

# Spin-reversed Quasiparticles in the Fractional Quantum Hall Effect – Finite System Calculations

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## Abstract

The elementary charged excitations at  $1/3$  Landau level filling have been studied for various spin polarizations for finite electron systems in a periodic rectangular geometry. In the absence of Zeeman energy, the spin-reversed excitations, studied for *three to six* electron systems show significant reduction of the energy gap, compared to the fully spin-polarized quasiparticle-quasihole gap, studied for upto *seven* electron systems. In the presence of Zeeman energy, the lowest energy excitations involve spin-reversed quasiparticles and spin-polarized quasiholes for low magnetic fields. With increasing magnetic fields, a crossover point is reached (in the region  $B < 10$  T), beyond which a fully spin polarized quasiparticle-quasihole state will be energetically favored. The Zeeman energy due to spin-flip explains qualitatively the linear magnetic field dependence of the activation energies observed experimentally.

## 1. Introduction

The fractional quantum Hall effect (FQHE) in the two-dimensional electron system, observed in modulation-doped GaAs-(AlGa)As, at low temperatures and high magnetic fields [1], has generated intense theoretical activities in recent years. Current understanding of the effect requires that the electron gas condenses into an *incompressible quantum fluid*, and dilation or contraction of the “incompressible” state creates fractionally charged quasiholes and quasiparticles [2–9]. (The incompressibility of the fluid is characterized by a positive discontinuity of the chemical potential at the stable states.) Recent measurements [10] on the exponentially small dissipation of the diagonal resistivity in the FQHE regime have established a single activation energy for the Landau level fillings of  $\nu = 1/3, 2/3, 4/3$  and  $5/3$ . It is also interesting to note that the magnetic field dependence of the activation energy observed in those experiments appears to be different from the current theoretical predictions. In all the theoretical calculations [4–9], the excitation energy gap scales with the natural unit of energy,  $e^2/\epsilon l_0$ , with  $\epsilon$  being the background dielectric constant and  $l_0 \equiv (\hbar c/eB)^{1/2}$  is the magnetic length. Instead of the expected behaviour of  $B^{1/2}$  dependence, the experimental data indicates [10] that the activation energy has a finite magnetic field threshold, above which it shows an almost *linear* increase with the magnetic field upto  $B \sim 12$  T. In our earlier works [11] we have studied the spin polarization of the ground state at various rational fillings. A natural extension of those calculations would be the *spin-reversed excitations*. Indeed, we would like to raise the possibility that the almost linear increase of the observed activation energies could perhaps be associated with the Zeeman energy due to the spin-reversed quasiparticles [12].

The energy gap,  $E_g \equiv \tilde{\epsilon}_p + \tilde{\epsilon}_h$  which corresponds to the energy required to create a quasiparticle ( $\tilde{\epsilon}_p$ ) and a quasihole ( $\tilde{\epsilon}_h$ ) well separated from each other, has been estimated by

several authors [4–9]. The hypernetted-chain estimate [5, 9] is not so reliable as the Monte Carlo result [6] for large but finite systems (upto 72 electrons),  $E_g \simeq 0.099 \pm 0.009$  (energies are quoted in units of  $e^2/\epsilon l_0$ , unless otherwise specified). The result from the collective excitation spectrum in analogy with the Feynman type excitations in liquid  $^4\text{He}$ , obtained by Girvin, MacDonald and Platzman [7], is  $E_g \simeq 0.106$ . Also, the estimate by Haldane and Rezayi [8], who computed the exact spectrum for small number of electrons (three to seven electrons) on a sphere and extrapolated the result to the thermodynamic limit, is  $E_g \simeq 0.105 \pm 0.005$ . From all these estimates, it is clear that the correct theoretical result for the energy gap in the case of spin-polarized quasiparticles and quasiholes is  $\sim 0.1$ . In the following we will demonstrate that, there exists other mechanism like spin reversal, where the energy cost is much lower than the above mentioned excitations.

