Mott-Hubbard Metal-Insulator Transition in Nonbipartite Lattices

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We reinterpret the Hubbard model in terms of doubly occupied sites and empty sites with an attractive interaction U whose pairing leads to the Mott-Hubbard transition. We develop a mean-field theory for this pairing which in a triangular lattice at $T=0$ leads to a first-order transition from a spiral, incommensurate metal to a commensurate insulator at $U \simeq 5.27t$ where a charge gap ($\simeq 0.085t$) opens up. We also discuss the effect of fluctuations.

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In this Letter we present some new results for the physics of the Hubbard model[1] and the Mott-Hubbard metal-insulator transition,[2,3] especially on nonbipartite lattices. Our discussion uses a reinterpretation of the model in terms of doubly occupied sites (doublons) and empty sites (holons), which carry opposite charges (with respect to a neutralizing background).[4] Then the Mott-Hubbard transition can be viewed as arising from the formation of bound, charge-neutral, pairs of doublons and holons. Their binding energy is the gap for charge excitations, i.e., the insulating gap. Our reinterpretation leads us to reexamine the Hartree-Fock (H-F) mean-field theory of the Hubbard model[5] but with the inclusion of spiral SDW (spin-density-wave) states. We find that it provides a useful, lattice-specific, zeroth-order description of the Hubbard model for any U and filling.

Using this theory, we derive some novel conclusions about the Hubbard model on the triangular lattice with nearest-neighbor hopping t (and generally in models with no nesting of the noninteracting Fermi surface). Specifically we find that in the *half-filled* triangular lattice at $T=0$, for small U the system is paramagnetic metal; at a critical $U=U_{c1}$ ($\simeq 3.97t$), it becomes a metal with an incommensurate spiral SDW, whose wave vector changes continuously as U is increased beyond U_{c1}, until at $U=U_{c2} \simeq 5.27t$ a *first-order metal-insulator transition* occurs. A finite charge gap at approximately $0.085t$ suddenly develops and the system goes into a commensurate, three-sublattice, 120° twist SDW state (which is just the ground state for the classical triangular antiferromagnet), which is insulating and stable for all $U > U_{c2}$. We argue that by considering the leading fluctuation corrections about the mean-field approximation, one obtains the essential qualitative physics of the Mott-Hubbard transition at finite temperatures, including the distinction[3] between Mott (paramagnetic) insulator and the antiferromagnetic insulator.

The Hubbard model Hamiltonian on a general lattice is[1]

$$H = -\sum_{\substack{ij\\ \sigma}} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} . \qquad (1)$$

A reinterpretation of this model in terms of doublons and holons is achieved by making a particle-hole transformation on the up-spin species, and relabeling the operators as $c_{i\uparrow} \to h_i^{\dagger}$ and $c_{i\downarrow}^{\dagger} \to d_i^{\dagger}$. The reference "vacuum" state $|\Omega\rangle$ has an up-spin particle at every site i; $h_i^{\dagger}|\Omega\rangle$ creates a holon and $d_i^{\dagger}|\Omega\rangle$ a doublon at i. The down-spin particle is obtained as $(d_i^{\dagger} h_i^{\dagger})|\Omega\rangle = S_i^{-}|\Omega\rangle$, where S_i^{-} is the spin-lowering operator. In terms of these operators, H can be rewritten as

$$H = \sum_{ij} t_{ij} h_i^{\dagger} h_i - \sum_{ij} t_{ij} d_i^{\dagger} d_j + U \sum_i d_i^{\dagger} d_i - U \sum_i d_i^{\dagger} d_i h_i^{\dagger} h_i . \qquad (2)$$

Note that doublons have a site energy U, and holons and doublons have an on-site *attractive interaction* U. The deviation away from half filling, δ, is given by $\delta = \bar{n}_0 - \bar{n}_2$, where $\bar{n}_0$ and $\bar{n}_2$ are the holon and doublon densities, respectively. Without loss of generality we can work in the ensemble where $S_z = 0$; since $S_z = (N/2) \times (1 - \bar{n}_0 - \bar{n}_2)$ it follows that $\bar{n}_0 = (1+\delta)/2$ and $\bar{n}_2 = (1-\delta)/2$.

