

# The Physics Behind High-Temperature Superconducting Cuprates: The “Plain Vanilla” Version Of RVB

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## Abstract

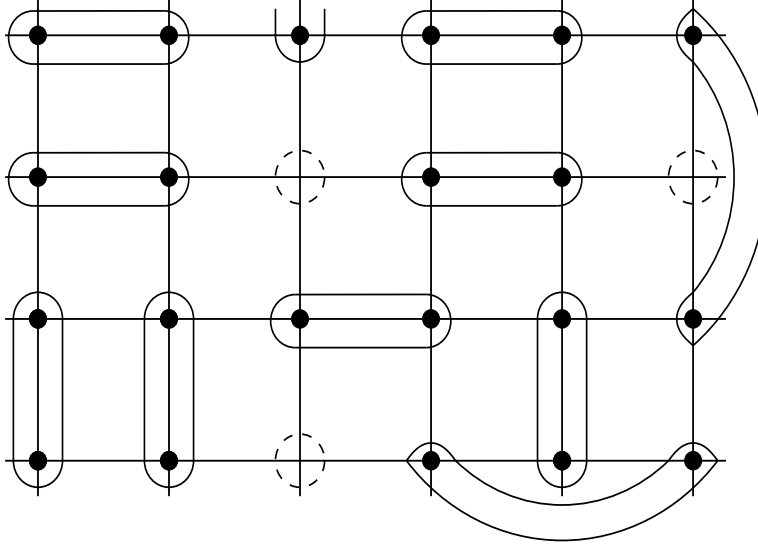
One of the first theoretical proposals for understanding high temperature superconductivity in the cuprates was Anderson’s RVB theory using a Gutzwiller projected BCS wave function as an approximate ground state. Recent work by Paramakanti, Randeria and Trivedi has shown that this variational approach gives a semi-quantitative understanding of the doping dependences of a variety of experimental observables in the superconducting state of the cuprates. In this paper we revisit these issues using the “renormalized mean field theory” of Zhang, Gros, Rice and Shiba based on the Gutzwiller approximation in which the kinetic and superexchange energies are renormalized by different doping-dependent factors  $g_t$  and  $g_S$  respectively. We point out a number of consequences of this early mean field theory for experimental measurements which were not available when it was first explored, and observe that it is able to explain the existence of the pseudogap, properties of nodal quasiparticles and approximate spin-charge separation, the latter leading to large renormalizations of the Drude weight and superfluid density. We use the Lee-Wen theory of the phase transition as caused by thermal excitation of nodal quasiparticles, and also obtain a number of further experimental confirmations. Finally, we remark that superexchange, and not phonons, are responsible for d-wave superconductivity in the cuprates.

## Introduction

The resonating valence bond (RVB) liquid was suggested in 1973 by Anderson and Fazekas (Anderson, 1973; Fazekas and Anderson, 1974) as a possible quantum state for antiferromagnetically coupled  $S = 1/2$  spins in a low dimensions. Their ideas were based on numerical estimates of the ground state energy. Instead of orienting the atomic magnets on separate, oppositely-directed sublattices, in the liquid they were supposed to form singlet “valence bonds” in pairs, and regain some of the lost antiferromagnetic exchange energy by resonating quantum-mechanically among many different pairing configurations. Such states form the basis of Pauling’s early theories of aromatic molecules such as benzene (as well as of his unsuccessful theories of metals), and are a fair description of Bethe’s (1931) antiferromagnetic linear chain. The  $S = 1/2$  antiferromagnetic Heisenberg model arises naturally in Mott insulators. Unlike conventional band insulators, Mott insulators have an odd number of electrons per unit cell and are insulating by virtue of the strong Coulomb repulsion between two electrons on the same site. Virtual hopping favors anti-parallel spin alignment, leading to antiferromagnetic exchange coupling  $J$  between the spins (Anderson, 1959). In the RVB picture,  $S = 1/2$  is important because strong quantum fluctuations favor singlet formation rather than the classically ordered Néel state.

