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Sign of equilibrium Hall conductivity in strongly correlated systems

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We consider the equilibrium current circulating in a cylindrical geometry, perpendicular to applied magnetic and electric fields in a strongly correlated system. We show that the sign of this current is determined by the derivative of the kinetic energy with respect to the chemical potential. We present exact numerical results from diagonalization of finite clusters to support our arguments. In the case of the Hubbard model with strong on-site repulsion the sign of the equilibrium Hall conductivity is electronlike for a small number of particles and holelike close to half filling.

There is considerable interest in the electronic properties of strongly correlated two-dimensional systems, in connection with the problem of high-T_c superconductivity.[1] Strong correlations give rise to departures from the ordinary Fermi-liquid picture. In particular, for one electron per lattice site, strong repulsion gives rise to the celebrated Mott transition.[2] The behavior of different physical quantities near this transition has been the subject of recent intensive investigation. In the large-U Hubbard model it has been shown that the plasma frequency is zero at vanishing densities and at half filling, and has a maximum at an intermediate filling factor. On the other hand, approaching half filling, the compressibility diverges as the inverse number of holes.[3] In this paper we study the strong-correlation effect on the equilibrium Hall current. For noninteracting electrons on a square lattice, the equilibrium Hall current changes sign at half filling as the Fermi surface changes its shape from electronlike to holelike. In the large-U limit we find an additional sign change below half filling which is purely due to correlations. We demonstrate this effect numerically, and understand it using simple analytical considerations.

We consider the Hubbard or t-J Hamiltonian in the presence of both a magnetic field B and an electric field E. We impose cylindrical boundary conditions, with the electric field parallel to the axis of the cylinder. The Hamiltonian will then be given by

$$H=-t\sum_{i,\tau,\sigma} c_{i,\sigma}^{\dagger} e^{i\varphi_{i,i+\tau}} c_{i+\tau,\sigma}+\text{H.c.}+E\sum_{i,\sigma} y_i c_{i,\sigma}^{\dagger} c_{i,\sigma}+H' \,, \tag{1}$$

where H' is the Hubbard repulsion, or the spin part in the case of the t-J Hamiltonian. In the latter, a projector over singly occupied sites is implicit in the kinetic term. $\tau=1,2$ denotes the basic lattice vectors. If $i=(l,m)$ is a lattice position then $y_i=m$, and the boundaries of the sample are chosen symmetrically in the y direction. We choose the gauge $\varphi_{i,i+1}=2\pi m\Phi/\phi_0$, $\varphi_{i,i+2}=0$, where Φ is the plaquette flux. We will be interested in the weak electric field regime, $EL_y \ll t$.

The total current circulating around the cylinder can be written as

$$J_x=\sum_i \langle \Psi_0 | \hat{j}_x^{(i)} | \Psi_0 \rangle \,, \tag{2}$$

with

$$\hat{j}_x^{(i)}=\frac{\partial H}{\partial \varphi_{i,i+1}} \equiv \hat{j}_{l,m;l+1,m} \,. \tag{3}$$

For $E=0$, $J_x=0$ because of symmetry around $y=0$; we have

$$\langle \Psi_0 | \hat{j}_{l,m;l+1,m} | \Psi_0 \rangle = -\langle \Psi_0 | \hat{j}_{l,-m;l+1,-m} | \Psi_0 \rangle \,. \tag{4}$$

Let us analyze the behavior of the local current as a function of the filling fraction $n=N_p/N_s$. N_p and N_s are the total particle number and the number of sites, respectively. We consider $E=0$ for the moment. If the lattice dimensions are large in the y direction we expect small charge modulations, and that the particle density is nearly uniform and equal to n on the whole sample. The local current $\mathcal{J}_{l,m}$ is given by

$$\mathcal{J}_{l,m}=\langle \Psi_0 | \hat{j}_{l,m;l+1,m} | \Psi_0 \rangle$$

$$=2\,\text{Im}\left[e^{i2\pi m\Phi/\phi_0} \left\langle \Psi_0 \left| \sum_\sigma c_{l,m,\sigma}^{\dagger} c_{l+1,m,\sigma} \right| \Psi_0 \right\rangle \right] . \tag{5}$$

It vanishes at $n=0$ and $n=1$ for all l and m. At $n=0$ there are no particles, and at $n=1$ the projector over the singly occupied subspace annihilates all the matrix elements of the current.

