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Gaps in Densities of States of Two Hubbard-Like Models

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Results are presented for the single-particle density of states of the one- and two-dimensional simplified Hubbard and Montorsi-Rasetti model. The former does not exhibit a metal-insulator transition as a function of U . With increasing temperature and for U not too large, the gap closes and spectral weight appears at the chemical potential. The Néel temperature and the temperature range for coexistence of magnetic long-range order and a gapless density of states are determined. The latter model exhibits a metal-insulator transition of the Mott type and does not show magnetic long-range order.

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The Hubbard model has been used extensively to describe properties of strongly correlated fermion systems [1,2]. An important issue is the occurrence of a metal-insulator (MI) transition as the Coulomb interaction U is varied. According to the Mott picture [3], for large coupling values and at half filling, the density of states (DOS) exhibits two bands of which the centers are separated by U . In the absence of electron correlation the width of each Hubbard band equals the free-particle bandwidth $W=2zt$, where z is the lattice coordination number and t is the hopping amplitude. The gap Δ between the bands is then expected to vanish at $U/W=1$, signaling a MI transition at zero temperature [3]. For the one-dimensional (1D) Hubbard model the exact solution yields a nonzero gap at half filling: The ground state is an insulator for all $U>0$ [4]. The repulsive half-filled two-dimensional (2D) Hubbard model at zero temperature is believed to be an insulator with antiferromagnetic long-range order (LRO) [1]. In both these cases the Mott picture for the behavior of the gap Δ does not seem to apply.

It is also of interest to consider the behavior of the gap as one goes away from half filling at zero temperature or upon changing the temperature at half filling. In both instances the question is whether spectral weight appears at the chemical potential [1]. For the 2D Hubbard model this question has recently been addressed [5,6].

In this Letter we present results for the half-filled simplified Hubbard (SH) [7] and Montorsi-Rasetti (MR) [8,9] model as obtained from exact diagonalization and quantum Monte Carlo simulations. For both models, the first term in the Hamiltonians $H_a \equiv H_0 + K_a$ ($a=SH, MR$) is diagonal in the occupation number rep-

resentation and is given by

$$H_0 = U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma}, \quad (1)$$

where $n_{i\sigma}$ is the number operator for an electron at lattice site i with spin $\sigma = \uparrow, \downarrow$, U is the on site Coulomb interaction constant and μ is the chemical potential. At half filling the electron density $\rho \equiv \sum_{i,\sigma} \langle n_{i\sigma} \rangle / N = 1$ (N denotes the number of lattice sites) and $\mu = U/2$.

The off-diagonal part of the Hamiltonian for the SH model reads

$$K_{SH} = -t \sum_{\langle i,j \rangle} (c_{i\uparrow}^\dagger c_{j\uparrow} + c_{j\uparrow}^\dagger c_{i\uparrow}), \quad (2)$$

where $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ are the creation and annihilation operators, respectively, for an electron with spin σ at lattice site i . The sum is over nearest-neighbor pairs. Hamiltonian H_{SH} is obtained from the Hubbard model by immobilizing the $\sigma = \downarrow$ electrons [7]. It can also be regarded as a model for crystallization [10], as the "symmetric" spinless Falicov-Kimball model [11,12] or as a model for an alloy in which the "impurities" ($\sigma = \downarrow$ electrons) are thermodynamically correlated by annealed averaging [10,11].

For bipartite lattices, it was rigorously shown [10,11] that the ground state of the half-filled SH model exhibits magnetic LRO in all dimensions. The immobile $\sigma = \downarrow$ electrons fully occupy one sublattice. For $U \neq 0$ the ground state is insulating [10,11]. For $d \geq 2$ the LRO vanishes above some (unknown) finite temperature [10,11]. In the limit of infinite dimensionality ($d \rightarrow \infty$) the SH model can be solved exactly [12,13].

