Hall Conductivity and Fermi Surface in Highly Correlated Systems

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We calculate exactly the one-particle spectral densities and Hall conductivity for the two-dimensional Hubbard model in the large-U limit, for two different finite clusters. The Fermi surface obtained from the one-particle spectral functions is consistent with Luttinger's theorem, but the Hall conductivity changes from electronlike for a dilute system to holelike for a nearly half-filled system, indicating the deconfinement of charge and spin excitations in a two-dimensional system.

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The electronic properties of doped Hubbard-Mott insulators have been studied for many years. The discovery of high-T_c superconductivity in the cuprate materials and the assumption that simple nearly half-filled one-band models retain the essential physics of these systems renewed the interest in this problem [1].

A central question in the theory of high-T_c superconductivity concerns the nature of the Fermi surface and the low-energy excitations in these materials. One of the most controversial questions is whether spin and charge are deconfined as in one-dimensional problems [2] or whether the excitations carry charge and spin together, being real electronlike quasiparticles [3].

Angle-resolved photoemission and inverse photoemission experiments in some of the high-T_c materials indicate the existence of a "large Fermi surface" consistent with that of a weakly interacting system [4,5]. In fact, band-structure calculations, which clearly cannot be used to describe the undoped insulating materials, predict for the doped systems a Fermi surface consistent with the one obtained by photoemission [6]. However, this successful prediction of one-electron-band calculations cannot be taken as evidence of weak interactions in these systems. If Luttinger's theorem [7] is obeyed, the Fermi volume is invariant under interaction effects and a strongly interacting system should also have a large Fermi surface. It has recently been shown that in a two-dimensional (2D) square lattice the Fermi surface of a t-J model is consistent with Luttinger's theorem [8]. Monte Carlo simulations for a nearly half-filled 2D Hubbard model also support this result [9].

In this Letter we study numerically the Fermi surface and the Hall resistivity of a 2D Hubbard model with strong on-site interactions. Consider the case of a nearly half-filled system (with the particle density $n \leq 1$): as we show below and in agreement with previous results, the one-particle spectral densities are consistent with a large Fermi surface. Moreover, the characteristic features of the spectral functions are strongly reminiscent of the experimental results. One of the important questions is whether this Fermi surface can be used to build a semiclassical theory for the dynamics of quasiparticles in an external magnetic field. If this were so, the Hall resistance should be negative for $n < 1$, indicating electronlike carriers. The de Haas–van Alphen effect should indicate the existence of such a large Fermi surface. If, on the other hand, charge and spin excitations were decoupled, the charge dynamics should be dominated by the existence of a pseudo Fermi surface for charge excitations which may be quite different from that observed in photoemission.

In the Hubbard model for large U, the kinetic energy and the integrated low-energy optical conductivity are decreasing functions of n for a nearly half-filled band [10]. Some authors have interpreted this result as an indication that charge carriers are holes, in accordance with the second point of view.

Recently Ioffe, Kalmeyer, and Weigmann [11] showed that a hole-doped Mott insulator has a positive Hall resistance and that its temperature dependence is consistent with experiments made in high-T_c materials. Their starting point is an effective Hamiltonian where charge and spin excitations are decoupled and consequently the positiveness of the Hall resistance they obtained is not surprising.

In order to put all the pieces together and build a consistent theory it is important to calculate in a good approximation and at the same footing the different properties of the system, i.e., the one-electron spectral densities, to obtain the Fermi surface and the Hall resistance of the system.

