Numerical Results for the Hubbard Model: Implications for the High T_c Pairing Mechanism

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Dedicated to Martin C. Gutzwiller on the occasion of his 75th birthday.

Abstract

Numerical studies of the Hubbard model and its strong-coupling form, the t-J model, show evidence for antiferromagnetic, $d_{x^2-y^2}$-pairing and stripe correlations which remind one of phenomena seen in the layered cuprate materials. Here, we ask what these numerical results imply about various scenarios for the pairing mechanism.

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In his 1963 article on the *Effect of Correlation on the Ferromagnetism of Transition Metals* [1], Gutzwiller suggested that it was “instructive” to consider a model Hamiltonian of the form

\[
H = \sum_{k,s} \epsilon_k n_{ks} + U \sum_i n_{i\uparrow} n_{i\downarrow} . \tag{1}
\]

He noted that the first term arose from solving Schrödinger’s equation for one electron in the effective periodic potential of the lattice while the second term described the Coulomb repulsion between two electrons of opposite spin which happen to be in the same orbit at site \(i\). In this same year, in a paper entitled *Electron Correlations in Narrow Bands* [2], Hubbard also studied this model. He wrote \(H\) in the form

\[
H = -\sum_{ijs} t_{ij} \left( c_{i,s}^+ c_{j,s} + c_{j,s}^+ c_{i,s} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{2}
\]

which is now called the Hubbard model. Here \(c_{i,s}^+\) created an electron of spin \(s\) in an orbital at site \(i\) and \(n_{i,s} = c_{i,s}^+ c_{i,s}\) was the orbital occupation number for electrons of spin \(s\) on site \(i\). For a 2D square lattice with \(t_{ij} = t\) for near-neighbor sites only, \(\epsilon_k\) of Eq. (1) is \(-2t(\cos k_x + \cos k_y)\). In this case, two parameters, \(U/t\) and the average site occupation \(n\) determine the state of the system. In his 1963 paper, Gutzwiller also proposed a new trial wave function for large \(U/t\). This wave function was obtained by applying a projection operator

\[
P_G(\eta) = \Pi_i \left( 1 - (1 - \eta) n_{i\uparrow} n_{i\downarrow} \right) \tag{3}
\]

to the usual Slater determinant of Bloch functions. In particular, for \(\eta = 0\), \(P_G(0)\) projects out all configurations with doubly occupied sites. The \(t\)-\(J\) model is the large \(U/t\) limit of the Hubbard model obtained by expanding to order \(t^2/U\) and dropping three-site terms which are proportional to the doping. Using the Gutzwiller projection operator, the \(t\)-\(J\) model has the form [3–5]

\[
H = P_G(0) \left[ -\sum_{(ij),s} t \left( c_{i,s}^+ c_{j,s} + c_{j,s}^+ c_{i,s} \right) + J \sum_{(ij)} \left( \vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j \right) \right] P_G(0) \tag{4}
\]

with the exchange interaction \(J = 4t^2/U\). Here the state of the system is determined by \(J/t\) and the site occupation \(n\).

Both Gutzwiller and Hubbard were interested in the strongly-correlated case in which \(U/t\) was large and in understanding what conditions favored ferromagnetism. Now, almost forty years later, we are still seeking to understand the behavior of the deceptively simple looking Hubbard and \(t\)-\(J\) models. In particular, we would like to know if these models contain the essential physics of the high \(T_c\) cuprate superconductors, and if so what they tell us about the basic pairing mechanism. The premise of this brief report is that numerical calculations have shown that the Hubbard and \(t\)-\(J\) models exhibit a number of the phenomena which have been observed in various cuprate materials. Nevertheless, as we will discuss, the question regarding the nature of the underlying pairing mechanism remains open with a diverse range of proposals set forth.
Turning first to our premise, we know from Monte Carlo calculations that the ground-state of the half-filled 2D Hubbard model has long-range antiferromagnetic order as does the 2D Heisenberg model, which is just the undoped $t$-$J$ model. It also has been shown from finite temperature Monte Carlo calculations that the low energy spin-fluctuations of the insulating cuprates are well described by the Heisenberg model. In particular, the instantaneous spin-spin correlation length calculated for the 2D $S = 1/2$ Heisenberg model with a near-neighbor exchange is in excellent agreement with neutron scattering measurements of $La_2CuO_4$ above its Neel Temperature. Thus, the 2D Hubbard and $t$-$J$ models provide an excellent description of the low energy magnetic behavior of the undoped layered cuprates. Likewise, DMRG calculations on half-filled $n$-leg Hubbard and $t$-$J$ ladders have shown that the even-leg ladders are spin-gapped while the odd-leg ladders are not. This is in agreement with experimental data on $SrCu_2O_3$ and $Sr_2Cu_3O_5$ which contain weakly-coupled arrays of 2- and 3-leg ladders respectively.