## 2. The energy gap

### 2.1. Periodic rectangular geometry

The finite electron system in a periodic rectangular geometry has been discussed earlier [3, 11] in the literature. Therefore, we will present here only a brief description of the formalism used in the present work. We assume that  $N_e$  number of electrons interact, via Coulomb interaction, in a rectangular cell of sides  $a$  and  $b$ . We impose the periodic boundary conditions, so that the electrons also interact with their periodic images, and the cell contains an integral number  $N_s$  of magnetic flux quanta. In the Landau gauge, the single-particle eigenfunctions for a rectangular cell are,

$$\phi_j(r) = \left[ \frac{1}{b\sqrt{\pi}l_0} \right]^{1/2} \sum_{k=-\infty}^{\infty} \exp[i(X_j + ka)y/l_0^2 - (X_j + ka - x)^2/2l_0^2]. \quad (1)$$

Here the integer  $j$ ,  $1 \leq j \leq N_s$  specifies the state, and  $X_j = 2\pi l_0^2 j/b$  is the center coordinate of the cyclotron motion, which is conserved by the electron-electron interaction. The Coulomb interaction is written in the form,

$$V(r) = \frac{1}{ab} \sum_q \frac{2\pi e^2}{\epsilon q} \exp(iq \cdot r), \quad (2)$$

where  $q = (2\pi s/a, 2\pi t/b)$  with  $s$  and  $t$  as integers. Considering only the lowest Landau level, the Hamiltonian is,

$$H = \sum_j W a_j^\dagger a_j + \sum_{j_1} \sum_{j_2} \sum_{j_3} \sum_{j_4} A_{j_1 j_2 j_3 j_4} a_{j_1}^\dagger a_{j_2}^\dagger a_{j_3} a_{j_4} \quad (3)$$

where  $a_j$  ( $a_j^\dagger$ ) is the annihilation (creation) operator for the  $j$ th

state. The single-electron part is a known constant [3], while the two-electron part is given by,

$$A_{j_1 j_2 j_3 j_4} = \frac{1}{2} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \phi_{j_1}^*(\mathbf{r}_1) \phi_{j_2}^*(\mathbf{r}_2) V(\mathbf{r}_1 - \mathbf{r}_2) \phi_{j_3}(\mathbf{r}_2) \phi_{j_4}(\mathbf{r}_1) \\ = \frac{1}{2ab} \sum_q' \sum_s \sum_t \delta_{q_x, 2\pi s/a} \delta_{q_y, 2\pi t/b} \delta_{j_1-j_4, t} \frac{2\pi e^2}{\varepsilon q} \quad (4) \\ \times \exp \left[ -\frac{1}{2} l_0^2 q^2 - 2\pi i s(j_1 - j_3)/m \right] \delta_{j_1+j_2, j_3+j_4}.$$

Here the Kronecker delta  $\delta$  with prime means that the equation is defined modulo  $N_s$ , and the summation over  $q$  excludes  $q_x = q_y = 0$ . The basis states are chosen to be the antisymmetrized products of single-particle eigenfunctions, eq. (1), denoted as  $|j_1 j_2 \dots j_{N_e}\rangle$ , with the quantum number  $J \equiv \sum_{i=1}^{N_e} j_i \pmod{N_s}$  being the total momentum along the axis fixed by the Landau gauge. The filling fraction is given by  $\nu = N_e/N_s$ , and the number of electrons is usually fixed by one's ability to diagonalize the huge Hamiltonian matrix. (In the present work, the biggest matrix we encountered had dimension 11 628.) The generalization of the present method to include the spin-reversal is rather straightforward [11]. The energy spectrum for the Hamiltonian is classified in terms of the total spin  $S$  and its  $z$ -component  $S_z$ . For a given  $S$ , the spectrum is identical for different values of  $S_z$ . In the present work, we will concern ourselves with only two cases, (a)  $S = S_z = N_e/2$ , and (b)  $S = S_z = N_e/2 - 1$ .

## 2.2. A cusp that is

As stated earlier, we wish to describe an incompressible electron fluid at the stable states, e.g., at  $\nu = 1/3$ . This means that, at  $1/3$  Landau level filling fraction, we expect to find discontinuities in the chemical potential, which would manifest itself as a cusp-like behavior in the energy vs. density curve at that filling fraction. The chemical potential is defined as,

$$\mu = E_0(\nu) + \nu \frac{\partial E_0}{\partial \nu} \quad (5)$$

where  $E_0(\nu)$  is the ground state energy per particle at  $\nu$ . For  $\nu = 1/3$ , the energy gap is then given by [12, 13],

$$E_g = \frac{1}{3}(\mu_+ - \mu_-) \quad (6)$$

with,

$$\mu_{\pm} \simeq E_0(\nu) + \nu[E_{\pm} - E_0]/(\nu_{\pm} - \nu).$$

Here  $\nu_{\pm} = N_e/(N_s \mp 1)$ ,  $E_{\pm} = E_0(\nu_{\pm})$  and the factor  $1/3$  is because of the fractional electron charge of the quasiparticles and quasiholes [9]. It is to be noted that the quasiparticle and quasihole excitations are obtained by changing the magnetic flux quantum from the stable filling fractions, keeping the total number of electrons,  $N_e$ , fixed. The spin-reversed quasiparticle and quasihole excitation energy gaps are obtained by calculating  $E_{\pm}$  in a system where the spin of one of the electrons is *reversed* relative to all the others. The ground state energy at  $\nu = 1/3$  [denoted by  $E_0(\nu)$  in eqs. (5) and (6)] is, however, calculated for the spin-polarized case.