At intermediate values of n, and because of rotational invariance around the axis of the cylinder $\mathcal{J}_{l,m}$ will be independent of l, and therefore we write $\mathcal{J}_{l,m}=\mathcal{J}(y)$. For small fields, we expect a current distribution *odd* in the y coordinate that is, $\mathcal{J}(y,n) \sim \alpha(n)\Phi f(y)$, with α some constant depending on the filling fraction but independent of the magnetic flux, and $f(y)$ an odd function. Since $\mathcal{J}(y,n) = -\mathcal{J}(-y,n)$, the total current $J_x = 0$.

In considering the effect of the electric field we *assume* that the current can be written as a function of the local density $n(y)$ in addition to its dependence on the y coordinate. That is $\mathcal{J} = \mathcal{J}(y, n(y))$. When E is turned on, due to the free boundary conditions in the y direction, there will be a charge redistribution with charges transferred from the region of $Ey > 0$ to the one with $Ey < 0$. This implies that there will be a dependence of the charge on the y coordinate that, in first order in the field will be given by

$$\delta n(y) \sim \beta E y \tag{6}$$

with β some constant that we assume to be uniform in sign in all the range of filling fractions from zero to one. This means that the charge will always increase (decrease) in the regions of negative (positive) potential energy. Of course, the electric field has to be small enough to satisfy $\beta E L_y \ll 1$. Now, due to this charge redistribution, and given the assumption $\mathcal{J} = \mathcal{J}(y, n(y))$, the current will no longer be an odd function of y, and therefore $J_x \neq 0$. This current circulates around the cylinder, and is thus transverse to the electric field; we identify it with the equilibrium Hall current of the problem. We want to find out the *sign* of the current to assign electronlike or holelike behavior. From (6) we have that (the y coordinate of the sample is in $-L_y \le y \le L_y$)

$$J_x = \int_0^{L_y} dy [\mathcal{J}(y) + \mathcal{J}(-y)] \simeq 2E\beta \int_0^{L_y} dy\, y \frac{\partial \mathcal{J}(y,n)}{\partial n} . \tag{7}$$

From the above considerations, $\partial \mathcal{J}/\partial n$ has a uniform sign for positive y, and changes sign for some filling fraction in the range $0 < n < 1$. Therefore there will be a sign change in the Hall current for some density n_0. The current J_x in our approach results from an unbalance of the (diamagnetic) local currents due to the charge rearrangement induced by the electric field. Therefore the sign of the equilibrium Hall conductance σ^e_{xy} is determined by the variation of the local current with the (local) density. For fixed field B, one expects the current to be a monotonic function of the kinetic energy, hence we conjecture that $\mathrm{sgn}[\sigma^e_{xy}]$ will correlate with $\mathrm{sgn}[\partial\langle T\rangle/\partial n]$. In the uncorrelated case this gives a sign change for half filling ($n = 1$). From numerical simulations[4] we know that in the case of the Hubbard model for large enough U, $\langle T\rangle$ has a local maximum for half filling, and therefore we expect a sign change in σ^e_{xy}. A sign change in σ_{xy} was reported in numerical simulations of the t-J model in Ref. 5. We can obtain the same qualitative behavior using the following hydrodynamic considerations.[6] In a static situation,

$$\mathbf{j} = 4\pi \nabla \times \mathbf{M} . \tag{8}$$

A static electric field $E_y = \nabla_y \delta\varphi$ produces a charge redistribution

$$\delta n = \frac{dn}{d\varphi} \delta\varphi . \tag{9}$$

Equation (8) is still valid when the boundaries in the y direction are open and hence $j_y = 0$. We take $\mathbf{M} = M\hat{\mathbf{z}}$. The current will then be given by

$$j_x = 4\pi \frac{\partial M}{\partial n} \frac{\partial n}{\partial \varphi} \frac{\partial \varphi}{\partial y} = 4\pi \frac{\partial M}{\partial n} \frac{\partial n}{\partial \mu} E_y \equiv \sigma^e_{xy} E_y . \tag{10}$$