To do so we have studied numerically a Hubbard Hamiltonian in the limit of strong on-site interaction U. All results presented below are obtained by exact diagonalization techniques [12]. To reduce the size of the Hilbert space, we eliminated, through the usual canonical transformation, the doubly occupied states. The resulting Hamiltonian reads

$$H=\sum_{\langle ij\rangle}(t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})+\sum_{\langle ij\rangle}\frac{4|t_{ij}|^2}{U}(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4}n_in_j)$$
$$+\sum_{\langle ijk\rangle}\frac{t_{ij}^{*}t_{kj}}{U}c_{k\sigma}^{\dagger}c_{j\sigma}n_{j-\sigma}c_{j\sigma'}^{\dagger}c_{i\sigma'}, \qquad (1)$$

where the operator $c_{i\sigma}$ destroys a fermion of spin σ at site i, $\mathbf{S}_i$ is the spin operator for site i, $n_{i\sigma}$ is the fermion num-

ber operator for site i and spin σ ($n_i = n_{i\uparrow} + n_{i\downarrow}$), the symbol $\langle ij \rangle$ denotes the sum over all pairs of nearest neighbors, $\langle ijk \rangle$ denotes the sum over all sets of three sites with i and k nearest neighbors of j, and t_{ij} is the hopping matrix element between sites i and j. All fermion operators are subject to the constraint of no double occupation. In what follows we indicate by t_x and t_y the hopping matrix element along the x and y directions, respectively, and we define $J_x = 4t_x^2/U$.

We solved exactly the problem in two finite clusters of $N = 12$ sites each and all possible numbers of particles N_e ($1 \leq N_e \leq N$). We considered rectangular clusters with periodic boundary conditions in the x direction and open boundary conditions in the y direction. The two types of clusters considered were 4×3 and 6×2 (the notation $m \times l$ indicates m sites in the x direction and l sites in the y direction). These geometries were chosen in order to be able to include an external magnetic field B of arbitrary intensity perpendicular to the plane. We considered only the diamagnetic coupling of the external field with the charged particles. This is done through Peierls substitution [13], which in the present case can be done by adding a phase to the hopping matrix elements in the x direction (this affects all terms except the spin-spin coupling). In what follows we present results for the one-particle spectral densities in the absence of magnetic field and the transverse conductivity σ_{xy} in the presence of a small magnetic field B.

For a rectangular $m \times l$ cluster with periodic boundary conditions only along the x direction the band structure of uncorrelated particles consists of l bands. Within each band the quantum number k_x varies between $-\pi/a$ and π/a, where a is the lattice parameter. Each band is characterized by a quantum number α corresponding to a different wave function in the y direction. For our 4×3 cluster we defined $\alpha = -1$, 0, and 1 for the lower, medium, and upper bands, respectively. As the one-particle states are filled, each band has a different Fermi momentum $k_{\alpha F}$. This collection of $k_{\alpha F}$ defines a "Fermi surface." Although this geometry is not the most appropriate for studying the Fermi surface, it is necessary for calculating the Hall conductivity and as mentioned above we calculate all the properties in the same cluster in order to minimize possible inconsistencies due to finite-size effects.

In the interacting system the expectation value for the occupation number $n_{\alpha k_x}$ of the state $|\alpha k_x\rangle$ is greater than 0 and lower than 1. We define $k_{\alpha F}$ as the momentum where this expectation value is equal to 0.5. With this criterion the Fermi surface in the interacting system is the same as in the noninteracting one. In Fig. 1 the expectation value of $\eta_{\alpha k_x}$ is shown; to present all the states in the same figure, we plotted $\langle n_{\alpha k_x} \rangle$ as a function of the noninteracting one-particle energies $\epsilon_{\alpha k_x}$. As is evident from the figure, for all densities $n = N_e/N$ the Fermi surface is consistent with Luttinger's theorem. In Fig. 1(c), corresponding to $N_e = 10$ particles and $J_x = 0.1 t_x$ in the