When a 2-leg Hubbard or $t$-$J$ ladder is doped away from half-filling, the added holes form $d_{x^2-y^2}$-like pairs with power law pair-field and CDW correlations and there are physically reasonable parameter regimes in which the pair-field correlations are dominant. Under pressure, the 2-leg ladder material $(SrCa)_{14}Cu_{24}O_{41}$ has a superconducting transition with $T_c \simeq 12K$, however transport evidence suggests that the pressure has made this system into an anisotropic 2D material rather than a weakly Josephson coupled array of 2-leg ladders. On doped 3-leg ladders, calculations indicate that the holes first go into the odd band and for doping $x \lesssim 0.05$ the system exhibits properties similar to a 1-leg, $t$-$J$ ladder, which is known to have charge-spin separation. At higher doping in the 3-leg ladder, pairs and domain walls form. When two holes are added to 4- and 6-leg ladders, they form $d_{x^2-y^2}$-like pairs and at finite doping, domain walls form. On doped 8-leg, $t$-$J$ ladders, DMRG calculations find domain walls with a linear hole density of 0.5 per $Cu$ separating $\pi$-phase shifted antiferromagnetic regions, similar to the stripes observed by neutron scattering from $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$. When a small next-near-neighbor hopping $t'$ is added, $d_{x^2-y^2}$-pairing correlations are favored over the striped domain wall configurations in the DMRG calculations.

Nevertheless, considerable difference of opinion remains about the nature of the correlations in the 2D system. While early RPA calculations for the doped 2D Hubbard model found that the exchange of antiferromagnetic spin fluctuations could lead to $d_{x^2-y^2}$-superconductivity, competing channels which arise from nesting and van Hove singularities lead to a breakdown of conventional perturbation theory. A number of authors have carried out renormalization group analyses which treat the various particle-hole and particle-particle channels on an equal footing. For the weak-coupling doped Hubbard model with a near-neighbor hopping $t$, a $d_{x^2-y^2}$-superconducting state is inferred from the divergence of the one-loop $d_{x^2-y^2}$-pairing susceptibility. More generally, the one-loop calculation can lead to divergencies of vertices associated with various channels. In particular, with a next-near-neighbor hopping $t'$, different instabilities arising from the position of Van Hove points on the fermi surface can compete. For example, from an analysis of the renormalization group flow, Furukawa et. al. have recently suggested that an Umklap-gapped, spin-liquid state might exist for a 2D Hubbard model with appropriate values of $t'$ and doping.

The original finite temperature Monte Carlo calculations were unable to reach low tem-
temperatures for the doped Hubbard model because of the fermion determinantal sign problem. They have, however, been used to study the momentum and Matsubara frequency dependence of the effective pairing interaction at temperatures of order one-half to one-third of the exchange energy scale $4t^2/U$. The leading eigenvalue in the singlet channel associated with this interaction was shown to have $d_{x^2-y^2}$ symmetry [23]. However, zero temperature constrained path Monte Carlo calculations [24] find only short-range pairing correlations in the groundstate of the 2D Hubbard model.