In 1986 the high  $T_c$  cuprates were discovered (Bednorz and Muller, 1986), and it was soon realized (Anderson, 1987a) that the operative element in their electronic structures was the square planar  $\text{CuO}_2$  lattice. In the “undoped” condition, where the Cu is stoichiometrically  $\text{Cu}^{++}$ , the  $\text{CuO}_2$  plane is just such an antiferromagnetically coupled Mott insulator. In many instances these planes are weakly coupled to each other. Anderson (1987a, 1987b), in response to this discovery, showed that an RVB state could be formally generated as a Gutzwiller projection of a BCS pair superconducting state. This is a much more convenient and suggestive representation than those based on atomic spins, and it immediately makes a connection with superconductivity.

The method of Gutzwiller (1963) was initially proposed as a theory of magnetic metals, in conjunction with the Hubbard model. His proposal was to take into account the strong local Coulomb repulsion of the electrons by taking a simple band Fermi sea state and simply removing, by projection, all (or, in the early version, a fraction) of the components in it which have two electrons on the same site. When one projects a half-filled band in this way the result is to leave only singly-occupied sites with spins. The new idea is to project a BCS



$$\mathbf{r} \text{ --- } \mathbf{r}' = \frac{|\uparrow_{\mathbf{r}}\downarrow_{\mathbf{r}'}\rangle - |\downarrow_{\mathbf{r}}\uparrow_{\mathbf{r}'}\rangle}{\sqrt{2}}$$

FIG. 1: Snapshot of a resonating valence bond (RVB) configuration showing singlet pairs of electrons and, in addition, a fraction  $x$  of doped holes. The many-body ground state wavefunction is a linear superposition of such configurations with the spatial dependence of the singlet pairing amplitudes determined by the function  $\varphi(r - r')$  defined in eq. (4).

paired superconducting state; then the spins are paired up in singlet pairs to make a liquid of pair “bonds”; see Fig. 1.

But of course, with exactly one spin at every site, this state is a Mott insulator, not a metal. Such an RVB liquid state is of rare occurrence in real Mott insulators, which usually exhibit either antiferromagnetic long range order as in the cuprates, or possibly have ordered “frozen” arrays of bonds. i.e., valence bond crystals rather than liquids. However, the importance of the RVB liquid was the suggestion that as one doped this state with added electrons or holes, the resulting metal would be a high  $T_c$  superconductor, retaining the singlet pairs but allowing them to carry charge and support supercurrents. The motivation for the pairing would be the antiferromagnetic superexchange of the original Mott insulator.

For over a decade and a half a number of theorists have been trying to implement this suggestion along a bewildering variety of routes. One main avenue has resulted from the proposal by several authors (Kotliar and Liu, 1988; Suzumura *et al.*, 1988; Gros, 1988;

Yokoyama and Shiba, 1988; Affleck *et al.* 1988; Zhang *et al.* 1988), that Anderson's original s-wave BCS be replaced by an exotic, d-wave state. The d-wave approach in the early days was quantitatively carried through by Gros (1989) using variational Monte Carlo methods and by Zhang, Gros, Rice and Shiba (1988) on a simplified model, and using very rough approximation methods. Recently the Gutzwiller-RVB wavefunction approach was revived by Paramakanti, Randeria, and Trivedi (2001; 2003) who used careful numerical methods to calculate many quantities of direct experimental relevance. Their results turn out to correspond remarkably well to the experimental phenomena observed in the cuprates across a very broad spectrum of types of data, a spectrum that was simply not available in 1987-88 when the original work was done. It may be because of this absence of data at the time that the original paper was for so long not followed up.