First consider the noninteracting limit in this language. Then holons and doublons with wave vector k have energies $\epsilon_{0k} = \mu_0 + t_k$ and $\epsilon_{2k} = \mu_2 - t_k$, where $t_k \equiv \sum_j t_{ij} e^{ikr_{ij}}$. The chemical potentials μ_0 and μ_2 are to be adjusted to fix S_z and δ. In particular, when S_z is 0, $\mu_2 = -\mu_0$. The doublons and holons then occupy nonintersecting regions of the Brillouin zone, separated by the Fermi surface (in the original language). This state has gapless charge excitations and is obviously metallic.

The effect of turning on the attractive interaction U between doublons and holons is to form pairs or "charge-density waves," which in terms of the original variables correspond to xy (spiral) or z (linear) spin-density waves. If this leads to long-range order, the corresponding order parameters are $\langle d_i^\dagger h_i^\dagger \rangle = \langle S_i^- \rangle = b_0 e^{i\mathbf{Q}\cdot\mathbf{r}_i}$ and

$$\langle 1-(h_i^\dagger h_i + d_i^\dagger d_i)\rangle = \langle S_i^z \rangle = \Delta \cos(\mathbf{Q}\cdot\mathbf{r}_i) .$$

A *coherent* Bose condensation of holon-doublon pairs into a *single* wave vector **Q** necessarily corresponds to an *xy* spiral SDW. Global spin rotations of this state can mix in spin ordering in the *z* direction but can never give a pure *z* linear SDW. Clearly, **Q** is also the center-of-mass (crystal) momentum of the pairs. In what follows, we focus attention on spiral states.

The simplest description of the pairing process is the BCS description.[6] It is the same as the H-F treatment of the Hubbard model which allows for *xy* ordering. For a pairing order parameter with a *single* wave vector **Q** (*even if incommensurate*), i.e., a spiral SDW, the mean-field theory can be implemented exactly.[7] One gets quasiparticles with energies E_{0k},

$$E_{2k} = R_k \pm [\mu_0 + (t_{Q-k} + t_k)/2] ,$$

where $R_k = \{[(t_{Q-k} - t_k)/2]^2 + (Ub_0)^2\}^{1/2}$. The mean-field energy is

$$\mathscr{E} = \sum_k [E_{0k} f^-(E_{0k}) + E_{2k} f^-(E_{2k})] - \sum_k R_k + NU\{b_0^2 + [(1-\delta)/2]^2\} - N\mu_0\delta , \quad (3)$$

when $f^-(x)$ is the Fermi function. The self-consistent equations which determine b_0 and μ_0 are

$$2b_0 = N^{-1}\sum_k (Ub_0/R_k)[1 - f^-(E_{0k}) - f^-(E_{2k})] , \quad (4a)$$

$$\bar{n}_0 - \bar{n}_2 = \delta = N^{-1}\sum_k [f^-(E_{0k}) - f^-(E_{2k})] . \quad (4b)$$

Consider the consequences of this description at half filling for $T=0$ and *large U*. Then $\mu_0 = 0$, both quasiparticles have a gap, and $b_0 \simeq \frac{1}{2}[1 - \frac{1}{2}\sum_k (t_{Q-k} - t_k)^2/U^2]$. The energy can be reexpressed as

$$\mathscr{E}_G/N = -\tfrac{1}{8}\sum_j J_{ij}[1 - e^{iQr_{ij}}] = -\tfrac{1}{8}[\tilde{J}(0) - \tilde{J}(Q)] ,$$

where $J_{ij} = 4(t_{ij})^2/U$ is just the Anderson superexchange interaction.[8] This is precisely the energy of the large-*U* projected Hamiltonian in the presence of a classical spiral SDW state $\langle S_i^- \rangle = \frac{1}{2} e^{i\mathbf{Q}\cdot\mathbf{r}_i}$, with maximal spin alignment of $\frac{1}{2}$. The choice of **Q** that minimizes the energy makes $\tilde{J}(Q)$ most negative within the Brillouin zone. For any bipartite lattice with nearest-neighbor (nn) coupling, the ground state is the Néel state, with $\mathbf{Q} = \mathbf{Q}_0$ such that $e^{i\mathbf{Q}_0\cdot\mathbf{R}} = \pm 1$ on the two sublattices. For the triangular lattice with nn coupling, **Q** is any of the six zone-corner vectors; e.g., $\mathbf{Q}_0 = (4\pi/3a, 0)$, and gives a three-sublattice antiferromagnetic state, with a 120° twist of the spins between the sublattice. In general, the optimal **Q** may not be commensurate with the lattice.

