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Effect of a charged impurity on the fractional quantum Hall effect: Exact numerical treatment of finite systems

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We investigate the role of a single charged impurity on the fractional quantum Hall effect by studying finite systems in spherical, toroidal, and disk geometries. Our qualitative results are independent of the geometry. We study the screening behavior systematically and find that screening charge accumulates at the impurity. The screening charge density shows an interesting oscillation with a characteristic scale of the magnetic length. We also find that the excitation gap is reduced significantly in the presence of the impurity.

The fractional quantum Hall effect (FQHE) is one of the most remarkable recent discoveries in condensed-matter physics. The original experimental discovery[1] by Tsui, Störmer, and Gossard has been followed by intense theoretical activity,[2–6] with most of the theoretical papers elucidating various aspects of the nature of the ground state giving rise to the remarkable experimental observations. The ground state of a two-dimensional electron gas in the presence of a strong perpendicular magnetic field at a fractional Landau-level filling $\nu = 1/m$ (m an integer) is now thought to be the Laughlin state,[2] an incompressible liquid described by a strongly correlated many-body wave function. The charge density of this electron liquid is uniform, except possibly at edges (which is unimportant in the thermodynamic limit). According to Laughlin, the ground state of this incompressible liquid is separated from the lower excited state by an energy gap (of the order of a fraction of a meV) which is responsible for the FQHE at temperatures low compared with the excitation gap. Laughlin's theoretical study,[2] as well as those of others[3–10] on the FQHE have concentrated on a *clean* two-dimensional (2D) electron system, whereas experiments are necessarily done on systems which contain impurities. Impurities may, in general, disrupt the highly correlated Laughlin state and ruin the FQHE. In fact, there is an already established experimental connection between the quality of a sample (as measured by the 2D mobility) and the existence of the FQHE. The FQHE has only been seen in samples of the highest purity with very high mobility values. An interesting theoretical issue associated with the presence of the impurity is the nature of screening by this highly correlated liquid, which cannot be studied by the standard many-body techniques because of the strong quantum correlation inherent in the system.

It is, therefore, important and interesting to investigate theoretically the effect of an impurity on the FQHE. In this Rapid Communication we provide the first systematic, theoretical investigation of the role of impurity in the FQHE. In particular, we consider the effect of a single, Coulombic-charged impurity center on the 2D electron system in the FQHE situation.

We report here *exact numerical* results for a *finite* 2D system containing a single charged impurity. In order to elucidate possible geometry and boundary effects, we have carried out our calculation in three different geometries: spherical,[3] toroidal,[4] and disk.[7,8] Exact numerical calculations[4,6–10] have earlier been carried out for *clean* 2D systems in these geometries by various authors. Our theory follows these earlier theoretical calculations except that we have an additional electron-impurity interaction term in our Hamiltonian. We find the expected accumulation of the electronic screening charge around the impurity and an interesting spatial oscillation in the screening density away from the impurity center. We also find that the excitation gap (defined simply as the energy difference between the ground state and the lowest relevant excited state) for our finite system is significantly reduced in the presence of the impurity. The results presented in this paper pertain to a positively charged static impurity center, which is, in fact, the most experimentally relevant case. We also make some remarks on the effect of a negatively charged impurity.

The Hamiltonian for our problem reads

$$H = H_0 + H_1 + H_i \, , \tag{1}$$

where H_0 is the noninteracting part of the Hamiltonian and H_1 is the electron-electron interaction. The part containing H_0 and H_1 has earlier been treated numerically[4,6–10] by a number of authors for different geometries. The H_i term is the contribution of the electron-impurity interaction which is given by

$$H_i = -\sum_j \frac{Ze^2}{\epsilon |\mathbf{R}_i - \mathbf{r}_j|} + E_{i-B} \, , \tag{2}$$

where Ze is the impurity charge, ϵ is the background static (lattice) dielectric constant, $\mathbf{R}_i, \mathbf{r}_j$ are the impurity and the jth-electron positions, respectively, and $E_{i\text{-}B}$ is the constant impurity-background interaction energy. We assume that the magnetic field is strong enough so that only the lowest spin-polarized Landau-level states can be occupied. We diagonalize the Hamiltonian defined by Eq. (1) numerically for a finite ($N = 3$ to 6) number of electrons in the different geometries. In this paper we concentrate on a filling factor of $\nu = \frac{1}{3}$ for the sake of brevity.