All of this work relies on one basic assumption, an assumption which has gone unquestioned among a large fraction of those theorists concerned with this problem, from the beginning. This is the assumption that the physics of these materials is dominated by the strong repulsive interactions of a single non-degenerate band of electrons on the  $\text{CuO}_2$  planes, and is specifically not at all similar to that of the conventional BCS superconductors. In the latter the direct electron interactions are heavily screened, and the lattice vibrations play the dominant role. We feel that the demonstration of d-wave superconductivity in particular makes phonons as major players difficult to support, even though there are some notable physicists, such as Mott, Friedel, Muller, and Abrikosov, who disagree. The phonon mechanisms are local in space, extended in time, making the dynamic screening mechanism emphasized by Schrieffer and Anderson relevant and leading to s-wave pairing (Schrieffer, 1964). This mechanism works better the more electrons there are per unit cell, and fails for monovalent metals. D-wave pairing, on the other hand, is essentially non-local in space and deals with strong repulsions by conventional space avoidance, as suggested by Anderson and Morel (1961) and by Kohn and Luttinger (1965). Phonon interactions, especially via optical phonons, are local and cannot easily lead to higher angular momentum pairing.

It has been argued that certain specific phonons in the presence of strong correlation can enhance d-wave pairing (Shen *et al.*, 2002). However, such couplings are reduced for small doping by the renormalization factor  $g_t^2$  as discussed later in the article. Even more cogent is the fact that, as we shall see, the attractive potential for d-wave pairing is more than adequate without phonons, and even if they contribute positively to it the effect will

be minor. (It has been argued that in some cases the contribution is negative (Anderson 2002)).

Furthermore, it is now known that the energy gap in high  $T_c$  superconductors is much larger than predicted by BCS theory, and can reach a value of order 50 meV. This is comparable to or exceeds typical phonon frequencies, making it obvious that a phonon cannot be the key player.

We prefer not to further burden this discussion with the equally strong chemical, angle resolved photoemission spectra and optical evidence for using only a single band; this subject is treated in, for instance, the paper by Zhang and Rice (1988), or in Anderson's book (1997).

These considerations suggested the use of models where the strong repulsive correlations are emphasized, specifically the Hubbard model, which takes as the only interaction a strong on-site repulsion. The Hubbard model can be transformed by a perturbative canonical transformation (Kohn 1964) into a block-diagonal form in which double occupancy is excluded, and replaced by an exchange interaction between neighboring sites as pointed out early on by Gros, Joynt and Rice (1986). This procedure converges well for sufficiently strong on-site interaction  $U$ , but presumably fails at the critical  $U$  for the Mott transition; the singly-occupied "undoped" case is unquestionably a Mott insulator in the cuprates and this transformation ipso facto works. The further simplified  $t - J$  model is often used; for refined calculations it has been argued (Paramekanti *et al.*, 2001; 2003) that this simplification may be too great, but for the semi-quantitative purposes of this article we will at least think in terms of that model.

The Mott insulator based theory for the cuprates has been expressed in a variety of forms other than straightforward Gutzwiller projection and we do not claim any great overall superiority for our method. Early on, Baskaran, Zou and Anderson (1987) (see also, Anderson (1987b) and Zou and Anderson (1988)) introduced the ideas of spin-charge separation (see also Kivelson, Rokhsar and Sethna, 1987) and of slave bosons and gauge fields introduced to implement the Gutzwiller constraint, and quite a number of authors (Ruckenstein *et al.*, 1987, Weng *et al.*, 1996) have followed this direction, most notably Baskaran (Anderson, Baskaran, Zou and Hsu, 1987; Baskaran and Anderson, 1988), Fukuyama (Suzumura *et al.*, 1988; Fukuyama, 1992) Kotliar (Kotliar and Liu, 1988), Ioffe and Larkin (1989) and a series of publications by P. A. Lee and co-workers (Nagaosa and Lee, 1990; Wen and Lee, 1996). A related method is the Schwinger boson, slave fermion technique which has been discussed

by a number of authors (Weigmann, 1988; Shraiman and Siggia, 1989; Lee, 1989). Undoubtedly for discussions of the precise nature of the phase transition and of the complicated mix of phenomena such as the pseudogap regime which occur above  $T_c$  these theories will be essential, but we here focus on properties of the ground state and of low-lying excitations, which by good fortune includes the basic physics of  $T_c$ . We feel that what we can calculate indicates the correctness of the fundamental Mott-based picture in such a way as to support the further effort needed to work out these theories.