The compressibility $\partial n/\partial \mu > 0$, but one expects a maximum in the dependence of $M(n)$, since, for example, in the t-J model it has to be zero for both $n = 0$ and $n = 1$. Hence the equilibrium σ^e_{xy} will change sign. In the weak field limit $M = \chi_d B$, where χ_d is the diamagnetic susceptibility. In this case $\sigma^e_{xy} = 4\pi B \partial \chi_d/\partial n$. Again, in the strong repulsion limit we expect χ_d to go to zero at half filling, thus giving a double minimum structure like that for $\langle T\rangle$ and the corresponding changes in sign for σ^e_{xy}.

In order to verify the above arguments we have solved exactly finite clusters using cylindrical boundary conditions, and evaluated the circulating current in the presence of an electric field. These results are shown in Figs. 1 and 2. In Fig. 1 we show results for spinless fermions with near-neighbor interactions. This case corresponds to the completely polarized Hubbard model, with H' in Hamiltonian (1) given by

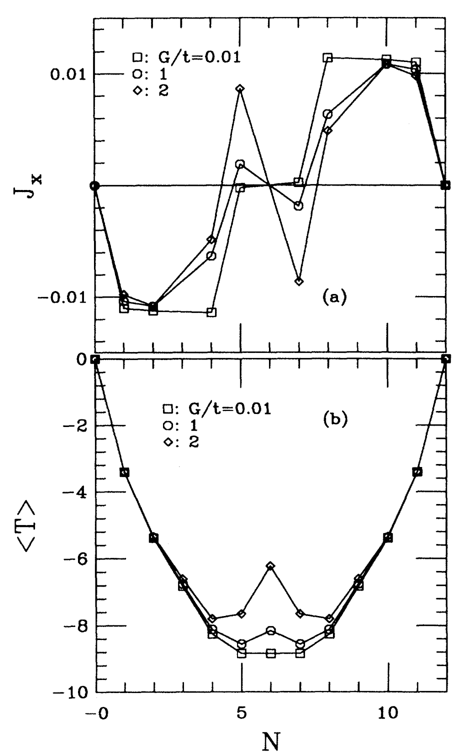

FIG. 1. (a) Dimensionless Hall current J_x and (b) kinetic energy $\langle T\rangle$ for a spinless fermion system with near-neighbor interaction as a function of particle number N, for a 12-site lattice ($L_x = 4$, $L_y = 3$). The results correspond to the fields $E/t = 0.02$ and $\phi/\phi_0 = 0.02$. We have checked that these values correspond to the linear response region. In all cases the continuous lines are guides to the eye.

$$H' = G \sum_{\langle i,j \rangle} (n_i - \langle n \rangle)(n_j - \langle n \rangle) ,$$

with $\langle n \rangle$ being the mean particle number. This correlated spinless Hamiltonian has the essential ingredients to exhibit the change in sign in the equilibrium transverse current, since in the strongly correlated limit ($G \gg t$) the kinetic energy vanishes at half filling because of the formation of a staggered charge-density wave. We therefore expect a double minimum in the dependence of the kinetic energy as a function of particle number and therefore a sign change in J_x. This is confirmed in our numerical calculations, an example of which is shown in Fig. 1(b). In Fig. 1(a) the point corresponding to $N=3$ (and $N=9$) was omitted. In general, in our simulations with fermions, to get sensible results we had to suppress points that for zero value of the electric field have a finite current, since we want the unperturbed states to carry no current. These degenerate states give a vanishing contribution to the current in the thermodynamic limit.