For the 2D $t$-$J$ model, questions of phase separation, stripe formation, and pairing arise. Our study of long $n$-leg $t$-$J$ ladders with $n$ up to 6 support the notion that the $t$-$J$ model does not phase-separate in the physically relevant $J/t$ region [27]. This conclusion disagrees with Green’s function Monte Carlo calculations of Hellberg and Manousakis [28] but is in agreement with other Green’s function Monte Carlo calculations with stochastic reconfiguration by Calandra and Sorella [29]. These latter authors also find evidence for long-range superconducting order for dopings $x > 0.1$ rather than stripes. Thus, while questions remain regarding the existence of long-range superconducting order, stripes, and phase separation, it is clear from a variety of numerical work that the Hubbard and $t$-$J$ model have low-lying states that exhibit a number of features which are seen in the cuprate materials.

So what can we conclude from this about the basic pairing mechanism? Certainly, in a general way, the fact that these models exhibit antiferromagnetism, $d_{x^2-y^2}$-pairing correlations and stripes imply that these phenomenon can arise naturally in systems with strong short-range Coulomb interactions in which there is a competition between kinetic and exchange energies: $d_{x^2-y^2}$ pairs as well as domain walls form as the doped holes locally arrange themselves so as to satisfy the competing requirements of minimizing both their kinetic energy and the disturbance of the background exchange interactions. However, beyond this general picture, forced by the minimalist nature of these models which after all have only $U/t$ or $J/t$ along with the band filling $n$ to parameterize the physics, there remain a remarkably diverse set of views regarding the underlying pairing mechanism.

In part, this diversity reflects the fact that for the parameter regime appropriate to the cuprates ($U/t \gg 1$ or $J/t < 0.5$) these models describe a strongly-coupled system which is delicately balanced. Thus, changes in the doping, the lattice or the next-near-neighbor hopping can alter the nature of the groundstate. While we believe that this delicacy in fact provides further evidence that these models contain much of the essential physics, it poses special problems for the theorist. One difficulty with a strongly-interacting system is that when a particular type of mean-field order is assumed, it has a good chance of being self-consistently “found”. That is, strongly-interacting systems can support a self-fulfilling ansatz, keeping the true nature of the groundstate hidden. One goal of the numerical work is to avoid this. However, it is easy to slip back into this framework in interpreting the numerical results. That is, one’s description of “the mechanism” may depend upon one’s starting ansatz. The delicate balance of the system suggests that one must simultaneously treat a variety of channels. In addition, one must ask if the weak-coupling regime of the Hubbard model is continuously connected to the strong-coupling regime. That is, what is the nature of the state out of which the superconducting state is formed as the temperature is lowered or at zero temperature as the doping is changed. Depending upon how one interprets the limited numerical data or what additional interactions or degrees of freedom one imagines including, different pairing scenarios arise.
Here, with this in mind, we’ll examine some of the numerical results. Consider the schematic phase diagram for the 2-leg Hubbard ladder shown in Fig. 1. Here the average site filling $\langle n \rangle$ is plotted along the horizontal axis and the ratio of the rung hopping $t_\perp$ to the leg hopping $t$ is plotted along the vertical axis. For the non-interacting system, the antibonding band is lifted above the bonding band for $t_\perp/t > 2$. Thus, at half-filling, $\langle n \rangle = 1$, for large values of $t_\perp/t$ the ladder is simply a typical band insulator with an even number of electrons per unit cell (2 per rung) filling the bonding band. In the absence of the interaction $U$, the bonding and antibonding bands of the half-filled system would overlap and it would become a metal for $t_\perp/t < 2$. However, with $U$ present it remains a spin-gapped insulator at half-filling. The important point is that for $\langle n \rangle = 1$, the spin-gapped small $t_\perp/t$ insulating state is adiabatically connected to the large $t_\perp/t$ Bloch band-insulating state.