Consider the small-*U* limit. Then the BCS instability sets in when $1 = U\chi(Q)$, where $\chi(Q)$ is the "pairing susceptibility" which is the spin susceptibility. As is well known[6,9] for bipartite lattices with nn coupling, at half filling, $\chi(Q)$ diverges for $\mathbf{Q} = \mathbf{Q}_0$ at $T \to 0$. Hence the ground state supports a nonzero b_0 for any finite *U*, no matter how small. We find that $Q = Q_0$ minimizes the ground-state energy for any *U*. The quasiparticle energies, now given by $E_{0k} = E_{2k} = (t_k^2 + U^2 b_0^2)^{1/2}$ always have a gap. The ground state is a two-sublattice antiferromagnetic insulator for all $U > 0$.

The situation for a nonbipartite lattice, such as the triangular lattice, even with just nn coupling, is more interesting. In this case, the Fermi surface at half filling does not nest[10] and $\chi(Q)$ is finite at $T=0$ for any Q. At half filling the Q at which $\chi(Q)$ peaks $[\mathbf{Q}_1 \equiv (0.73\pi/a, 0)$ or its "star"] is different from the zone-corner wave vector $\mathbf{Q}_0$ $[(4\pi/3a, 0)]$ which characterizes the pairing for large *U*. Thus the pairing instability is to an incommensurate (spiral) SDW, and occurs at a nonzero *U* given by $U_{c1} = \chi^{-1}(\mathbf{Q}_1) = 0.66zt$, where z $(=6)$ is the coordination number.

How does the wave vector of the spiral state change from $\mathbf{Q}_1$ to $\mathbf{Q}_0$, and the quasiparticle spectrum vary as *U* increases from U_{c1} to ∞? A numerical solution of the self-consistent equations and a minimization of the energy with respect to **Q** leads us to the results shown in Fig. 1. There is an upper critical $U_{c2} = 0.86zt$ such that for $U_{c1} < U < U_{c2}$, $\mathbf{Q}^*$, the optimal **Q** changes continuously from $\mathbf{Q}_1$ to $\mathbf{Q}_0$. In this range of *U*, there are pockets in the zone where E_{0k} or E_{2k} is negative. Thus, gapless charge excitations exist and this is a spiral *metallic* phase.

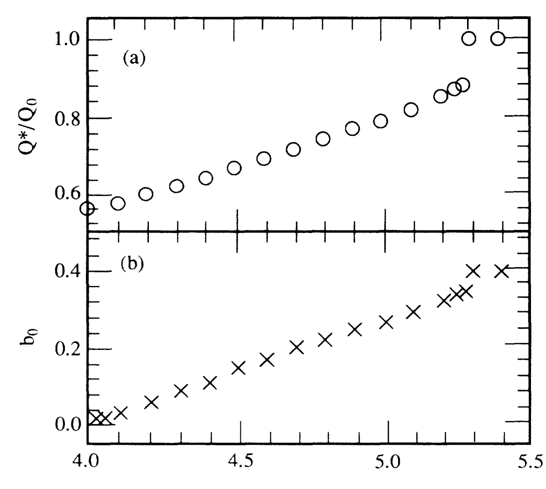

FIG. 1. (a) Magnitude of the ordering wave vector Q^* in units of $Q_0 = 4\pi/3$ and (b) magnetization b_0 vs U/t. The incommensurate phase first occurs at $U_{c1} \approx 3.97$ (not shown), the first-order transition into the insulating antiferromagnetic phase occurs at $U_{c2} = 5.27$. For $U < U_{c1}$, b_0 is zero.

Exactly at U_{c2} there is a first-order metal-insulator transition. The wave vector Q^* jumps from approximately $0.88Q_0$ to Q_0, the magnetization jumps from 0.34 to 0.39, and an insulating gap at approximately $0.085t$ suddenly opens up. Beyond U_{c2}, $\mathbf{Q}^*$ sticks at $\mathbf{Q}_0$ and the charge gap has the value Ub_0-2t—this is the three-sublattice antiferromagnetic *insulating* state.