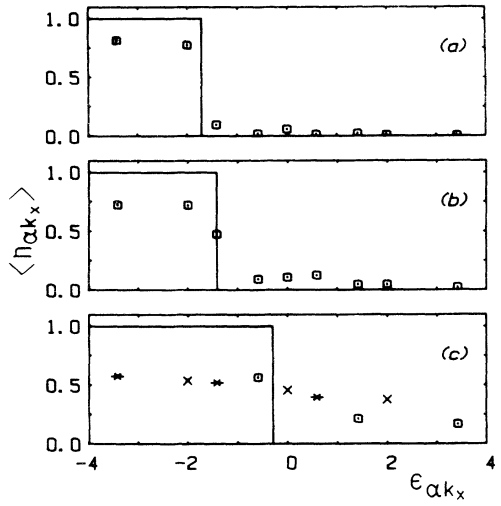

FIG. 1. Occupation numbers $\langle n_{\alpha k_x} \rangle$ as a function of the noninteracting one-particle energies $\epsilon_{\alpha k_x}$ for $J_x/t_x = 0.1$ in the 4×3 cluster. (a) $N_e = 4$, (b) $N_e = 6$, and (c) $N_e = 10$. In (c), different symbols indicate different values of the quantum numbers α: $\alpha = -1$ (stars), $\alpha = 0$ (crosses), and $\alpha = 1$ (squares). Continuous lines indicate the occupation numbers for the noninteracting systems.

4×3 cluster, there are some oscillations in $\langle n_{\alpha k_x} \rangle$. This is a consequence of plotting all bands on the same scale; with each band, however, the behavior of $n_{\alpha k_x}$ is monotonous. The same results are obtained for infinite U ($J_x = 0$).

The one-particle spectral densities obtained from the Green functions $\langle\langle c_{\alpha k_x}, c^\dagger_{\alpha k_x} \rangle\rangle$ are shown in Fig. 2. The spectral densities show a lot of structure that extends far from the Fermi energy. There is a strong peak that crosses the Fermi energy as k_x crosses the corresponding Fermi momentum $k_{\alpha F}$. These spectral densities are in qualitative agreement with photoemission spectra obtained in high-T_c materials. Although the clusters studied are small and do not have x-y symmetry, these results together with those obtained in Refs. [8,9] are evidence that the Fermi surface in these strongly interacting systems is consistent with Luttinger's theorem if the number of holes is large enough. The case of a single hole may have a particular behavior [8,14].

We now present results for the transverse conductivity σ_{xy}. The Hall resistance $R_H = R_{yx}/B$ or the Hall number n_H must be calculated by inverting the conductivity tensor, and have the same sign as σ_{xy}. We calculated the transverse conductivity using linear response theory. We included a magnetic field perpendicular to the plane and considered the perturbation produced by a small transverse electric field. The coupling of the electrons to the electric field is given simply by $H_{\rm int} = -eE \sum_i y_i$, where e is the electron charge, E is the electric field, and y_i is the y coordinate of the ith electron. The transverse conduc-

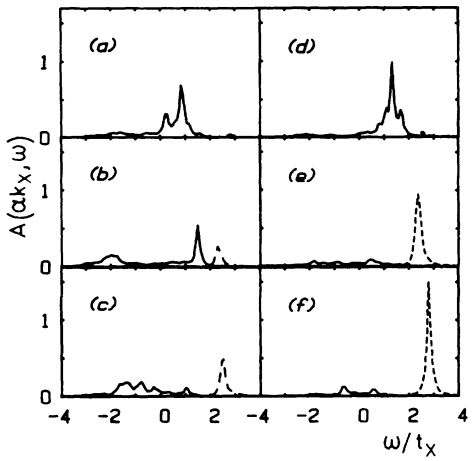

FIG. 2. One-particle spectral densities for ten particles in the 4×3 cluster with $J_x/t_x=0.1$. (a)–(c) correspond to $\alpha=0$ with $k_x=0$, $\pi/2$, and π, respectively; (d)–(f) correspond to $\alpha=1$ with $k_x=0$, $\pi/2$, and π. The solid and dashed lines correspond to the photoemission and inverse photoemission spectra, respectively. The spectral functions are plotted with a Lorentzian broadening of $\delta=0.08t_x$. The Fermi energy is located at $\omega\simeq 2t_x$.