We discuss our results for the spherical geometry first. This geometry was first considered[3] by Haldane for the clean system. We put the impurity at the north pole and calculate the Coulomb potential using the geometric distance as the interparticle separation. In the absence of the impurity, the ground state at $\nu = \frac{1}{3}$ fractional filling is the

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$L = 0$ state, where L is the total angular momentum of the electrons. The excited states correspond to higher values of the angular momentum. Our calculated energies for the clean system agree with the results[9] of Haldane. In the presence of the impurity, the spherical symmetry is broken and L is no longer a good quantum number. However, azimuthal symmetry is still preserved and the states can be classified according to L_z, the z component of the angular momentum. The ground state has $L_z = 0$ and the (degenerate) excited states split because of the level mixing by the impurity potential. We define the excitation gap as the energy difference between the ground state and the lowest excited state. In Fig. 1(a) we show the excitation gap in the spherical geometry as a function of the impurity strength Z for two different finite systems with the number of electrons $N = 5$ and 6. It is obvious from the figure that the excitation gap is significantly reduced in the presence of the impurity. In Fig. 2(a) we show the screening behavior in the spherical geometry. In the absence of the impurity the electronic charge density is uniform. The screening charge accumulates at the impurity if one is present. The screening charge density oscillates away from the impurity with a characteristic length scale of the magnetic length. The period of this local screeening oscillation can be seen to be independent of the strength of the impurity charge. In Fig.

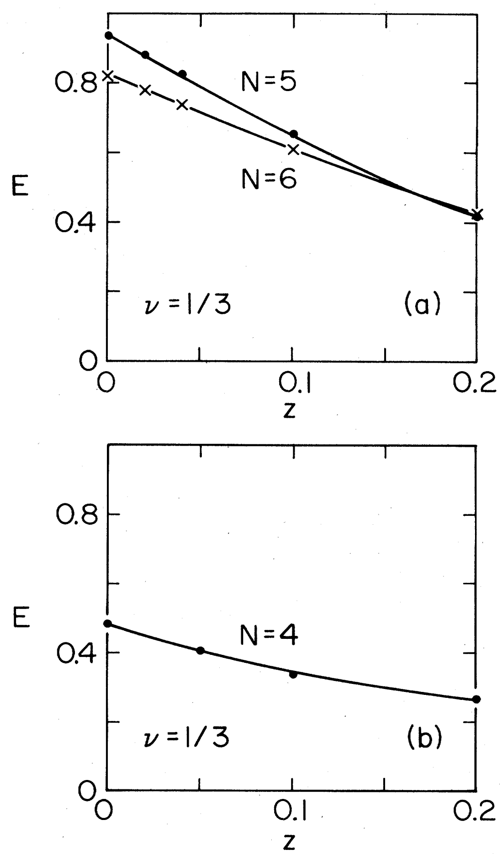

FIG. 1. Excitation gap E for $\nu = \frac{1}{3}$ in the units of $e^2/\epsilon l$ (where l is the magnetic length) as a function of the impurity strength Z for (a) the spherical and (b) the toroidal geometry. For (a), two different calculations with the total number of electrons $N = 5$ and 6 are shown, whereas for (b) $N = 4$.

