cusp at $\nu = 1$.

Figure 2 shows the various corrections to the spin-flip energy of a 2D system that are needed to interpret Kukushkin and co-workers' experiment.[2] We chose the impurity distance to be $z_0 = 180$ Å from the 2DEG to produce the best fit. Since the 2DEG has its maximum density at approximately 100 Å from the interface, this is in satisfactory agreement with the experimentalists' specification that the impurities lie between 250 and 400 Å from the interface. Moreover, the excellent fit between the photoluminescence results and the theoretical calculations is not very sensitive to the choice of z_0: varying z_0 between 140 Å and 300 Å changes our final result by less than 1.4 meV at $B = 15$ T, and by 0.2 meV at $B = 1$ T.

In addition to the photoluminescence studies, activated transport[3] measurements have also been made to determine the spin gap. The interpretation of these experiments does not involve the KEC and the FDC terms, so for these cases our theory predicts the spin gap to be as indicated on Fig. 2 by the line labeled (c). Our calculated results do not match these experiments as well as photoluminescence. However, impurity effects, which were not included in the present study, are expected to affect the transport data interpretation.[10] Nevertheless, the present calculation represents significant improvement over perturbation theoretical and HFA calculations, since it gives better agreement with both transport and photoluminescence experiments than any of these techniques.

In conclusion, we present a VQMC study on the spin excitations of the $\nu = 1$ quantum Hall liquid. We found strong evidence that Landau-level mixing effects are very important, even at the lowest experimentally achievable density parameter r_s. Further, our formalism, being well suited to study previously neglected experimental corrections, is able to quantitatively interpret photoluminescence data for the spin gap.

This work was supported by National Science Foundation Grant No. DMR91-20269 and by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. Calculations were done using the CRAY-C90 computer at the San Diego Supercomputer Center and the Cray-YMP computer at National Energy Research Supercomputer Center.

[1] *The Quantum Hall Effect*, edited by R. E. Prange and S. M. Girvin (Springer, Berlin, 1990).
[2] I. V. Kukushkin *et al.*, Europhys. Lett. **22**, 287 (1993); (private communication).
[3] A. Usher, R. J. Nicholas, J. J. Harris, and C. T. Foxton, Phys. Rev. B **41**, 1129 (1990).
[4] K.-S. Kim *et al.*, J. Korean Phys. Soc. **26**, S46-9 (1993).
[5] T. Ando and Y. Uemura, J. Phys. Soc. Jpn. **37**, 1044 (1974).
[6] A. Pinczuk *et al.*, Phys. Rev. Lett. **68**, 3623 (1992).
[7] C. Kallin and B. I. Halperin, Phys. Rev. B **30**, 5655 (1984).
[8] S. L. Sondhi, A. Karlhede, S. A. Kivelson, and E. H. Rezayi, Phys. Rev. B **47**, 16 419 (1993).
[9] H. A. Fertig, L. Brey, R. Cõté, and A. H. MacDonald, Phys. Rev. B **50**, 11 018 (1994).
[10] A. P. Smith, A. H. MacDonald, and G. Gumbs, Phys. Rev. B **45**, 8829 (1992).
[11] E. H. Rezayi, Phys. Rev. B **36**, 5454 (1987); **43**, 5944 (1991).
[12] F. D. M Haldane and E. H. Rezayi, Phys. Rev. B **31**, 2529 (1985).
[13] X.-J. Zhu and S. G. Louie, Phys. Rev. Lett. **70**, 335 (1993).
[14] D. Ceperley, Phys. Rev. B **18**, 3126 (1978).
[15] Balázs Králik and S. G. Louie (unpublished).
[16] W. L. McMillan, Phys. Rev. **138**, A442 (1965).
[17] S. Fahy, X. W. Wang, and S. G. Louie, Phys. Rev. B **42**, 3503 (1990).
[18] S. L. Sondhi, Ph.D. thesis, UCLA, 1992.
[19] R. P. Laughlin, Phys. Rev. Lett. **50**, 1395 (1983).
[20] T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. **54**, 437 (1982).
[21] V. M. Apalkov and E. I. Rashba, Pis'ma Zh. Éksp. Teor. Fiz. **53**, 420 (1991) [JETP Lett. **53**, 442 (1991).