The Mott Metal-Insulator transition in the half-filled Hubbard model on the Triangular Lattice.

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We investigate the metal-insulator transition in the half-filled Hubbard model on a two-dimensional triangular lattice using both the Kotliar-Ruckenstein slave-boson technique, and exact numerical diagonalization of finite clusters. Contrary to the case of the square lattice, where the perfect nesting of the Fermi surface leads to a metal-insulator transition at arbitrarily small values of $U$, always accompanied by antiferromagnetic ordering, on the triangular lattice, due to the lack of perfect nesting, the transition takes place at a finite value of $U$, and frustration induces a non-trivial competition among different magnetic phases. Indeed, within the mean-field approximation in the slave-boson approach, as the interaction grows the paramagnetic metal turns into a metallic phase with incommensurate spiral ordering. Increasing further the interaction, a linear spin-density-wave is stabilized, and finally for strong coupling the latter phase undergoes a first-order transition towards an antiferromagnetic insulator. No trace of the intermediate phases is instead seen in the exact diagonalization results, indicating a transition between a paramagnetic metal and an antiferromagnetic insulator.

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The Mott metal-insulator transition (MIT), i.e. the transition from a metallic to an insulating phase driven by the electronic correlation, is one of the most relevant issues in condensed matter theory. In the last few years it has been also the object of an intensive study, due to many experimental evidences of Mott insulators ranging from the parent compounds of the superconducting cuprates to the alkali fullerenes of the type $A_4C_{60}$. The simplest model in which the competition between the delocalizing effect of the kinetic energy and the electronic correlation can give rise to a MIT is the Hubbard model

$$\mathcal{H} = - t \sum_{\langle i,j \rangle} (c_{i,\sigma}^\dagger c_{j,\sigma} + h.c.) - \mu \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow},$$

where $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) creates (destroys) an electron with spin $\sigma$ on the site $i$ and $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$ is the number operator; $t$ is the hopping amplitude, $U$ is the Hubbard on-site repulsion, $\mu$ is the chemical potential. The hopping is restricted to nearest-neighbors and the indices $i,j$ label the points $r_i$ and $r_j$ of a $d$-dimensional lattice.

At half-filling (i.e. for a number of electrons equal to the number of sites), this model is known to undergo a MIT by increasing the interaction strength $U$. On the $d$-dimensional cubic lattice the perfect nesting property of the Fermi surface makes the model unstable towards antiferromagnetism as soon as a non-zero $U$ is turned on, driving the system to the insulating state. In this paper we focus on the triangular lattice as a prototype for a model where the perfect nesting is absent for the uncorrelated metal. Since in the $U/t \rightarrow \infty$ (Heisenberg) limit the model is likely to display a Néel ordered (insulating) ground state (GS), the MIT is expected to occur for finite $U$.

Besides its theoretical relevance, our analysis has also an experimental counterpart. In fact, the adlayer structures on semiconductor surfaces, such as SiC(0001) or K/Si(111) : B, have recently turned out to be an almost ideal environment for the study of Mott insulators and are characterized by a $\sqrt{3} \times \sqrt{3}$ arrangement of the dangling-bond surface orbitals, which are likely to be well described by bidimensional strongly correlated Hamiltonians on the triangular lattice.

Hartree-Fock (HF) calculations, performed by Krishnamurthy and co-workers, produce a rather rich phase diagram: for small $U$ the system is a paramagnetic metal (PM), which turns to a metal with incommensurate spiral spin-density-wave (Spiral Metal, SM) at $U = U_{c1} = 3.97t$. Two successive first order transitions occur further increasing the coupling: at $U = U_{c2} = 4.45t$ a semi-metallic linear spin-density wave (LSDW) is stabilized, and a first order MIT to an antiferromagnetic insulator (AFMI) occurs at $U = U_{c3} = 5.27t$. In the same work it has also been argued that at finite temperature the model should present a Mott transition between a paramagnetic metal and a paramagnetic insulator.
However, the above transitions only occur at relatively large $U/t$ and the HF approximation is unreliable in the intermediate- and strong-coupling regime. Therefore we adopt the more appropriate slave-boson (SB) approach \[13,14\] as an interpolating scheme between the $U/t = 0$ and the $U/t \to \infty$ regimes. To allow for the presence of incommensurate spiral spin ordering, we introduce the spin-rotational invariant formulation \[15\] of the Kotliar-Ruckenstein SB approach \[14\]. The reader can find further details in Ref. \[15\].