### The Method

Starting from the Hubbard Hamiltonian (which may be generalized in various ways without affecting the following arguments)

$$H = T + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

where  $T$  is the kinetic energy. We suppose that there is a canonical transformation  $e^{iS}$  which eliminates  $U$  from the block which contains no states with  $n_{i\uparrow} + n_{i\downarrow} = 2$ , and which presumably contains all the low-lying eigenstates and thus the ground state; there are no matrix elements of the transformed Hamiltonian connecting these to doubly-occupied states. Thus

$$e^{iS} H e^{-iS} = H_{t-J} = P T P + J \sum_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \quad (2)$$

Here  $P = \prod_i (1 - n_{i\uparrow} n_{i\downarrow})$  is the Gutzwiller projection operator, which projects out double occupancy. The kinetic energy  $T$  is actually modified to include a 3-site hopping term, which we will neglect here, realizing that our Fermi surface and velocity are heuristically adjusted in any case. The low-lying eigenstates of this Hamiltonian are necessarily of the form  $P |\Phi\rangle$ , where  $|\Phi\rangle$  is a completely general state of the appropriate number of electrons in the band. Thus Gutzwiller projection is necessary if one is to use the canonical transformation to eliminate  $U$ .

We make the fundamental assumption that the correct  $|\Phi\rangle$  may be approximated by a general product wave function of Hartree-Fock-BCS type, so that

$$P |\Phi\rangle = P \prod_{\vec{k}} \left( u_{\vec{k}} + v_{\vec{k}} c_{\vec{k}\uparrow}^\dagger c_{-\vec{k}\downarrow}^\dagger \right) |0\rangle. \quad (3)$$

In fact, one can simply rewrite  $P|\Phi\rangle$  for a fixed number of electrons ( $N$ ) as

$$P|\Phi\rangle = P \left[ \sum_{\vec{r}, \vec{r}'} \varphi(\vec{r} - \vec{r}') c_{\vec{r}\uparrow}^\dagger c_{\vec{r}'\downarrow}^\dagger \right]^{N/2} |0\rangle, \quad (4)$$

where  $\varphi(\vec{r} - \vec{r}')$  is the Fourier transform of  $v_{\vec{k}}/u_{\vec{k}}$ . This real space wavefunction may be visualized in terms of a linear superposition of configurations consisting of singlet pairs and vacancies with no double occupancy. Each valence bond is the snapshot of a preformed pair of electrons, while the vacancies correspond to doped holes; see Fig. 1.

In the conventional theory of metals, the Hartree-Fock BCS ansatz turns out to be justifiable as the first step in a perturbation series which preserves many of the properties of the non-interacting particle model, relying on adiabatic continuation arguments in a qualitative way. We see no reason why it cannot be equally effective in this case. We emphasize that we are *not* approximating the actual wavefunction  $e^{iS}P|\Phi\rangle$  as a product function, but the function to be projected,  $|\Phi\rangle$ , and we are searching for an effective mean field Hamiltonian which determines this function. The projected Hamiltonian is a hermitian operator which acts on this function, in complete analogy to an ordinary interacting Hamiltonian, and we may treat it in mean field theory if we so desire. We accept that the wave functions are enormously underspecified by this Hamiltonian, but in fact that makes it more likely, rather than less, that a simple product will be a fairly good approximation.

The philosophy of this method is analogous to that used by BCS for superconductivity, and by Laughlin for the fractional quantum Hall effect: simply guess a wave function. Is there any better way to solve a non-perturbative many-body problem?