## 2.3. Finite-thickness correction

In our discussions so far, we have ignored the finite spread of the electron wavefunction perpendicular to the two-

dimensional plane. It is well-known [14–16] that inclusion of the finite thickness correction effectively softens the short-range divergence of the bare Coulomb interaction, when the interelectron spacing is comparable with the inversion layer width. Consequently, many important energies in the FQHE are drastically reduced. While the reduction of the ground state energy still keeps the incompressible quantum fluid state energetically favorable over the crystalline state [15], the reduction of the collective excitation gap provides a better comparison with the experiment. The most common form for the charge distribution normal to the plane is by the Fang–Howard [14] variational wave function,

$$g(z) = \frac{1}{2} b^3 z^2 \exp(-bz) \quad (7)$$

where the effects of only the lowest subband is considered. The variational parameter is given by,

$$b = [33\pi m^* e^2 n / 2\epsilon \hbar^2]^{1/3} \quad (8)$$

where  $m^* = 0.067m_e$  is the effective mass,  $n$  is the electron density fixed by the Landau level filling  $\nu$ . The depletion layer electron density is negligible as compared to the electron density [14–16] and is not included in eq. (8).

The effective electron–electron interaction is then written as [16],

$$V(r) = \frac{e^2}{\varepsilon} \int dz_1 \int dz_2 g(z_1) g(z_2) [r^2 + (z_1 - z_2)^2]^{-1/2}. \quad (9)$$

Using the result,

$$F(q) \equiv \frac{q}{2\pi} \int \frac{d\mathbf{r} e^{i\mathbf{q}\cdot\mathbf{r}}}{[(z_1 - z_2)^2 + r^2]^{1/2}} \\ = \exp[-q|z_1 - z_2|] \quad (10)$$

and  $g(z)$  from eqs. (7) and (8), eq. (9) can be rewritten as,

$$V(r) = \left[\frac{1}{2} b^3\right]^2 \left(\frac{e^2}{\varepsilon}\right) \int_0^\infty dq J_0(qr) \int dz_1 dz_2 z_1^2 z_2^2 \\ \times e^{-bz_1} e^{-bz_2} e^{-q|z_1 - z_2|}$$

which after some algebra, leads to

$$V(r) = \left(\frac{e^2}{\varepsilon}\right) \int_0^\infty dq F(q) J_0(qr) \quad (11)$$

with

$$F(q) = \left[1 + \frac{9}{8} \frac{q}{b} + \frac{3}{8} \left(\frac{q}{b}\right)^2\right] \left(1 + \frac{q}{b}\right)^{-3}.$$

For large  $r$ ,  $V(r)$  has the usual  $1/r$  behavior, and for small  $r$ , the  $\ln r$  behavior is obtained.

## 3. Numerical results and discussions

The major bottleneck of the numerical diagonalization method, such as the one used here, is the dimension of the Hamiltonian matrix, which grows very rapidly with the electron number  $N_e$ . In the case of one spin reversal considered in the present work, the situation is even worse, since the electrons with different spin can now occupy states with same  $j$ . The matrix dimension in that case, is increased approximately by a factor  $\sim (N_e + 1)$  as compared to that for the spin-polarized case. A straightforward diagonalization of the matrix is thus not possible for  $N_e > 4$  with one spin reversed.

