Electronic Properties of the Insulating Half-Filled Hubbard Model

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Monte Carlo results for the frequency dependent conductivity $\sigma_1(\omega)$, the angular resolved photoemission spectral weight $A(p, \omega)$, and the electron momentum distribution $\langle n_p \rangle$ are calculated for a half-filled Hubbard model with the on-site Coulomb interaction $U$ equal to the bandwidth $8t$. We find that even for $U = 8t$, a spin-density-wave approximation provides a sensible description of this data and hence a useful picture of the electronic degrees of freedom in the insulating state.

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Neutron scattering experiments show that the spin degrees of freedom of the insulating cuprates are well described by an $S = 1/2$ antiferromagnetic Heisenberg model. However, the interpretation of the frequency dependent conductivity and angular resolved photoemission spectroscopy (ARPES) studies of the insulating cuprates require that the charge degrees of freedom also be included. A spin-density-wave (SDW) description provides a weak-coupling approach, in which both the collective antiferromagnetic spin fluctuation and the itinerant electronic charge degrees of freedom can be taken into account. Furthermore, Schrieffer, Wen, and Zhang [1] showed that a random phase approximation (RPA) calculation of the spin-wave spectrum in an SDW state not only give the correct weak-coupling results, but in addition provide a sensible fit to the strong-coupling behavior.

Here we report quantum Monte Carlo (QMC) results for the conductivity, the one-electron spectral weight, and electron momentum occupation of a two-dimensional, half-filled Hubbard model with an on-site Coulomb interaction $U$ equal to the one-electron bandwidth. Thus, we are well out of the weak-coupling regime. For these parameters, local moments are well formed and the ground state is characterized by long-range antiferromagnetic order. The frequency dependent conductivity and the single-particle spectral weight exhibit a well developed insulating gap set by the Coulomb interaction. Nevertheless, we find that the frequency dependent conductivity, the momentum dispersion, and relative spectral weights of the peaks in the single-particle spectral weight and the momentum distribution $\langle n_p \rangle$ of the electrons are in good agreement with the SDW picture.

In the Hubbard model

$$H = -t \sum_{\langle i,j \rangle,s} (c^\dagger_{i,s} c_{j,s} + c^\dagger_{j,s} c_{i,s}) + U \sum_i n_{i\uparrow} n_{i\downarrow},$$

the operator $c^\dagger_{i,s}$ creates an electron of spin $s$ on site $i$ and $n_{i,s}$ is the number operator for spin $s$ and site $i$. For the simple near-neighbor form of the kinetic energy, the band energy $\varepsilon_p$ is

$$\varepsilon_p = -2t[\cos(p_x) + \cos(p_y)].$$

When $U$ is comparable to or larger than the bandwidth $8t$, the spin degrees of freedom are well described by a spin-1/2 antiferromagnetic Heisenberg Hamiltonian with an exchange interaction $J = 4t^2/U$. Here we will consider the half-filled band ($n_{\uparrow} + n_{\downarrow} = 1$) with $U = 8t$. In this case, for temperatures well below $8t$, local moments form with $\sqrt{\langle (n_{\uparrow} - n_{\downarrow})^2 \rangle} = 0.95$. As the temperature decreases below $J$, antiferromagnetic correlations develop and at low temperatures the antiferromagnetic correlation length grows exponentially. For the temperature $T = 0.125t$, at which we have carried out the Monte Carlo simulations discussed below, the antiferromagnetic correlation length is larger than the $12 \times 12$ lattice we have used.

The real part of the frequency dependent $q = 0$ conductivity is given by the Kubo relation

$$\sigma_1(\omega) = \text{Re} \int_{i\omega_m}^{i\omega_m + i\beta} \frac{\Delta_s(i\omega_m)}{i\omega_m - \omega + i\delta}$$

with

$$\Delta_s(i\omega_m) = \int_0^\beta d\tau e^{-i\omega_m \tau} \langle j_s(\tau) j^\dagger_s(0) \rangle.$$  \hspace{1cm} (4)

Here $\omega_m$ is a Matsubara frequency $2\pi m T$, $j_s(\tau) = \exp(H\tau) j_s \exp(-H\tau)$, and

$$j_s = -itea \sum_{i,s} \left( c^\dagger_{i,s} c_{i+sx} - c^\dagger_{i+sx} c_{i,s} \right).$$  \hspace{1cm} (5)

The current-current Green’s function given in Eq. (4) is evaluated with the usual Monte Carlo method [2,3]. Note that at half filling there is no fermion sign problem. The analytic continuation in Eq. (3) is carried out using a maximum entropy procedure [4,5].

The results obtained for $\sigma_1(\omega)$ versus $\omega$ are shown as the solid curve in Fig. 1. A clear gap is seen which is consistent with the vanishing Drude weight discussed in
The Monte Carlo results give $\frac{1}{2} ( -k_x ) = 0.77$ and the area under the solid curve in Fig. 1 showing the Monte Carlo data for $\sigma_1 (\omega)$ gives 0.74. The small difference reflects the difficulty in analytically continuing the numerical data. The spin-density-wave result

$$\frac{1}{2} ( -k_x ) = - \frac{1}{2N} \sum_p \frac{1}{E_p} \left( 1 - \frac{e_p}{E_p} \right)$$

(10)

gives 0.85. This approximation overestimates the size of the kinetic energy, and hence the area under $\sigma_1 (\omega)$. Nevertheless, the simple spin-wave result for $\sigma_1 (\omega)$ is similar to the Monte Carlo data.