With appropriate values for Q^*, U_{c1}, and U_{c2}, this scenario can most likely accommodate general lattices and general couplings t_{ij}. For example, in the case of the square lattice with a small next-nearest-neighbor hopping,[11] t_2, we find again a paramagnetic metal for small U, then an incommensurate metal for intermediate U, and an antiferromagnetic insulator for large U.

Next consider what happens at finite temperatures. As is well known, on bipartite lattices, *at small U*, H-F theory is a good guide. At $T_c(U)$ given by $U=\chi^{-1}(T_c)$, a pairing instability occurs accompanied by a formation of quasiparticles with a charge gap and long-range Néel order. Thus, there is *one transition*, from a paramagnetic metallic phase to an antiferromagnetic insulating phase.[12] As long as $T_c(U)/zt \ll 1$, the transition is well described by mean-field theory.[13]

But this picture is obviously incorrect for large U. In this case, for $U \gg zt$, the doublons and holons will form real-space[14] bosonic pairs[15] with a binding energy of order U. Now there are two temperature scales: (1) an upper temperature scale T_u, primarily determined by U, at which the bosons form and a *charge gap* opens up; and (2) a lower temperature T_l, determined by the hopping amplitude for the pairs, at which the pairs Bose condense. In spin language, the formation of doublon-holon pairs is simply the formation of local moments and their hopping amplitude is the exchange energy of the spins; their Bose condensation results in long-range magnetic order.

Mean-field theory leads to a transition[16] at T_u and describes the physics associated with it. For large T, the (noninteracting) doublons and holons are nondegenerate with $\chi_{\text{pair}}(Q) \sim 1/T$ leading to the H-F instability at $T \simeq U$. For $T \ll U$, charge excitations have a gap $\sim U$. Thus, the region $T_l < T < T_u$ corresponds to a *paramagnetic* insulating[10] phase. For $T < T_l$, after the Bose condensation occurs, one has an antiferromagnetic (or spiral) insulating phase. It should be noted that in 2D t_l is always zero..

The processes that are responsible for the distinction between T_u and T_l are contained only in the fluctuations about mean-field theory. Given one H-F solution, other degenerate solutions can be obtained by performing global-spin rotations. Hence there are long-wavelength boson modes which have low energies—these are the spin waves; the hopping amplitude of the bosons determines the spin-wave stiffness constant J_{SW}. These spin waves destroy long-range order at any finite temperature in 2D and for $T > T_l$ (determined by J_{SW}) in 3D and at $T=0$, reduce the value of b_0 from its mean-field value.[17] There are two limits in which J_{SW} is easy to calculate: In the limit of $U \gg zt$ and $T \to 0$, J_{SW} is proportional to $4t^2/U$. In the other limit, that of small U in a bipartite lattice, $J_{\text{SW}} \sim U\xi_0^2$, where ξ_0 is the pairing coherence length,[6] which is very large. In this case $T_l > T_u$, which is in fact responsible for there being only one transition. A precise elucidation of the details of the phase diagram and whether or not T_u corresponds to a true transition needs a careful and involved calculation of J_{SW} and of the fluctuation effects for intermediate values of U/zt, which we will report in a separate publication.

We have also explored the mean-field theory outlined above for δ nonzero, and find that it gives a useful zeroth-order description of the physics of the Hubbard model, for all U and δ. In particular, for large U, and $\delta \neq 0$, we find a spiral metallic phase,[18,19] which evolves continuously into a ferromagnetic phase for $\delta \gg t/U$. The results are very similar to what we have obtained using the Schwinger-boson-slave fermion mean-field theory.[20] Of course, the "elementary" excitations of mean-field theory are not weakly interacting, as is evident from the fluctuation corrections. For example, for $U \to \infty$ and $\delta > 0$ the "spin-flip bosons" $b_i^\dagger \equiv d_i^\dagger h_i^\dagger$ have a hard-core repulsion between themselves and with the (renormalized) holon quasiparticles, and spin fluctuations lead to interactions between the holon quasiparticles. Thus, questions as to whether the holons can form Cooper pairs leading to superconductivity,[21] and how particle-hole fluctuations of the holon Fermi sea destroy[22] the ferromagnetic state for finite U and large δ, etc., are to be addressed as questions of second-level instabilities due to the interactions between the elementary excitations of the Hartree-Fock theory. We will discuss such issues elsewhere.