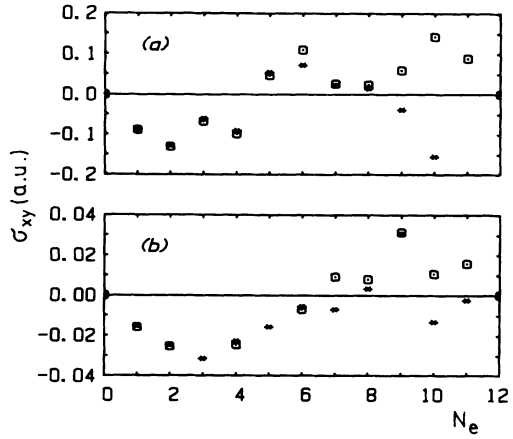

FIG. 3. Transverse conductivity as a function of the total number of particles for (a) a 4×3 cluster with $t_y=t_x$, and (b) a 6×2 cluster with $t_y=2t_x$. Squares and stars correspond to $J_x/t_x=0$ and 0.1, respectively.

tivity is

$$\sigma_{xy}=-e^2a^2t_x\langle\langle\bar{j}_x,\bar{y}\rangle\rangle_{\rm ret}|_{\omega=0}\,, \qquad (2)$$

where $\bar{j}_x$ and $\bar{y}$ are adimensional current and position operators. This equation yields for a noninteracting system in the two clusters studied a negative transverse conductivity for all densities ($0<n<1$), in agreement with the semiclassical theory.

In Fig. 3, we show the results obtained as a function of N_e for both the 4×3 and 6×2 clusters and different values of U. There are three points which are not included; for these points, because of quasidegeneracy of the ground state in these geometries the computation of σ_{xy} is subject to large numerical uncertainties.

There are several features which deserve comment: The transverse conductivity for $J_x=0$ is electronlike for low n and holelike for larger n. The Hall number changes sign when the lower Hubbard band is approximately half filled ($n\simeq0.5$). The single-hole problem is a special point. The total spin of the system for one hole and $J_x=0$ is maximum in agreement with the Nagaoka theorem; consequently the transverse conductivities for a single hole and a single electron are equal in absolute value and of different sign. For all other densities in the 4×3 cluster the total spin is zero for even N_e and $\frac{1}{2}$ or $\frac{3}{2}$ for odd N_e. For this system, the behavior of even and odd number of holes appears to be slightly different; this is probably due to finite-size effects. In the 6×2 cluster, both the eleven- and nine-particle ground states are completely polarized, but for all other densities the total spin is between 0 and $\frac{3}{2}$. Note that, although there is no electron-hole symmetry in the lower Hubbard band, the absolute value of the transverse conductivity for the case of a few electrons N_e is of the same order of magnitude as the conductivity for a few holes $N-N_e$. As U decreases there is a tendency towards a disappearance of holelike behavior for $n\simeq1$. This could be a consequence of the antiferromagnetic correlations, which increase rapidly as U decreases. In fact, as shown in Fig. 4 the Hall conductivity for the 4×3 cluster with $N_e=10$ changes sign when strong short-range antiferromagnetic correlations appear.

As a general behavior, these results show that for large U ($J_x\leq0.1t_x$) the Hall number changes sign when the lower Hubbard band is approximately half filled, the car-

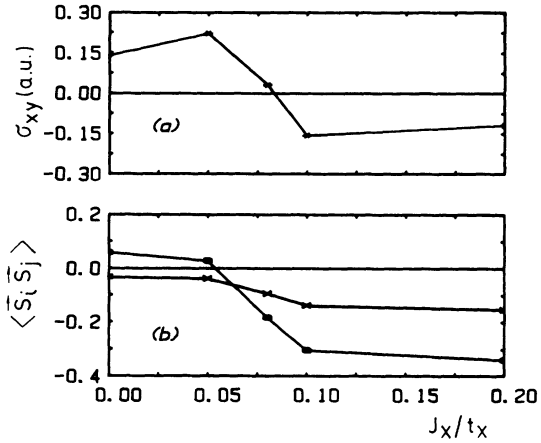

FIG. 4. (a) Transverse conductivity as a function of J_x/t_x for the 4×3 cluster with $N_e=10$ and $t_y=t_x$. (b) Nearest-neighbor spin-spin correlations. Parameters are the same as in (a). Squares indicate correlations along the upper and lower chains, and crosses indicate the correlations of the central chain. The lines are only to guide the eye.