We introduce on each site a set of four SB operators $e_i, s_i, \tau_i, s_i \downarrow$ and $d_i$ to label empty ($e$), singly ($s$), and doubly ($d$) occupied sites, respectively. The spin projection $\zeta = \uparrow, \downarrow$ is measured with respect to a local quantization axis, which is allowed to vary from site to site. The resulting SB Hamiltonian is

$$
\mathcal{H} = -t \sum_{\langle i,j \rangle} \left[ c_{i,\zeta}^\dagger c_{j,\zeta} + (R_{\zeta,j}^\dagger R_{\zeta,j}) c_{i,\zeta} z_{j,\zeta} c_{j,\zeta}^\dagger + H.c. \right] - \mu \sum_{i,\zeta} \left[ c_{i,\zeta}^\dagger c_{i,\zeta} + U \sum_{i} d_{i}^\dagger d_{i} \right] + \sum_{i} \lambda_i \left( e_{i}^\dagger e_{i} + d_{i}^\dagger d_{i} + \frac{1}{2} \sum_{\zeta} s_{i,\zeta}^\dagger s_{i,\zeta} - 1 \right) + \sum_{i,\zeta} \Lambda_{i,\zeta} \left( c_{i,\zeta}^\dagger c_{i,\zeta}^\dagger - s_{i,\zeta}^\dagger s_{i,\zeta} - d_{i}^\dagger d_{i} \right)
$$

(2)

where $c_{i,\zeta}^\dagger$, $c_{i,\zeta}$ are the pseudofermion operators, the Lagrange multipliers $\lambda_{i,\zeta}$ and $\Lambda_{i,\zeta}$ enforce on each site the completeness constraint and the correct fermion counting respectively, the operator $R_{\zeta,i}$ rotates the local reference frame back to the laboratory frame, and the operator

$$
z_{i,\zeta} = \frac{e_{i}^\dagger s_{i,\zeta} + s_{i,\zeta}^\dagger d_{i}}{\sqrt{1 - d_{i}^\dagger d_{i} - s_{i,\zeta}^\dagger s_{i,\zeta}^\dagger}} \sqrt{1 - e_{i}^\dagger e_{i} - s_{i,\zeta}^\dagger s_{i,\zeta}^\dagger}$$

reconstructs the hopping amplitude in the enlarged Fock space, and yields the correct $U \to 0$ limiting behavior in the mean-field approximation \[14,15\]. When the angle between two local quantization axes depends only on their relative position, up to a global phase factor one can assume $R_{\uparrow,i}^\dagger R_{\downarrow,j} = \exp[i \mathbf{Q} \cdot (\mathbf{R}_{i} - \mathbf{R}_{j}) \tau_{y}/2]$, where $\tau_{y}$ is the Pauli matrix and $\mathbf{Q}$ is the (incommensurate) modulating wavevector \[13\]. In such a case a mean-field description with real site-independent expectation values for the SB operators

$$
\langle e_{i}^{\dagger} \rangle = e_{0}; \quad \langle s_{i,\uparrow}^{\dagger} \rangle = s_{0,\uparrow}; \quad \langle d_{i}^{\dagger} \rangle = d_{0},
$$

(3)

and for the Lagrange multipliers

$$
\langle \lambda_{i} \rangle = \lambda_{0}; \quad \langle \Lambda_{i,\zeta} \rangle = \Lambda_{0,\zeta},
$$