The behavior of this system under doping is, of course, quite different depending upon the size of $t_\perp/t$. In the shaded 2-band region, doped holes enter as quasi-particles with charge $e$ and spin $s = 1/2$. Above a value of $t_\perp/t$ which, for the interacting system depends upon $U$, the doped holes enter a single band Luttinger liquid and exhibit spin-charge separation. In the shaded region of the phase diagram, the doped holes form pairs consisting of superpositions of rung and leg singlets with the $d_{x^2-y^2}$-like phasing shown in Fig. 2. Here, power-law pairing correlations compete with CDW correlations [12–15]. How should these results be interpreted? One might have thought that the 2-leg ladder geometry is ideally suited for an RVB description. In the limit in which the rung exchange $J_\perp$ is large, one can imagine that the groundstate of the undoped ladder contains a set of rung valence-bond singlets with a spin gap $-\frac{3}{4}J_\perp$. Upon hole doping, these latent rung singlet pairs are free to move and power law pairing correlations develop. In the isotropic case in which the leg and rung exchange couplings are equal, the undoped groundstate still has a robust spin gap of order $J/2$ and one can again picture that the pairing correlations arise when the system is hole-doped and the singlet pairs (shown in of Fig. 2) are free to move. Thus, there is a continuous transition from the spin-gapped Mott insulating phase to the $d_{x^2-y^2}$-superconducting phase as the chemical potential exceeds a critical value. However, contrary to some of the original RVB tenents [30], there are no spinon excitations in the undoped, 2-leg ladder and the type of spin-charge separation found in the one-leg system is absent. In fact, for the 2-leg Hubbard ladder the weak and strong-coupling regions appear to be adiabatically connected.

Another view argues that the exchange of short-range antiferromagnetic spin fluctuations mediate the pairing [22,31]. Indeed, Monte Carlo calculations [32] of the effective pairing interaction $V(q, \omega_m)$ show that it resembles the spin susceptibility $\chi(q, \omega_m)$ as suggested by weak-coupling RPA calculations. Fig. 3 shows Monte Carlo results for $V(q,0)$ and $\chi(q,0)$ versus $q_x$ for $q_y = \pi$. As the temperature is lowered and the short-range, spin-spin correlations develop, the pairing interaction $V$ shown in Fig. 3(a) exhibits a $q$ and $T$ dependence similar to $\chi$ shown in Fig. 3(b). This same behavior is seen on $8 \times 8$, 2D clusters [23]. However, because of the fermion sign problem these Monte Carlo calculations are limited to temperatures greater than of order $J/3$. Moreover, the simple RPA framework clearly fails to describe the spin-gapped nature of the undoped ladder and an approach such as the RNG-bozonization [33,34] method is needed. In this approach, a weak-coupling renormalization group calculation is used which treats all channels on an equal footing until the dominant couplings emerge and can be treated by abelian bosonization. Lin, Balents, and
Fisher [34], and Arrigoni and Hanke [35] have shown that in weak coupling a generic ladder model, including both longer-range Coulomb interactions and hopping [35], flows to a manifold with $SO(5)$ symmetry. This is the symmetry group originally proposed by Zhang [36] in which the antiferromagnetic and superconducting order parameters are combined into a five-dimensional superspin. For an $SO(5)$ symmetric ladder, the magnon dispersion about $(q_x = \pi, q_y = \pi)$ should be identical to the hole pair dispersion about $(q_x = \pi, q_y = \pi)$. This was shown to be the case for an explicitly constructed $SO(5)$ ladder [37]. However, this need not be the case for the Hubbard and $t$-$J$ models in the physically relevant region of parameter space. The point is that the RNG results were obtained in the weak-coupling regime. Thus, for example, for the Hubbard ladder, the question is whether there is room for a sufficient renormalization group flow to approach the region in which $SO(5)$ provides a useful description of the low energy properties when $U$ is of order the bandwidth. A similar question, of course, also arises for the $t$-$J$ ladder. One test of $SO(5)$ is to compare the magnon and pair dispersions which would be identical for an $SO(5)$ ladder. The question is whether they are close so that $SO(5)$ provides a good starting point for describing the collective modes of the $t$-$J$ ladder, or whether they are significantly different. With the open boundary conditions on a $2 \times L$ ladder used in the DMRG calculations, the coefficient of the $q^2$ dispersion measured relative to $(\pi, \pi)$ for the magnon and $(0, 0)$ for the pair, is given by the slope of the $L^{-2}$-dependence of the energy $E_m = E_0(S = 1) - E_0(S = 0)$ to add a magnon and the energy to add a pair $E_p = E_0(n_n = 2) - E_0(n_n = 0)$, respectively. As shown in Fig. 4, for a 2-leg $t$-$J$ ladder with $J/t = 0.5$ these two slopes differ by a factor of 2. Thus, in the strong-coupling limit the 2-leg Hubbard model, or here the $t$-$J$ model, does not exhibit an exact $SO(5)$ symmetry. However, recent work on the Hubbard model and $SO(5)$ symmetry [38] has shown that in intermediate to strong coupling, the presence of the on-site $U$ requires one to implement a projected $SO(5)$ symmetry in which the high-energy double occupancies, responsible for the Mott-Hubbard gap, are Gutzwiller-projected out. This restores $SO(5)$ symmetry for static correlation functions but introduces changes in dynamic ones [39], such as the differences in the magnon and pair dispersions discussed above.