While the main focus of this paper is on the physical properties of the projected wavefunction, we briefly mention what is known about its energy as a variational state for the  $t$ - $J$  model (Hsu, 1990; Yokoyama and Ogata, 1996). At half filling, the projected  $d$ -wave BCS state does remarkably well, with an energy of  $-0.3199 J$  per bond compared with the best estimate of  $-0.3346 J$  (Trivedi and Ceperley, 1989). Interestingly, projecting the BCS state does just about as well as projecting a spin density wave state which has long range order ( $-0.3206 J$ ). This state also has an ordering moment which is much too large (0.9). The best trial state is obtained by combining the two, which achieves an energy of  $-0.3322 J$  and a staggered magnetization of 0.75, which is close to the best numerical estimates. Upon doping, AF co-exists with  $d$ -wave superconductivity up to  $x = 0.11$  for

$J/t = 0.3$  (Giamarchii and Lhuillier, 1991; Himeda and Ogata, 1999; Ogata and Himeda, 2003). This is in disagreement with experiments which show that AF order is destroyed beyond 3 to 5% doping. However, more recent work which combines Gutzwiller projection with a Jastrow factor finds that the energy of the  $d$ -wave superconductor is considerably lowered and Sorella *et al.* (2002a) have presented numerical evidence that the ground state of the 2D  $t - J$  model has  $d$ -wave superconducting long range order over a wide doping range; see also the work of Maier *et al.* (2000) on the Hubbard model. This issue is controversial (Zhang *et al.*, 1997; Shih *et al.*, 1998; White and Scalapino 1999; Lee *et al.*, 2002; Sorella *et al.*, 2002b) and not easy to settle because of technical difficulties with fermion simulations. Nevertheless, the most important point from our perspective is that the superconducting ground state is energetically highly competitive over a broad range of doping, and thus the variational state whose properties we are describing in this paper will be a good approximation to the ground state of a model close to the  $t - J$  model.

## Mean Field Theory

In evaluating the energy of these wave functions Zhang *et al.* (1988) used a rough approximation first proposed by Gutzwiller (1963) which involves assuming complete statistical independence of the populations on the sites; see also Vollhardt's (1984) review for a clear explanation. This is not too bad, since the one-particle states are defined as momentum eigenstates, but not perfect, as pointed out by Zhang *et al.* (1988) by comparing with Monte Carlo calculations for a particular case. But in order to understand the results qualitatively we will follow this simple procedure here. The evaluations in Paramekanti *et al.* (2001; 2003) are carried out without this approximation.

In the product wave function  $|\Phi\rangle$  with the chemical potential fixed so that there are, on average,  $1 - x$  electrons per site, with  $x$  the fraction of holes, the states with 0, 1 and 2 electrons on a given site have probabilities  $(1 + x)^2/4$ ,  $(1 - x^2)/2$  and  $(1 - x)^2/4$ , respectively. The corresponding numbers after projection are  $x$ ,  $1 - x$  and 0. Thus the relative number of pairs of sites on which a hole can hop from one to the other may be calculated to be  $g_t = 2x/(1 + x)$ , while the relative number of pairs of sites which can experience spin exchange is  $g_S = 4/(1 + x)^2$ . These are taken to be the renormalization factors for the kinetic energy and superexchange terms in the  $t - J$  Hamiltonian; that is, the Hubbard Hamiltonian is first transformed into the  $t - J$  Hamiltonian, and then its effect on



the actual product wave-function is estimated in this way. More accurate estimates could be calculated using Monte-Carlo methods, and the extra correlated hopping terms could be included, but we actually doubt if the latter change things much.

Essentially, in this approximation all terms of the nature of spin interactions have a single renormalization factor,  $g_S$  while all terms in the kinetic energy are renormalized by a factor  $g_t$ . The ratio of these is quite large, being about a factor of 8 even at 20% doping. Thus this method results in an approximate (or quantitative) spin-charge separation, which is as effective for experimental purposes (Anderson, 2000) as the qualitative one of more radical theories. In reality, the wave function will have some correlations of occupancy, but these are higher order in  $x$  – in the limit of small  $x$  the holes move independently. Also in reality the dispersion relation may not scale perfectly, but again we do not think this is a very large effect.