To emphasize the basic point of our argument we also solved the same Hamiltonian for the case of hard core bosons (HCB's), where the above-mentioned degeneracies are absent. From the point of view of the exclusion principle, the HCB's behave as fermions.[7] Hence we expect the same qualitative behavior for the change in sign of J_x as in the case of the fermions. This is illustrated in Fig. 2 where we show also the kinetic energy as a function of particle number. We see that it exhibits a double-minimum structure that is correlated as predicted with the change in sign of J_x. Since the ground state of this system is superfluid away from half filling, we expect the diamagnetic susceptibility (and $\partial \chi_d / \partial n$) to be much larger than in the fermion case, and this is consistent with the numerical results. This also would suggest that this current would be readily observable in a superconducting ground state of fermions.

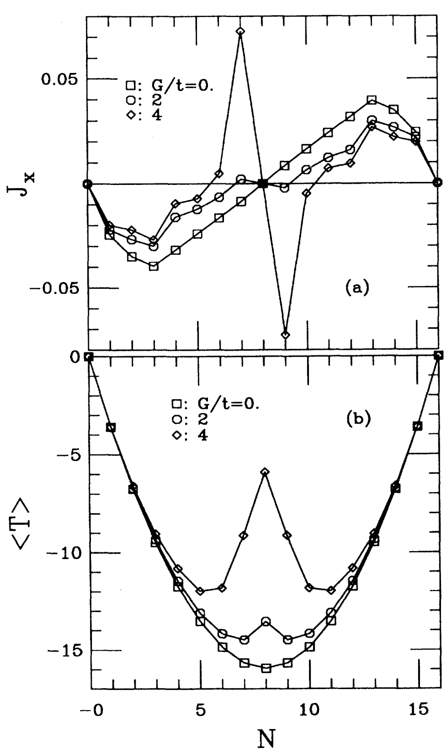

FIG. 2. (a) Hall current J_x and (b) kinetic energy $\langle T \rangle$ for the ground state of a hard core boson system with near-neighbor interaction. The results are for a 4×4 lattice and the values of the fields are the same as in Fig. 1. Note the correspondence of $\mathrm{sgn}[\sigma^e_{xy}] = \mathrm{sgn}[\partial\langle T \rangle/\partial n]$ (note that $J_x \propto \sigma^e_{xy}$).

The above considerations apply for the case of thermodynamic equilibrium. By this we mean that the electric field acts as a perturbation that modifies the ground state from a non-current-carrying state to one with a finite equilibrium current circulating around the cylinder in our geometry. If time-dependent perturbation theory is applied, this regime corresponds to the "slow" limit in which the frequency of the applied perturbation goes to zero faster than the wave vector, and the system has time to reach a new equilibrium state in the presence of the field. That is,

$$\sigma^e_{xy} = \lim_{q\to 0} \lim_{\omega\to 0} \frac{\langle [j_x, j_y] \rangle (q,\omega)}{i\omega} .$$

The transport regime corresponds to the "fast" limit[8] where the system stays homogeneous (does not have time to adjust to the spatially varying potential). If the spectrum has a gap, or if the velocity matrix elements are zero between the ground state and states with zero excitation energy, there is in principle no distinction between the transport and the equilibrium currents.[9]. In the slow limit, when $\omega=0$, the charges adjust to the spatially varying potential and clearly no current flows in the direction of the field. In the presence of a magnetic field, however, there is a finite current transverse to the electric field, modulated with a wave vector q. If we focus on a strip of width $L = 1/2q$, the current and charge distribution will be qualitatively similar to a finite sample of transverse dimensions $\sim L$. We therefore conclude that the equilibrium response of a finite sample corresponds to the slow limit, with $q \sim 1/L$, L being the dimensions in the sample in the direction of the electric field (parallel to the axis of the cylinder in our geometry). This is the limit which has been studied in our numerical simulations, and in the numerical experiments of Castillo and Balseiro.[5] A very important question is the evaluation of the off-diagonal current-current correlation function in the opposite (i.e., $q=0$ first) limit, which corresponds to the standard Hall conductivity measurements. Our discussion above applies to the case of small magnetic field B. In the case of large $B(\omega_c \tau \gg 1)$, we expect the limits to commute since in this case the magnetic length provides a small length scale $\ell_B \sim 1/B$ that allows us to take the small-q limit first. This makes our results applicable to the transport regime, and in particular this limit could be realizable in the "low-T_c" materials.

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