riers being electronlike for low density and holelike for intermediate densities. For larger densities ($n \simeq 1$) the behavior of the transverse conductivity is dominated by the spin-spin correlations. If U is large enough, the Hall number remains positive up to $n = 1$; if U is smaller, however, the transverse conductivity becomes negative for low hole doping. For the system we studied there is a region of densities which depends on the cluster (typically $0.5 < n < 0.75$) where the Hall number is positive for a wide range of values of U. The interplay between antiferromagnetism and the Hall conductivity in the region $n \simeq 1$ cannot be studied in detail in these small clusters; unfortunately the Hilbert spaces for larger clusters are too large for our computing facilities.

Our results can be taken as indirect evidence that in the 2D Hubbard model, in the large-U limit, charge and spin excitations are decoupled, and, although one-particle band-structure calculations may correctly predict the shape of the Fermi surface, they cannot be used to predict the dynamics of charge excitations.

Another interesting point is what is the "Fermi surface" that a de Haas–van Alphen experiment probes. This problem is much more difficult to study in a small cluster, although we are currently working on the problem.

To summarize, we have for the first time calculated exactly the spectral densities and the Hall conductivity in the same strongly interacting system. Our results show that the Fermi surface calculated from the one-particle spectral functions is consistent with Luttinger's theorem and the Hall conductivity for a nearly half-filled system ($n \simeq 1$) indicates holelike carriers if the parameters are such that the antiferromagnetic correlations are weak. This makes evident the failure of the one-particle theories which would predict the wrong sign for the conductivity. This apparent contradiction between the shape of the Fermi surface and the Hall conductivity can be taken as evidence of the deconfinement of charge and spin excitations.

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[1] P. W. Anderson, Science **235**, 1196 (1987).
[2] P. W. Anderson, Phys. Rev. Lett. **64**, 1839 (1990).
[3] A. Kampf and J. R. Schrieffer, Phys. Rev. B **41**, 6399 (1990).
[4] J. C. Campuzano *et al.*, Phys. Rev. Lett. **64**, 2308 (1990).
[5] B. O. Wells *et al.*, Phys. Rev. Lett. **65**, 6636 (1990); C. G. Olson *et al.*, Phys. Rev. B **42**, 381 (1990); T. Takahashi *et al.*, *ibid.* **39**, 6636 (1989).
[6] S. Massida, J. Yu, and A. J. Freeman, Physica (Amsterdam) **152C**, 251 (1988); L. F. Mattheiss, Phys. Rev. Lett. **58**, 1028 (1987); J. Yu, A. J. Freeman, and J. H. Xu, *ibid.* **58**, 1035 (1987).
[7] J. M. Luttinger, Phys. Rev. **121**, 942 (1961).
[8] W. Stephan and P. Horsch, Phys. Rev. Lett. **66**, 2258 (1991).
[9] D. J. Scalapino, in *High Temperature Superconductivity: Proceedings of the Los Alamos Symposium, 1989,* edited by K. S. Bedell, D. Coffey, D. E. Meltzer, D. Pines, and J. R. Schrieffer (Addison-Wesley, New York, 1990).
[10] A. Moreo and E. Dagotto, Phys. Rev. B **42**, 4786 (1990); W. Stephan and P. Horsch, *ibid.* **42**, 8736 (1990).
[11] L. B. Ioffe, V. Kalmeyer, and P. B. Weigmann, Phys. Rev. B **43**, 1219 (1991).
[12] E. R. Gagliano *et al.*, Phys. Rev. B **34**, 1677 (1986); E. R. Gagliano and C. A. Balseiro, Phys. Rev. Lett. **59**, 2999 (1987); R. Haidock, V. Heine, and M. Kelly, J. Phys. C **5**, 2845 (1972).
[13] D. R. Hofstadter, Phys. Rev. B **14**, 2239 (1976), and references therein.
[14] E. Dagotto *et al.*, Phys. Rev. B **41**, 2585 (1990); **41**, 9049 (1990); K. J. von Szczepanski *et al.*, *ibid.* **41**, 2017 (1990).