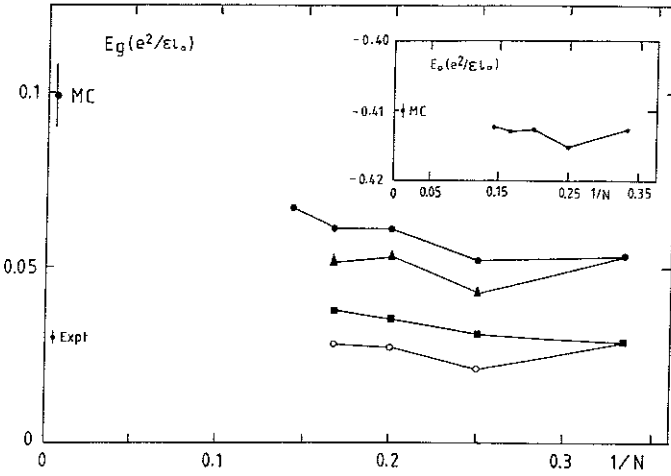


Fig. 1. The energy gap  $E_g$  (in units of  $e^2/\epsilon_0$ ) for different spin polarization of the quasiparticle (q.p.) and quasihole (q.h.) excitations for three to seven electron systems, in the absence of Zeeman energy. The Monte Carlo result (MC) is from Ref. [6] for the spin-polarized q.p. and q.h. (●). The other three cases are: spin-polarized q.p. + spin-reversed q.h. (▲); spin-reversed q.p. + spin-polarized q.h. (■); and spin-polarized q.p. + q.h. (○). The experimental data is from Ref. [10]. The ground state energy at  $\nu = 1/3$  from Refs [3] and [6] are given as inset for comparison.

The computational method used in the present work is described briefly in the appendix.

In Fig. 1, we have plotted the energy gap for three to seven electron systems for various spin polarization of the quasiparticles and quasiholes. The four-electron spin-polarized result was first obtained by Yoshioka [13]. However, as shown in the figure,  $E_g$  depends on the system size somewhat, and the extrapolation of our results for the spin-polarized (three to seven) electron system (plotted as ●) approximately leads to  $E_g \approx 0.10$ . The result is thus in agreement with the earlier estimates, described in the introduction. The reliability of our approach is best seen in the case of the ground-state energy at  $\nu = 1/3$  [3] plotted as inset in Fig. 1, for three to seven electron systems. The results are very close to the accurate Monte Carlo results of Ref. 6 with the Laughlin wave function.

In Fig. 1, we have also plotted the energy gap for different spin polarizations of the quasiparticles and quasiholes. The four cases we have studied are: (a) spin-polarized quasiparticle–quasihole gap, (b) spin-polarized quasiparticle and spin-reversed quasihole gap (▲), (c) spin-reversed quasiparticle and spin-polarized quasihole (■) and (d) spin-reversed quasiparticle and quasihole (○). It is clear in Fig. 1, that the lowest energy excitations (in the absence of Zeeman energy) at  $\nu = 1/3$  involve spin-reversal. The origin of this could perhaps be traced to the earlier findings [11] that, for any state other than  $1/m$  with  $m$  odd integer, which is spin-polarized, the electron–electron interaction decreases the tendency to spin polarization, resulting in lower energies for the spin-reversed cases. The spin reversal is found to cost much less energy for  $E_+$  (reduction of a flux quanta) than that for  $E_-$  (addition of a flux quanta). Therefore, in the absence of Zeeman energy, the lowest energy excitations correspond to the case where  $E_+$  and  $E_-$  are evaluated for spin-reversed systems.

The Zeeman energy (per particle) contribution to the energy gap for various cases are, (a) zero for fully spin polarized quasiparticle–quasihole case, (b)  $(1 + 1/3N_e)\epsilon_z$  for the spin-reversed quasihole-spin polarized quasiparticle case, (c)

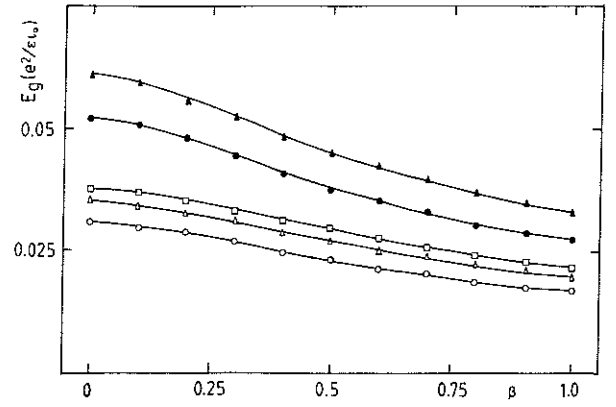


Fig. 2. Energy gap  $E_g$  (in units of  $e^2/\epsilon_0$ ) as a function of the dimensionless parameter  $\beta = (b l_0)^{-1}$  for four (● and ○), five (▲ and △) and six (□) electron systems. The filled points are for spin-polarized q.p. + q.h. case, while the empty points correspond to the spin-reversed q.p. + spin-polarized q.h. case. The five and six electron results in the former case are not distinguishable in the present figure.