In summary, we have shown that a reinterpretation of the Hubbard model provides some new insights into the physics of the Hubbard model and the metal-insulator transition. We have also shown that a H-F mean-field theory for pairing (or spiral SDW) can be implemented to yield meaningful results (especially when one includes fluctuation effects). It would be interesting to look for spiral SDW states and other consequences of our theory in conventional strongly correlated systems showing the Mott-Hubbard metal-insulator transition.

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[1]J. Hubbard, Proc. Roy. Soc. London A **276**, 238 (1963); **281**, 401 (1964).

[2]N. F. Mott, *Metal Insulator Transitions* (Taylor and Francis, London, 1974).

[3]For a recent review, see T. V. Ramakrishnan, in *The Metallic and Nonmetallic States of Matter,* edited by P. P. Edwards and C. N. R. Rao (Taylor and Francis, London, 1985).

[4]Such a representation has been used earlier by G. Kemeny and co-workers in a series of papers [e.g., see G. Kemeny and L. G. Caron, Rev. Mod. Phys. **40**, 790 (1968)], but we put it to quite a different use.

[5]For example, see D. R. Penn, Phys. Rev. **142**, 350 (1966).

[6]For example, J. R. Schrieffer, *Theory of Superconductivity* (Benjamin, Reading, 1971).

[7]In contrast, if we allowed for a linear SDW, the H-F mean-field theory for the ordered phase becomes difficult to implement as it involves the diagonalization of an incommensurate Hamiltonian. We have yet to check the relative stability of the spiral SDW with respect to the linear one. It appears likely that for large U the spiral phase should be favored.

[8]P. W. Anderson, Phys. Rev. **86**, 694 (1952).

[9]See J. E. Hirsch, Phys. Rev. B **31**, 4403 (1985).

[10]For example, see E. Tosatti and P. W. Anderson, Solid State Commun. **14**, 773 (1974).

[11]This model has been discussed recently by H. Q. Lin and J. E. Hirsch, Phys. Rev. B **35**, 3359 (1987).

[12]We refer to the phase with a charge gap and an exponentially activated conductivity, loosely, as being insulating.

[13]In two dimensions, however, this transition is destroyed by fluctuations in the phase of the order parameter (see below).

[14]P. Nozieres and S. Schmitt-Rink, J. Low Temp. Phys. **59**, 195 (1985).

[15]This is obvious if one describes the large-U perturbation theory using the new language. At $U=\infty$, at half filling, only spins are present—equivalently doublons and holons are bound on the same site; to order t/U, the ground state has mixed in pair of doublons and holons which are one lattice spacing apart, and so on.

[16]If across a portion of $T_u(U)$ there is a first-order jump in the gap, it could survive the inclusion of fluctuations while a continuous transition is unlikely to survive as such.

[17]Indeed, for U close to U_{c1} where b_0 is small, these fluctuations may completely destroy the long-range order.

[18]B. I. Shraiman and E. D. Siggia, Phys. Rev. Lett. **62**, 1564 (1989).

[19]The H-F theory for the square lattice Hubbard model for $\delta\neq0$ has been recently studied by H. Schulz (to be published), who also considers linear SDW states. We disagree with his suggestion that within this mean-field theory there can be a spiral insulating phase for $\delta\neq0$.

[20]C. Jayaprakash, H. R. Krishnamurthy, and S. Sarker, Phys. Rev. B **40**, 2610 (1989).

[21]This question is of obvious interest in the context of high-T_c superconductors; P. W. Anderson, in *Frontiers and Borderlines in Many-Particle Physics,* International School of Physics "Enrico Fermi," Course CIV, edited by J. R. Schrieffer and R. A. Broglia (North-Holland, Amsterdam, 1989).

[22]B. S. Shastry, H. R. Krishnamurthy, and P. W. Anderson (to be published).