Turning next to the 8-leg, $t$-$J$ ladder results, the DMRG calculations [19] for the doped system find evidence for the formation of charged stripes separating $\pi$-phase shifted antiferromagnetic regions as illustrated in Fig. 5. Both site-centered “one-leg” and bond-centered, “two-leg” stripes with a linear charge density $\rho_L = 0.5$ have been found in these calculations, depending upon the length of the open end $8 \times L$ system. While the existence of striped domain walls was found in early Hartree-Fock calculations [10], Emery and Kivelson [11] have argued that stripes arise when phase separation in the $t$-$J$ model is frustrated by long-range Coulomb forces. In addition, they have suggested that the holes on the stripes exhibit charge-spin separation, at least over some suitable length scale, so that spinons can fluctuate into the “insulating spin-gapped” regions between the stripes. In this spin-gap proximity effect scenario, these spinons then transfer the spin-gap from the “insulating spin-gapped” region back onto the charged stripe leading to enhanced pairing correlations [12]. Ultimately the pairing correlations on different stripes couple through a Josephson coupling to form the superconducting state.

The DMRG calculations certainly do find striped domain walls in a variety of $n$-leg ladder calculations. Furthermore, there is a significant spin gap of order $J/2$ on an undoped 2-leg ladder which could make such regions attractive candidates for inducing a “spin-gap
proximity effect”. Nevertheless, our numerical calculations on the $t$-$J$ model imply that it does not phase-separate in the physically relevant region of parameter space [27]. Rather, we find that stripe formation in the $t$-$J$ model is driven by the competition between the kinetic and exchange energies. Furthermore, when we turn on a next-nearest-neighbor hopping $t'$, the stripes and stripe-stripe correlations decrease as the pairing correlations increase in strength. The pairing correlations are present when the static stripes have disappeared as well as any evidence for the fluctuation stripe correlations in the density-density correlation function. It appears from these calculations that in this region the stripes have evaporated [21].

Still other theories propose additional order parameters such as the $d$-wave density state which has antiferromagnetic orbital currents. Monte Carlo calculations on a Gutzwiller projected BCS $d$-wave variational state are reported to have a power law decay of the orbital currents [13]. It has also been suggested that the pseudogap phase of the cuprates is associated with a $d$-wave density phase which is prevented from fully developing by disorder [14]. However, we find that the antiferromagnetic orbital currents decay exponentially on the 2-leg $t$-$J$ ladder [13] and also decay rapidly on 6-leg $t$-$J$ ladders. In addition, were a phase transition to a $d$-wave density phase to occur for the lightly-doped 2D Hubbard model at a temperature $T^*$ well above the superconducting transition temperature, one would have expected to see some indication of this in the finite temperature Monte Carlo results.

There has also been a recently proposed $Z_2$ gauge theory in which electrons can fractionalize into separate charge and spin degrees of freedom in dimensions greater than one [10]. Here the spin of the electron is carried by a neutral fermionic excitation, the spinon, and the charge is carried by a bosonic excitation, the chargon. Central to this fractionalization is an underlying topological order. If this $Z_2$ topological order is present, the groundstate of such a system on a 2D periodic lattice should exhibit a 4-fold degenerate groundstate. Here, we comment on the relationship of such a theory to what is known numerically about the 2D Hubbard and $t$-$J$ models. For the 2D Heisenberg model with periodic boundary conditions, exact diagonalization calculations on finite sized clusters find a “Neel tower of states” with the groundstate energy $E_0$ varying with the total spin as $S(S + 1)$. This implies that the groundstate of the half-filled $t$-$J$ model is not a “topological antiferromagnetic” state which would have had an $S = 0$, 4-fold degenerate groundstate in the limit of a large 2D lattice with periodic boundary conditions. Similarly, in the weak-coupling limit of the half-filled 2D Hubbard model, renormalization group calculations imply that the system has a Neel antiferromagnetic groundstate and electron-like quasi-particles above a gap. Since, in strong coupling, the Hubbard model goes to the $t$-$J$ model, which at half-filling is Heisenberg-like, it seems likely that the groundstate of the half-filled Hubbard model is the traditional antiferromagnetic state for all $U/t$. It may be that additional 4-site ring exchange interactions, or other interactions laying outside the simple near-neighbor exchange-coupled Heisenberg model, can lead to such a topological state. This remains to be studied.