(4)

is possible. Eqs. (3) and (4) refer to the case in which the translational symmetry is not broken and the expectation values of the bosons and of the Lagrange multipliers do not depend on the site. We have also studied configurations with broken translational symmetry. In particular we considered solutions in which in the bosons have different values on each of the three sublattices, and analogous to LSDW found in Hartree-Fock \[12\]. The latter solutions can be found considering a four-sites unit cell. A similar SB calculation has been performed in Ref. \[16\], where, however, the generalization of the SM phase found in HF was never recovered as an energy minimum. In the case of spiral spin ordering, the Hamiltonian \[2\] can be analytically diagonalized by adopting the Bloch representation, and performing a unitary transformation with respect to spin indices, yielding

$$
E_{k,\pm} = \frac{1}{2} \left[ t(z_{0,\uparrow}^2 + z_{0,\downarrow}^2) T_{e} + \Lambda_{0,\uparrow} + \Lambda_{0,\downarrow} \right] + \mu \left[ - \frac{1}{2} \sqrt{\left( t(z_{0,\uparrow}^2 - z_{0,\downarrow}^2) T_{e} + \Lambda_{0,\uparrow} - \Lambda_{0,\downarrow} \right)^2 + 4 t^2 z_{0,\uparrow}^2 z_{0,\downarrow}^2} - T_{e}^2 \right]
$$

where $T_{e} = - \sum_{k} \cos(\mathbf{Q} \cdot \mathbf{1}/2) \cos(\mathbf{k} \cdot \mathbf{1})$, $T_{e} = - \sum_{k} \sin(\mathbf{Q} \cdot \mathbf{1}/2) \sin(\mathbf{k} \cdot \mathbf{1})$, and $1 = (1,0),(1/2, \pm 3/2)$ are the nearest-neighbor displacements. The self-consistency equations are obtained by minimizing the free energy

$$
\mathcal{F} = \mathcal{F}_{0} - T \sum_{\mathbf{k},\alpha=\pm} \log \left( 1 + e^{-E_{k,\alpha}/T} \right),
$$

where $\mathcal{F}_{0} = N[U d_{0}^2 + \lambda_{0}(e_{0}^2 + d_{0}^2 + s_{0,\uparrow}^2 + s_{0,\downarrow}^2) - 1) - \Lambda_{0,\uparrow}(d_{0}^2 + s_{0,\uparrow}^2) + \Lambda_{0,\downarrow}(d_{0}^2 + s_{0,\downarrow}^2) + \mu n]$, $N$ is the number of sites, and $n$ is the electron density per site, and read

$$
\frac{\partial \mathcal{F}}{\partial \mathbf{X}} + \sum_{\mathbf{k},\alpha=\pm} \frac{\partial E_{k,\alpha}}{\partial \mathbf{X}} f(E_{k,\alpha}) = 0,
$$

(5)

where $f(E) = [e^{E/T} + 1]^{-1}$ is the Fermi function and $\mathbf{X}$ represents generically one of the parameters \[3\], \[4\] and the two components of the pitch vector $\mathbf{Q}$. The chemical potential $\mu$ is fixed by the condition

$$
\sum_{\mathbf{k},\alpha=\pm} f(E_{k,\alpha}) = nN.
$$

In this paper we assume henceforth $n = 1$ (half-filling).

The self-consistency equations \[3\] yield the same solutions found in HF, namely a paramagnetic metal, a metal with incommensurate spiral ordering, a linear spin-density-wave and an antiferromagnetic insulator. As in HF, the PM-SM transition is continuous, and the other two transitions are of first order, but all of them occur at larger coupling values, $U_{c1} = 6.68t$, $U_{c2} = 6.84t$, and $U_{c3} = 7.68t$. The energy curves corresponding to the above phases are reported in Fig. \[1\]. Our results agree with Ref. \[16\] as far as the PM, AFM, and LSDW phases are concerned, but we also find a region of stability for the SM phase, which was not detected in Ref. \[16\]. These authors were indeed looking for spiral phases starting from the strong-coupling side, and following them to weaker coupling. On the other hand, our analysis shows that a
spiral phase develops continuously from the PM at intermediate coupling and it ends in a critical point soon after the level-crossing with the AFMI (see the inset in Fig. 1), and does not exist at strong-coupling. Therefore, our SM phase is the generalization of the corresponding phase found within HF [12], and it is unrelated to the high-energy SM phases of Ref. [10]. However, the region of existence of the SM is narrower within SB as compared to HF, and the magnetization $m = \frac{1}{2}(n_\uparrow - n_\downarrow)$ is always less than 0.1, a really small value with respect to the HF value ($\leq 0.4$). Therefore the jump of the magnetization at the SM-AFMI transition is substantially larger than in the HF approximation. We point out that, contrary to nesting models, where the presence of free particles (doping) is a necessary condition for spiral ordering [15,17,18], here the spiral phase exists at half-filling, as previously shown in Ref. [11], within the HF approximation. Despite the overall qualitative agreement between the HF and the SB phase diagrams, the main outcome of the comparison between them is that the stability of the SM phase is strongly reduced. Furthermore, the SM is hardly distinguishable from the PM in its whole region of stability. It is reasonable to expect that the inclusion of quantum fluctuations washes out these phases leaving the way open for a transition between a PM and the AFMI.