The off-diagonal contribution to the MR Hamiltonian is given by [8]

$$K_{MR} = -\frac{1}{2} \sum_{\langle i,j \rangle} \sum_{\sigma,\sigma'} t^{(\sigma,\sigma')} (c_{i\sigma}^\dagger c_{j\sigma'} + c_{j\sigma'}^\dagger c_{i\sigma}) + \frac{1}{2} \sum_{\langle i,j \rangle} \sum_{\sigma,\sigma'} \tilde{t}^{(\sigma,\sigma')} (c_{i\sigma}^\dagger c_{j\sigma'} + c_{j\sigma'}^\dagger c_{i\sigma}) (n_{i-\sigma} + n_{j-\sigma'} - \gamma n_{i-\sigma} n_{j-\sigma'}), \quad (3)$$

and includes spin-flip hopping terms which may be ascribed to spin-orbit coupling [14]. In addition, different hopping processes can be assigned different amplitudes using the parameters $\{t^{(\sigma,\sigma')}, \tilde{t}^{(\sigma,\sigma')}, \gamma\}$. These differences may arise because of bond-charge effects [8]. For several sets of model parameters, the transformation $A_i \equiv (c_{i\uparrow} + c_{i\downarrow})/\sqrt{2}$, $B_i \equiv (c_{i\uparrow} - c_{i\downarrow})/\sqrt{2}$ brings K_{MR} into a form where the off-diagonal part for the spinless B fermions drops out and only the A fermions can hop [8,9,15]. For the particular choice $t^{(\sigma,\sigma')} = \tilde{t}^{(\sigma,\sigma')} \equiv t$, which we also adopt, H_0 and K_{MR} commute, so that the total numbers of empty and doubly occupied sites are conserved [8]. For $t^{(\sigma,\sigma')} \equiv t$ and $\tilde{t}^{(\sigma,\sigma')} = 0$ the

FIG. 1. Density of states $N(\omega)$ for the half-filled SH model for $U=1$, $t=1$, and several temperatures. (a) $T=0.01$. (b) $T=0.05$. (c) $T=0.1$. (d) $T=0.05$. Parts (a)–(c) are for 8×8 lattices. Part (d) is the exact result for a 4×4 lattice.

MR Hamiltonian reduces to the SH Hamiltonian with $n_{i\downarrow}$ and $c_{i\downarrow}^\dagger$ replaced by $B_i^\dagger B_i$ and $A_i^\dagger$, respectively.

An important feature of the SH and MR model is that they allow for an accurate and efficient calculation of static and dynamical quantities [9,15]. No minus sign or instability problems characteristic of quantum Monte Carlo simulations of fermion models are encountered [2]. Real-time correlation functions such as $\langle \{A_i(t), A_i^\dagger\} \rangle$ can be evaluated directly without using any approximation [9,15]. From the knowledge of these quantities the spectral functions and DOS readily follow [9,15]. The results

presented below for lattices up to sixteen sites are exact. For larger lattice sizes we made use of a Monte Carlo (MC) method [2].

In Figs. 1 and 2 the DOS for the half-filled SH model on square lattices are shown for $U=1$ and $U=15$ at various temperatures T . In all DOS figures energies are measured in units of t , relative to the chemical potential. The DOS gives the probability for removing or adding $\sigma=\uparrow$ electrons from or to the system. At half filling the densities of the spin-up and spin-down electrons are equal and independent of the temperature and U . Our results

FIG. 2. Density of states $N(\omega)$ for the half-filled SH model on 8×8 lattices for $U=15$, $t=1$, and several temperatures. (a) $T=0.01$. (b) $T=0.1$.

FIG. 3. The 2D SH model. Estimated temperatures T_0 (dotted line) at which gaps in the DOS close as a function of coupling strength U , $t=1$. Critical temperature T_c for antiferromagnetism as a function of U . ■: numerical results. Drawn line is a guide to the eye. For $T_0 < T < T_c$ a gapless DOS coexists with magnetic LRO.

for the gap Δ in the DOS show no size dependence for lattices containing up to 64 sites. At very low temperatures and $U \neq 0$, the gap $\Delta = U$, in agreement with the rigorous result [11]. For small and intermediate U , the bandwidth of both bands decreases with increasing U . For $U > 8$ the bandwidth approaches a nonzero value as $U \rightarrow \infty$. For $U > 8$ and increasing T the bandwidths increase somewhat, but a finite gap remains for all temperatures. For $0 < U < 8$ the gap closes as the temperature is raised. At the chemical potential ($\omega=0$) no peak is observed as the gap disappears. For larger temperatures substantial spectral weight is found at $\omega=0$ for $0 < U < 4$ and the model exhibits metallic behavior. The temperature T_0 at which the gap closes for $4 < U < 8$ increases very strongly (e.g., $U=5$, $T_0 \approx 0.15$ and $U=7.5$, $T \approx 10$). For fixed large temperatures the weight at the chemical potential decreases with increasing U . For $4 < U < 8$ one only finds a pseudogap for large enough temperatures: $N(\omega=0)$ remains small. The size dependence of the spectral weight $N(\omega=0)$ was very small for

all U using lattices with up to 64 sites. Estimates for the temperatures T_0 at which gaps in the DOS close are shown in Fig. 3. Similar results were found for the 1D SH model.