Thus the renormalized Hamiltonian simply takes the form of a modified  $t - J$  Hamiltonian,

$$H_{eff} = g_t T + g_S J \sum \mathbf{S}_i \cdot \mathbf{S}_j \quad (5)$$

(Again, we ignore the three-site hopping terms). Zhang *et al.* (1988) showed that if we treat this within Hartree-Fock-BCS approximation, we arrive at a modified BCS gap equation. The kinetic energy is renormalized downwards, and the interaction term  $\mathbf{S}_i \cdot \mathbf{S}_j$ , which can be written in the form of four fermion operators  $c^\dagger c^\dagger c c$  alike, can be factorized in two ways. It can be factorized in such a way that it leads to an anomalous self-energy term of the form,  $J \langle c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \rangle c_{j\downarrow} c_{i\uparrow} + h.c.$ , which will lead to a gap; or it can be factorized in such a way as to give a Fock exchange self-energy  $\chi_{ij} = \langle c_{i\sigma}^\dagger c_{j\sigma} \rangle$ , with  $\chi_{\vec{k}}$  its Fourier transform, which is of nearly the same form as the kinetic energy, and adds to it. Exhaustive study of this form of wave function has led to the conclusion that the optimum gap equation solution is a d-wave of symmetry  $d_{x^2-y^2}$  (Kotliar and Liu, 1988; Suzumura *et al.*, 1988; Gros 1988; Yokoyama and Shiba, 1988; Affleck *et al.*, 1988; Zhang *et al.*, 1988). The outcome is a pair of coupled equations, one for the anomalous self-energy and the other for the effective particle kinetic energy:

$$\Delta_{\vec{k}} = \frac{3}{4} g_S J \sum_{\vec{k}'} \gamma_{\vec{k}-\vec{k}'} \frac{\Delta_{\vec{k}'}}{2E_{\vec{k}'}} \quad (6)$$

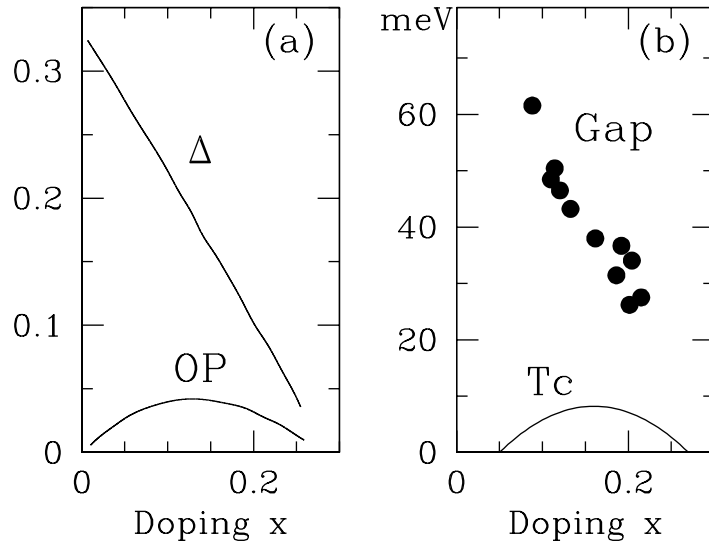


FIG. 2: (a) The amplitude of the (dimensionless) d-wave gap  $\Delta$  (called  $\tilde{\Delta}$  in Zhang *et al.*, (1988)) and the superconducting order parameter (OP) as functions of hole doping  $x$  in the  $t - J$  model for  $J/t = 0.2$  calculated in the renormalized mean field theory of Zhang *et al.* (1988). (b) The spectral gap (in meV) for Bi2212 as measured by ARPES (Campuzano *et al.*, 1999) and  $T_c$  as a function of doping. The  $x$  values for the measured  $T_c$  were obtained by using the empirical relation  $T_c/T_c^{\max} = 1 - 82.6(x - 0.16)^2$  (Presland *et al.*, 1991) with  $T_c^{\max} = 95\text{K}$ .