Despite the strong frustration of the antiferromagnetic (AFM) order on the triangular lattice [16], both the HF and SB approaches indicate no paramagnetic Mott insulating phase in the zero-temperature phase diagram of the half-filled Hubbard model.

In particular, within the SB approach, we can indicate how far the system is from the Brinkman-Rice transition [3] to a paramagnetic Mott insulator. In fact, if the possibility for magnetic ordering is neglected, the paramagnetic metallic phase undergoes a Brinkman-Rice transition with vanishing double occupancy and effective hopping amplitude, for a critical value (at $T = 0$) of the Hubbard interaction $U_{BR} = 32t N^{-1} \sum_\mathbf{k} \varepsilon_\mathbf{k} \Theta(2|\varepsilon_\mathbf{k}| + \mu)$ ($\varepsilon_\mathbf{k} = -T_c(Q = 0)$) [3,4], i.e. $U_{BR}/t \simeq 15.8$ on the triangular lattice. As we see this value is much larger than $U_{c1}/t$, $U_{c2}/t$ and $U_{c3}/t$ found above. The system is therefore not even close to the Brinkman-Rice transition when the MIT occurs.

In order to understand to which extent the picture we found within the mean-field SB theory survives in an exact treatment of the model, we performed exact diagonalization of small clusters by means of the standard Lanczos algorithm. The largest lattice compatible with all the symmetries of the model that can be handled with exact diagonalization is a $N = 12$ site cluster [6]. We always used twisted boundary conditions with a suitable phase such that the half-filled system is in a closed-shell configuration. This is important in order to perform a reasonable investigation of the conduction properties of the finite-size system. It turns out that the boundary conditions that minimize the energy in a closed-shell configuration for $U = 0$ leave the system in a closed-shell configuration at all $U$. The energy is shown as a function of $U$ in Fig. 1. The overall agreement with the mean-field SB results is good, the largest deviations ($\sim 20\%$) being, as expected, at intermediate coupling ($U/t \sim 7$).

To check the occurrence of a discontinuous phase transition we evaluated the overlap between the GS wave function and the two limiting cases of $U = 0$, and for large $U$ (namely, $U = 100t$). As shown in Fig. 2 on the large-$U$ side of the diagram the GS has a large overlap to the AFM strong-coupling state and a vanishing overlap with the non-interacting metallic one. On the metallic side the overlap with the non-interacting state is always finite, but it is a decreasing function of $U$; in this regime the GS has anyway a vanishing overlap to the AFM state. We have therefore a clear evidence for a strongly correlated metal with a decreasing coherent part. In particular the sharp
change of the GS wave function at \( U_{\text{MIT}} \approx 12.07t \) is due to a level-crossing occurring between a metallic and an antiferromagnetic solutions, as it is shown in the inset of Fig. 2. These results, however, do not rule out the possibility of a continuous transition within the metallic phase, i.e. the PM-SM transition found with SB.