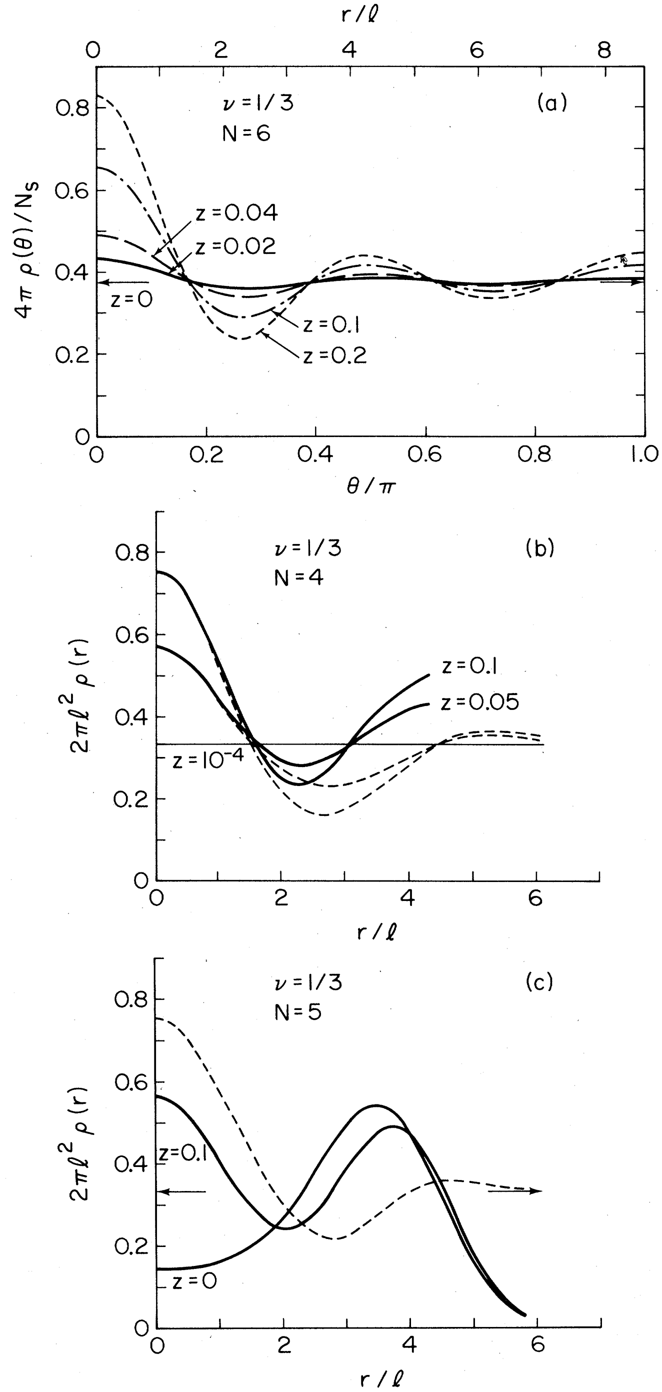

FIG. 2. Spatial behavior of the screening charge density ρ is shown for different impurity strengths in (a) spherical [$\rho(\theta)$ is density per unit solid angle], (b) toroidal, and (c) disk geometries. N_s is the total number of states and θ is the azimuthal angle, whereas r is the distance from the impurity center (which is always at the origin). Note that rotational symmetry is absent in the toroidal geometry, with the solid curves giving the charge density in the (0,1) direction and the dash-dotted curves giving the same in the (1,1) direction of the rectangle (b). In (c) the dashed curve gives the screening charge density (i.e., the difference between the electronic charge densities corresponding to $Z = 0.1$ and 0, shown by the solid curves). The arrows indicate the average normalized charge density in the disk at $\nu = \frac{1}{3}$.

3 we plot the charge density for systems of $N=4$, 5, and 6 electrons for a fixed Z. Except near the edge, the screening is quite independent of the system size. This leads us to believe that the occurrence of a local charge-density wave around the impurity is a general feature of the physics of the system, not restricted to the finite systems we are studying numerically. Using symmetry considerations we can obtain the effect of a negatively charged impurity in the sphere.

To investigate whether the above qualitative results are geometry dependent, we have also considered the toroidal and disk geometries with a finite number of electrons and a single charged impurity. In the toroidal geometry[4,10] the ground state at $\mu=\frac{1}{3}$ is triply degenerate for the clean system. In the presence of the impurity (which, by virtue of the periodic boundary condition, lies in every single rectangular cell), the degeneracy is lifted because the impurity potential mixes the momentum eigenstates. Because of this reduced symmetry in the presence of the impurity we can only diagonalize up to a $N=4$ system in the toroidal geometry. Both the ground and the excited states of the clean system become nondegenerate in the presence of the impurity and we define the excitation gap as the energy difference between the "lowest" ground-state and the "lowest" excited-state levels.[11] In Fig. 1(b) we show this excitation gap as a function of the impurity strength Z for $N=4$. The result is qualitatively the same as that in Fig. 1(a), showing that the excitation gap is significantly reduced in the presence of the impurity. In Fig. 2(b) we show the screening behavior in the toroidal geometry, which is similar to that [Fig. 2(a)] in the spherical geometry.