The DOS for the MR model on a 8×8 lattice is presented in Fig. 4 for $U=4$ and $U=15$ and $T=0.01$. At very low temperatures a MI transition as a function of U was found [9]. The development of the gap for varying coupling strength exactly fits the Mott picture, i.e., $\Delta = U - W^3$. As mentioned above, the MR model with spin-flipping terms and $\tilde{t}^{(\sigma,\sigma')} = 0$ is equivalent to the SH model, so that the bond-charge hopping processes, see (3), are essential for the occurrence of a MI transition. For the MR model studied here the widths of the Hubbard bands are independent of U , because $[H_0, K_{MR}] = 0$ [15]. This may be the reason that the critical coupling equals the free-particle bandwidth. For $U < W$ the DOS is the sum of two bands with width W . For $U \geq W$ the DOS does not change with temperature. Hence, for $U=W$ the two Hubbard bands just touch each other but $N(\omega=0)=0$ for all temperatures. The salient features of the gap Δ in the DOS as a function of U for both the SH and MR model do not significantly depend on dimensionality or size of the lattice.

The critical (Néel) temperature for antiferromagnetism in the 2D SH model as a function of U is shown in Fig. 3. At very low temperatures the $\sigma=\downarrow$ electrons fully occupy one sublattice and we find LRO for $T < T_c$, in concert with rigorous results [10,11]. For $T < T_c$ the static magnetic-structure factor, $S(\mathbf{q}) = \sum_{i,j} \exp[i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)] \langle (n_{i\uparrow} - n_{i\downarrow})(n_{j\uparrow} - n_{j\downarrow}) \rangle / N$, scales linearly with the lattice size N for $\mathbf{q} = (\pi, \pi)$. The mean-squared staggered magnetization, $\langle M_S^2 \rangle \equiv S(\pi, \pi) / N$ ($\langle M_S \rangle = 0$), decreases with decreasing U . At low temperatures this is due to the increasing quantum fluctuations of the $\sigma=\uparrow$ electrons. At the critical temperature T_c where the LRO vanishes, the specific heat C/N exhibits a sharp maximum. The value of C/N at T_c increases slowly (less than linearly) with the number of lattice sites. For all purposes the estimates for the critical temperature T_c as obtained from

FIG. 4. Density of states $N(\omega)$ for the MR model on half-filled 8×8 lattices with $t=1$ and $\gamma=2$ for several coupling strengths and temperature $T=0.01$. (a) $U=4$. (b) $U=15$.

4×4 , 6×6 , and 8×8 lattices are the same. We find that the value of T_c is not of the order of t or U . A similar conclusion was reached by Brandt and Mielsch for the $d=\infty$ SH model [12]. The "phase diagram" of the 2D SH model, shown in Fig. 3, is qualitatively the same as the one of the Hubbard model obtained from a random one-body approximation [16]. Figure 3 clearly demonstrates the coexistence of magnetic LRO and metallic behavior. In the SH model the closing of the gap at T_0 in the DOS is not related to the disappearance of antiferromagnetism. The metallic behavior reflects the motion of the $\sigma=\uparrow$ electrons, while the magnetic properties are mainly displayed by the $\sigma=\downarrow$ electrons. For the 1D SH model we conclude that there is LRO only for $T=0$ and $U\neq 0$. On the other hand, the 1D and 2D MR model do not exhibit magnetic LRO.

We have also computed the Drude coefficient D for both models [17]. For the MR model $D=0$ if the DOS exhibits a gap and the chemical potential is located in the gap and $D\neq 0$ otherwise [15]. For the SH model we find that $D\rightarrow 0$ as $U\rightarrow \infty$, but for the small lattices used ($N\leq 16$) we find $D\neq 0$ for small U , in conflict with the observation that at low temperatures the chemical potential lies in the gap. For small U one expects large finite-size effects [17].

In summary, we have calculated the DOS and magnetic properties of the half-filled SH and MR model. In contrast to the MR model the SH model displays magnetic LRO and does not exhibit a MI transition as a function of U . The MI transition of the MR model is in complete accordance with the Mott picture [3]. For $U < 4d$ and increasing temperature the gap in the DOS of the SH model closes and spectral weight appears at the chemical potential. The vanishing of the gap is not related to the disappearance of magnetic LRO.

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