In Fig. 3 we show the spin structure factor, \( S(q) = \sum_{i,j} S_i^z S_j^z \exp[i \cdot (r_i - r_j)]/N \), for different values of \( U \). The results do not suggest any intermediate state between a metallic state without magnetic order and the AFM insulator, as \( S(q) \) abruptly changes from a structureless behavior to an AFM pattern peaked at the classical ordering wavevector, i.e. \( Q_0 = (4\pi/3, 0) \). Although we suspect that the intermediate phases are an artifact of the mean-field approach, the weakness and the strong size-dependence of the spiral phases suggested by the SB results, may make them unaccessible on our 12-site lattice.

All the results of exact diagonalization point towards the same direction: the metal-AFMI level-crossing found within the SB mean-field approach is shifted to larger values of \( U \). The metallic solution exhibits a continuous loss of metallicity with increasing \( U \). The Drude weight is finite up to the MIT on the 12-site lattice although it is quite small (4% of the non-interacting value). We remark that, due to finite-size effects, we cannot exclude the possibility that \( D_{xx} \) vanishes before the transition to the AFMI is reached. In such a case, there would be a region of parameters in which the paramagnetic insulator exist, though the SB results point in the opposite direction.

In conclusion, using the slave boson technique and the exact diagonalization, we have investigated the zero-temperature phase diagram of the half-filled Hubbard model on a two dimensional triangular lattice. The mean-field SB approach displays a rich phase diagram which qualitatively resembles the one from HF calculations, but, on the other hand, drastically reduces the stability of the spiral metal and of the linear spin-density-wave states. Namely, the weak-coupling paramagnetic metal continuously evolves into a spiral metal at \( U = U_{c1} = 6.68t \), which crosses the linearly polarized spin-density-wave ground-state at \( U = U_{c2} = 6.84t \). The latter phase undergoes a further first-order transition towards an antiferromagnetic insulator at \( U = U_{c3} = 7.68t \). All these transitions occur for coupling constants substantially smaller than the critical value for the real part of the \( xx \) component of the conductivity tensor for a tight-binding model at zero temperature may be expressed in terms of the Kubo formula 

\[
\sigma_{xx}(\omega) = D_{xx} \delta(\omega) + \Im\langle 0|J_x^I \frac{1}{\omega - H + E_0 - i\delta} J_x |0\rangle, \tag{6}
\]

where \( J_x = \sum_{l,\sigma} l_x (c_{l,\sigma}^\dagger c_{l+1,\sigma} - h.c.) \) is the \( x \)-component of the current operator. The coefficient of the zero-frequency delta function contribution \( D_{xx} \), the Drude weight, is given by the f-sumrule (13)

\[
D_{xx} = \frac{\pi e^2}{2} \langle \mathcal{H}_x^I \rangle - \sum_{n \neq 0} \frac{|\langle \phi_n | J_x | \phi_n \rangle|^2}{E_n - E_0}, \tag{7}
\]

where \( \mathcal{H}_x^I = \sum_{l,\sigma} l_x^2 (c_{l,\sigma}^\dagger c_{l+1,\sigma} + h.c.) \), and \( |\phi_n\rangle \) is the eigenfunction of \( \mathcal{H} \) with eigenvalue \( E_n \).

The latter quantity, which is reported in Fig. 4 is a direct measure of the metallic character of the state, and the MIT is signaled by the vanishing of \( D_{xx} \) (20). For a finite system, \( D_{xx} \) does not vanish for any value of \( U \), but an abrupt change takes place at the level-crossing point. For \( U < U_{\text{MIT}} \), \( D_{xx} \) is a decreasing function of the interaction, which resembles the overlap in Fig. 3. An abrupt change takes place at the level-crossing point and for \( U > U_{\text{MIT}} \) it becomes negative, a common phenomenon in the insulating phase of a small-size system (21).

Using the Lanczos algorithm we have also calculated the finite-frequency optical conductivity \( \sigma(\omega) \) and the Drude weight, measuring the electronic mobility. The
Brinkman-Rice transition to a paramagnetic insulator ($U_{BR} = 15.8t$). The exact-diagonalization results present a first order transition between the paramagnetic metal and the antiferromagnetic insulator at $U_{MIT} = 12.07t$, without intermediate “exotic” phases.

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