The disk model we consider has a positive background charge density, which is uniformly distributed over the disk and which exactly neutralized the total charge in the system. The uniform charge density is therefore $\rho=\nu/2\pi l^2$, where l is the magnetic length. The ground state of a finite disk for up to $N=6$ electrons at $\nu=\frac{1}{3}$ is found to have total angular momentum $L=N(N-1)/2\nu$, which is consistent with Laughlin's wave function, but is somewhat different from that of the earlier work.[7,8] The energy levels in the disk geometry are not reliable and there is no downward cusp in the ground-state energy at $\nu=\frac{1}{3}$. We believe that this is related to the open boundary condition (edge effects) present in the disk geometry. In Fig. 2(c) we show the electronic charge density in the disk geometry both with and without the impurity (which is placed at the center of the disk). The charge density for the clean disk is seen to be quite different (in particular, *nonuniform*) from that in the other geometries (sphere or torus), where the charge density in the clean system is uniform. The nonuniformity of the charge density in the disk geometry is a finite size effect, and, in fact, for small systems ($N=2,3,4$, etc.) Laughlin's wave function also gives a charge density having similar nonuniform behavior. As one can see from Fig. 2(c), the screening behavior in the disk geometry is quite similar to that in the other geometries, even though the charge density for the clean system behaves differently. In particular, the screening charge accumulates at the impurity and oscillates away from the impurity with the characteristic length scale of the magnetic length.

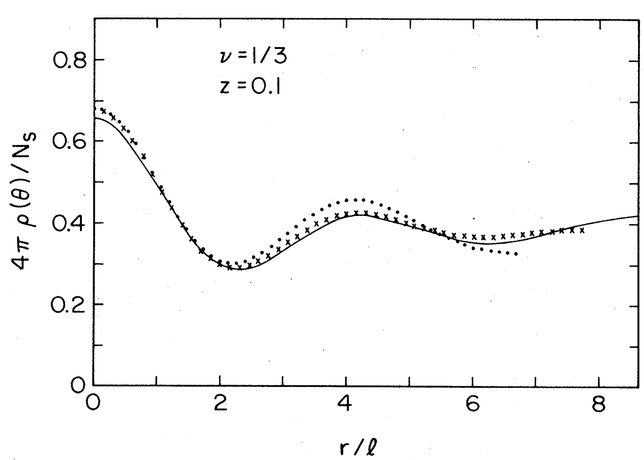

FIG. 3. Spatial behavior of the screening charge in the spherical geometry for a fixed $Z=0.1$ and for different system sizes: $N=6$ (solid curve), $N=5$ (crosses), and $N=4$ (dots). The distance γ is along the surface.

In summary, we have investigated the effects of a single charge impurity on the FQHE by numerically studying finite sytems in different geometries. To the extent that one can neglect impurity-impurity interaction effects, our one-impurity model may be an approximation for experimental systems with a *dilute* impurity concentration. It should be noted that the actual 2D systems showing the FQHE are modulation doped and, hence, the impurities are spatially separated from the 2D electrons. In our model this fact is easily incorporated by making the impurity strength $Z<1$. In practice,[12] a value of Z around 0.1 may be the realistic value for the actual high-mobility GaAs samples.

By far the most interesting and unanticipated result is the oscillatory screening behavior (Figs. 2 and 3) around the impurity. The result is geometry independent, and, to the extent we are able to investigate, independent of the system size as well. Results for the spherical case [Figs. 2(a) and 3] clearly indicate this charge-density oscillation to be an intrinsic property of the 2D system. We should emphasize that this screening oscillation is unrelated to the Friedel oscillation, which arises because of the existence of a sharp Fermi surface in the system. The screening oscillation in our case is a consequence of the imcompressible nature of the strongly interacting system. The corresponding noninteracting dielectric screening does not show[13] any oscillatory behavior. Our results give some hints that the highly correlated Laughlin-liquid state may actually be destroyed by impurities through the formation of local charge-density waves around each impurity as shown in Figs. 2 and 3. Our result for the (30–50%) reduction in the excitation gap (Fig. 1; $Z\sim0.1$) of the system is much more difficult to interpret theoretically, since this is clearly a strongly size-dependent phenomenon. Our calculated excitation energies are those of localized levels around the impurity and should not be related to the experimental[14] mobility gap. One can perhaps try to probe their localized levels directly by some sort of finite-frequency experiment using low-energy photons or phonons.

Our work raises a number of interesting and intriguing questions. In particular, the local charge-density wave around the impurity needs to be understood in detail. The question of how clean a sample has to be in order for FQHE to be observable is another such question. Our calculational details and additional numerical results will be reported in a forthcoming longer publication.

Note added. Our results are in excellent quantitative agreement with the recently published[15] theoretical results of Girvin, MacDonald, and Platzman. In particular, we find that the shift in the ground-state energy due to the presence of the impurity can be written as αZ^2, where Z is the impurity charge. We find numerically $\alpha \simeq 1.2$ for $\nu = \frac{1}{3}$ and for a five-electron spherical system, whereas Ref. 15 gives $\alpha = 1.15$. The oscillation period of the screening charge also agrees well with the results of Ref. 15.

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