In order to learn more about the one-electron properties of this system, we have calculated the single-particle spectral weight

$$A (p, \omega) = - \frac{1}{\pi} \lim \left. G(p, i\omega_n) \right|_{i\omega_n - \omega + i\delta}$$

(11)

by analytically continuing the Monte Carlo data with the maximum entropy technique. Figure 2 shows plots of $A(p, \omega)$ versus $\omega$ for various momentum slices through the Brillouin zone, and Fig. 3 shows the single-particle density of states

$$N(\omega) = \frac{1}{N} \sum_p A(p, \omega).$$

(12)

The insulating gap is clearly evident. However, it is also clear from Fig. 2 that the peak in $A(p, \omega)$ disperses. In Fig. 2(a), the spectral weight exhibits two peaks which disperse symmetrically about $\omega = 0$. The relative spectral weight shifts from negative to positive energies as the momentum moves from below $(\pi/2, \pi/2)$ to above this value. At the $(\pi/2, \pi/2)$ point, the spectral weight is symmetrically distributed. In an ARPES experiment, only the $\omega \approx 0$ spectral weight is observable. Thus at first glance, it might appear that the peak in $A(p, \omega)$ passed through a “Fermi surface” as the momentum is changed from $(\pi/2, \pi/2)$ to $(2\pi/3, 2\pi/3)$. However, one would also see that the zero of energy is displaced from the peak at $(\pi/2, \pi/2)$ by a gap $\Delta$ and in addition a small peak disperses away from the Fermi energy as the momentum is increased beyond $(\pi/2, \pi/2)$. An angular resolved bremsstrahlung isochromat spectroscopy (BIS) experiment would show that as $p$ increases along the diagonal, spectral weight is transferred to an image peak lying symmetrically above the Fermi energy. For a system with only a near-neighbor hopping the spectral weight is evenly divided for $(\pi/2, \pi/2)$ and then shifts heavily to the BIS side as $p$ increases further. Figures 2(b) and 2(c) show the $\omega$ variation of the spectral weight for various values of the momentum $p$ taken along several additional cuts in the Brillouin zone.

In Fig. 4, the solid points show the position of the peaks in $A(p, \omega)$ versus $p$. Here the solid curves correspond to the SDW dispersion relation $E_p = \pm \sqrt{\epsilon_p^2 + \Delta^2}$ for
\[ A(\mathbf{p}, \omega) = \frac{1}{2} \left( \frac{1 - \frac{\varepsilon_\mathbf{p}}{E_p}}{E_p} \right) \delta(\omega + E_p) + \frac{1}{2} \left( 1 + \frac{\varepsilon_\mathbf{p}}{E_p} \right) \delta(\omega - E_p) \] (14)

provides a natural explanation for the spectral weight transfer found in the Monte Carlo data. In particular, the spectral weight for \( \omega \leq 0 \) determines the electron momentum distribution

\[ \langle n_\mathbf{p} \rangle = \int_{-\infty}^{0} d\omega A(\mathbf{p}, \omega). \] (15)

In Fig. 5, Monte Carlo results for \( \langle n_\mathbf{p} \rangle \) are shown as the solid points and the curve corresponds to the SDW result \( \frac{1}{2} (1 - \frac{\varepsilon_\mathbf{p}}{E_p}) \).

Thus it appears that even in the case where \( U \) is equal to the bandwidth \( 8t \), the spin-density-wave picture provides a useful framework for understanding the electronic

\[ E_\mathbf{p} = \sqrt{\varepsilon_\mathbf{p}^2 + \Delta^2} = \Delta + J(\cos p_x + \cos p_y) \] (13)

with \( J = 4t^2/U \). Thus in this limit, the dispersion only depends upon \( J \). Also in this limit, the kinetic energy of the half-filled band \( \langle k_x \rangle \) varies as \( t^2/U \) [2] so that the \( f \)-sum rule is also set by \( J \).
properties of the half-filled insulating state of the Hubbard model. In particular, it provides a reasonable description of $\sigma_1(\omega)$ and the insulating nature of the system. Furthermore, it gives a single-particle spectral weight which disperses in the same way as the Monte Carlo data and in addition exhibits the same shift in the relative spectral weights of the peaks [8].

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[7] The broadening of $0.5\tau$ used in plotting the SDW results provides a rough estimate of the temperature and frequency dependent quasiparticle lifetime which varies from $T = 0.125\tau$ to of order $\tau$ as $\omega$ increases. The resolution of the analytic continuation also varies with frequency and ranges from $-(0.25-0.5)\tau$ at low $\omega$ to $(1-2)\tau$ at higher frequencies.
[8] In order to compare theory with experiment we have also carried out Monte Carlo calculations for a Hubbard model with a next-nearest-neighbor hopping $t'$. Within the SDW framework this simply alters $\epsilon_p$ by adding a term $-4t'\cos p_x\cos p_y$. Calculations of the quasiparticle lifetimes due to fluctuations of the sublattice magnetization are also being carried out. The results will be presented in a longer paper.