For the doped 2D Hubbard and $t$-$J$ models, it is possible that a topological phase exists. This would, of course, be a key finding and would lay the groundwork for a spin-charge fractionalization mechanism in which the electron separates into a spinon which carries the electron’s spin and fermi statistics and a chargon which can bose condense giving superconductivity [10]. While it seems unlikely that this can happen at infinitesimal doping, it could be that it occurs at some finite doping. At present, our numerical work on the Hubbard and
t-J models has failed to find evidence of such a topological state. However, these studies are limited and there are of course additional interactions present. For example, we know that the cuprates are actually charge transfer insulators rather than Mott-Hubbard insulators. While we believe that this enhances the pairing tendencies that one sees in the Hubbard and t-J models due to the extra exchange paths and increased pair mobility \[47\], it is possible that these additional interactions produce more profound effects.

To summarize, the Hubbard model and its strong-coupling limit, the t-J model, have certainly proven “instructive” as originally suggested by Gutzwiller. The numerical results exhibit a variety of antiferromagnetic, \( d_{x^2-y^2} \)-pairing and stripe correlations reminding us of the phenomena seen in the cuprates and providing tests for various pairing scenarios. The numerical results suggest that (1) the competing requirements of minimizing the kinetic energy and the disturbance of the exchange energy background underlie both pairing and stripe domain wall formation, (2) the momentum and temperature dependence of the effective pairing is similar to the spin susceptibility, and (3) stripes compete with superconductivity.

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FIG. 1. Schematic groundstate phase diagram of the 2-leg Hubbard model showing $t_\perp/t$ along the vertical axis and the average site filling along the horizontal axis. For $U = 0$, the solid curve separates the region in which the bonding and antibonding bands both have electrons (shaded) from the region in which the electrons only occupy states in the bonding band.

FIG. 2. Schematic drawing of the pair-wave function showing the values of the off-diagonal matrix element $\langle N - 2| (c_{i\uparrow}c_{j\downarrow} - c_{i\downarrow}c_{j\uparrow})|N \rangle$ for removing a singlet pair between near-neighbor sites.
FIG. 3. (a) Momentum dependence of the effective interaction \( V(q) \) at various temperatures for a 2-leg Hubbard ladder with \( U = 4t \), \( \langle n \rangle = 0.875 \) and \( t_\perp = 1.5t \). Here, \( V(q) \) is measured in units of \( t \), \( q_y = \pi \) and \( V(q) \) is plotted as a function of \( q_x \). (b) Momentum dependence of the magnetic susceptibility \( \chi(q) \) for the same parameters.

FIG. 4. Magnon and hole-pair energies versus \( (\pi/L)^2 \) for a \( 2 \times L \), \( t-J \) ladder with \( J/t = 0.5 \). Exact \( SO(5) \) symmetry would imply that the slopes of the two curves would be the same.
FIG. 5. Hole density and spin moments for a $16 \times 8$, $t$-$J$ lattice with $J/t = 0.35$ and a hole doping $x = 0.125$. The diameter of the circles is proportional to the hole density $1 - \langle n_i \rangle$ on the $i^{th}$ site and the length of the arrow is proportional to $\langle S_i^z \rangle$ according to the scales shown. The lattice has periodic boundary conditions in the $y$-direction and open boundary conditions in the $x$-direction with a staggered magnetic field of strength $h = 0.1t$ applied at the open ends.