$(1 - 1/3N_e)\epsilon_z$  for the spin-reversed quasiparticle-spin polarized quasihole case and (d)  $2\epsilon_z$  for the spin-reversed quasiparticle–quasihole case. Here  $\epsilon_z = g\mu_B B$ , with  $\mu_B = e\hbar/2m_e c$  the Bohr magneton and the Landé  $g$ -factor,  $g \approx 0.529$  for GaAs. As we shall see later, in the presence of Zeeman energy, only case (c) for low magnetic fields and (a) for high magnetic fields are energetically favorable.

In Fig. 2, we have plotted the energy gap  $E_g$  as a function of the dimensionless parameter  $\beta = (b l_0)^{-1}$  for four- to six-electron systems at  $\nu = 1/3$ . In the case of spin-polarized quasiparticles and quasiholes (filled points), five and six electron system results are indistinguishable in the figure. The interesting point, however, is that there is a substantial reduction of the gap in the range of  $\beta = 0.5$ – $1.0$ , compared to the ideal case of  $\beta = 0$ . In fact, the ratio of  $E_g(\beta = 1)/E_g(\beta = 0)$  is 0.53, 0.52 and 0.54 for four (●), five (▲) and six-electron (■) system respectively. In the case of spin-reversed quasiparticle and spin-polarized quasihole (empty points), the reduction is slightly less: 0.55, 0.56 and 0.57 for four (○), five (△) and six-electron (□) systems respectively.

At  $\nu = 1/3$ , the magnetic field dependence of the finite-thickness parameter  $\beta$  is given as,  $\beta = 0.525B^{1/6}$  and the Zeeman energy (in units of  $K$ ) as  $\epsilon_z = 0.355B$  with  $B$  given in Tesla. From these relations, we can easily obtain the magnetic field dependence of the energy gap,  $E_g$ . The results for five-electron system is shown in Fig. 3. The six-electron result is not distinguishable in the figure. The experimental data, obtained from six different samples, by Boebinger *et al.* [10] is also presented for comparison. For low magnetic fields, the lowest energy excitations rises linearly as a result of the spin-reversed quasiparticles, which include the dominant contribution from the Zeeman energy. The slope of this curve is very similar to the linear type part of the experimental results. As the magnetic field is increased further, the  $B^{1/2}$  dependence (modified by the magnetic field dependence of  $\beta$ ) is then obtained due to the spin-polarized quasiparticles and quasiholes. This part of the theoretical curve is also qualitatively similar to the experimental results. The point we wish to make in this work is that, for low magnetic fields, the spin-reversal presumably plays an important role in the elementary excitations in the FQHE. The observation of a finite magnetic field threshold has been explained qualitatively as due to disorder [10].

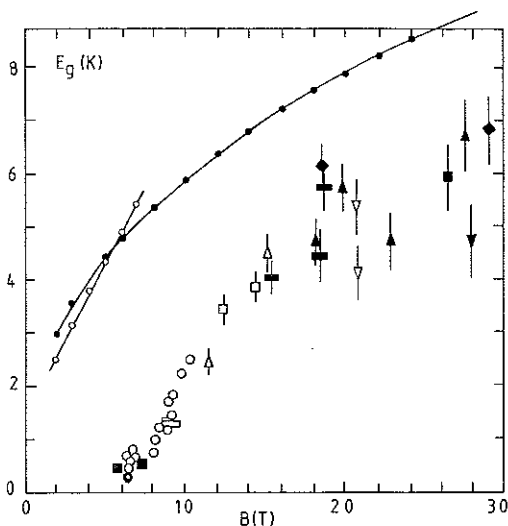


Fig. 3. Energy gap  $E_g$  (in units of K) as a function of magnetic field  $B$  (given in Tesla) for five-electron system. The filled and empty points have the same meanings as in Fig. 2.

The present work is open to some improvements. Most important of them could be that at low magnetic fields, where the spin-reversed quasiparticles seem to be important, mixing of higher Landau levels should be considered. This correction is at most 10% for four-electron (spin-polarized) system [13], in the region of magnetic fields of interest. Though difficult, larger system results would also be interesting. Suitable approximations are needed for such calculations.

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### Appendix

As the dimension of the Hamiltonian matrix is quite large — more than 11 000, for the spin-reversed systems — which in turn requires that the arithmetic be done in double precision, the straightforward diagonalization of the matrix is impossible. Furthermore, in the present work, we are dealing with the number of electrons and flux quanta such that they have no common divisor greater than unity. Therefore the symmetries based on the magnetic translation group [17] cannot be used to reduce the size of the matrix. It should however be noted that the two-body operator of the Hamiltonian, eq. (4), can connect only those states which differ by at most two indices labelling the occupied single-particle states. The majority of the matrix elements is therefore zero. Moreover, the coefficients of the two-body operator in fact, depends only on the difference between the indices and hence there are only a few (roughly the number of flux quanta squared) different matrix elements. When we store the matrix

in the computer by rows keeping only non-zero elements and represent these as offsets to the array containing the different elements together with the corresponding column indices, only four bytes of storage per non-zero element is required. The matrix being symmetric only the upper or lower triangle need to be stored.

The lowest eigenvalue and the corresponding eigenvector can be obtained by minimizing the Rayleigh quotient

$$\lambda(x) = \frac{x^T H x}{x^T x}$$

where  $x$  represents the column vector of the coefficients in the superposition of the basis states. The next lowest eigenvalue can then be found in a similar manner by working in the subspace orthogonal to this eigenvector. Repeating the procedure we can extract the required number of the lowest eigenvalues together with the eigenvectors. For the minimization of the Rayleigh quotient we choose the conjugate gradient method in which the quotient is approximated by a quadratic function and the minimum in each iteration step is searched in the plane spanned by the gradient and the search direction of the previous iteration step. It is in fact possible to iterate all the required eigenvalues simultaneously using, e.g., the method developed by Döhler [18]. This treatment of eigenvalues is quite convenient since the Hamiltonian matrix is needed only for multiplication of vectors which can be easily performed even though the matrix is represented in a rather complicated fashion.

### References

1. Tsui, D. C., Störmer, H. L. and Gossard, A., Phys. Rev. Lett. **48**, 1559 (1982); Störmer, H. L., Chang, A., Tsui, D. C., Hwang, J. C. M., Gossard, A. C. and Wiegmann, W., Phys. Rev. Lett. **50**, 1953 (1983).
2. For a review see, Halperin, B. I., Helv. Phys. Acta **56**, 75 (1983).
3. Yoshioka, D., Halperin, B. I. and Lee, P. A., Phys. Rev. Lett. **50**, 1219 (1983); Yoshioka, D., Phys. Rev. **B29**, 6833 (1984).
4. Halperin, B. I., Phys. Rev. Lett. **52**, 1583, 2390(E) (1984).
5. Chakraborty, Tapash, Phys. Rev. **B31**, 4026 (1985).
6. Morf, R. and Halperin, B. I., Phys. Rev. **B33**, 2221 (1986).
7. Girvin, S. M., MacDonald, A. H. and Platzman, P. M., Phys. Rev. Lett. **54**, 581 (1985).
8. Haldane, F. D. M. and Rezayi, E. H., Phys. Rev. Lett. **54**, 237 (1985).
9. Laughlin, R. B., Phys. Rev. Lett. **50**, 1395 (1983); Surf. Sci. **142**, 163 (1984).
10. Boebinger, G. S., Chang, A. M., Störmer, H. L. and Tsui, D. C., Phys. Rev. Lett. **55**, 1606 (1985); Boebinger, G. S., Private communications (1986).
11. Chakraborty, Tapash and Zhang, F. C., Phys. Rev. **B29**, 7032 (1984); Zhang, F. C. and Chakraborty, Tapash, Phys. Rev. **B30**, 7320 (1984).
12. Chakraborty, Tapash, Pietiläinen, P. and Zhang, F. C., Phys. Rev. Lett. **57**, 130 (1986); Chakraborty, Tapash, Phys. Rev. **B34**, 2926 (1986).
13. Yoshioka, D., J. Phys. Soc. Jpn **53**, 3740 (1984); *ibid.* **55**, 885 (1986).
14. Ando, T., Fowler, A. B. and Stern, F., Rev. Mod. Phys. **54**, 437 (1982); Fang, F. F. and Howard, W. E., Phys. Rev. Lett. **16**, 797 (1966).
15. MacDonald, A. H. and Aers, G. C., Phys. Rev. **B29**, 5976 (1984).
16. Zhang, F. C. and Das Sarma, S., Phys. Rev. **B33**, 2903 (1986).
17. Haldane, F. D. M., Phys. Rev. Lett. **55**, 2095 (1985).
18. Döhler, B., Numer. Math. **40**, 79 (1982).