which is an orthodox BCS equation, and

$$\chi_{\vec{k}} = -\frac{3}{4}g_s J \sum_{\vec{k}'} \gamma_{\vec{k}-\vec{k}'} \frac{\xi_{\vec{k}'}}{2E_{\vec{k}'}}. \quad (7)$$

Here  $\xi_{\vec{k}} = g_t \varepsilon_{\vec{k}} - \mu - \chi_{\vec{k}}$ , and  $\varepsilon_{\vec{k}}$  is the band energy, and  $\mu$  is an effective chemical potential,  $\gamma_{\vec{k}}$  is the Fourier transform of the exchange interaction, initially simply the nearest neighbor result

$$\gamma_{\vec{k}} = 2(\cos k_x + \cos k_y) \quad (8)$$

and  $\mu$  is set to give the right number of electrons  $N_e$ , which commutes with the projection operator.  $E_{\vec{k}} = \sqrt{\xi_{\vec{k}}^2 + \Delta_{\vec{k}}^2}$ , which has the same form as in the BCS theory.

Zhang *et al.* (1988) gave the result of solving these gap equations in the oversimplified case where only nearest neighbor hopping is allowed, and we reproduce their figure here as

Fig. 2(a). We see that  $\Delta$ , the magnitude of the d-wave symmetry gap, falls almost linearly with  $x$  from a number of order  $J$ , and vanishes around  $x = 0.3$  for  $J/t = 0.2$ . The more realistic model of Paramekanti *et al.* (2001; 2003) gives a similar result. We presume that this quantity represents the pseudogap, which is known to vary experimentally in this way. (A calculation by an entirely different method (Anderson, 2001) gave the same result.)

Also plotted on this graph is the physical amplitude of the order parameter (OP)  $\Delta_{SC} = \langle c_{i\uparrow}c_{j\downarrow} \rangle$ , which is supposed to renormalize with  $g_t$ . This is actually true but the argument is more subtle than that given in Zhang *et al.* (1988). It is necessary to recognize that the two states connected by this operator contain different numbers of particles. The simpler argument is to realize, as was remarked in Paramekanti *et al.* (2001; 2003) that the physically real quantity is the off diagonal long range order eigenvalue of the density matrix, which is the square root of the product of  $\langle c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger c_{i+l\uparrow} c_{j+l\downarrow} \rangle$  for large distance  $l$  which is renormalized by a factor of  $g_t^2$ . This quantity in this early graph, and in the more accurate work of Paramekanti *et al.* (2001; 2003), bears a striking resemblance to the variation of  $T_c$  with doping, and was by implication suggested to be a measure of  $T_c$ ; but it was not until 1997 that the Wen-Lee theory for the renormalization of  $T_c$  (to be discussed below) appeared, and it is not quite true that the order parameter and  $T_c$  are identical.

Before turning to  $T_c$ , we briefly mention results on nodal quasiparticles (“nodons”) obtained from our approach. These are the important low-lying excitations in the superconducting state and dominate low temperature thermodynamics, transport and response functions (Hardy *et al.*, 1993; Krishana *et al.*, 1995; Zhang *et al.*, 2000; Chiao *et al.*, 2000), in addition to controlling  $T_c$  (see below). The Gutzwiller projected d-wave superconducting ground state supports sharp nodal quasiparticle excitations (Paramekanti *et al.*, 2001; 2003) whose coherent spectral weight  $Z$  goes to zero as  $g_t$  but whose Fermi velocity  $v_F$  is very weakly doping dependent and remains non-zero as the hole doping  $x \rightarrow 0$ . These results imply that the real part of the self-energy  $\Sigma'(k, \omega)$  for the gapless nodal quasiparticles has singular energy and momentum dependences:  $Z \sim x$  means that  $|\partial\Sigma'/\partial\omega| \sim 1/x$  which in turn implies  $\partial\Sigma'/\partial k \sim 1/x$  in order to have a non-zero nodal  $v_F$ . These predictions are in very good agreement with recent ARPES data as shown in Fig. 3, and in addition also explain the remarkable doping dependence of the “high energy” dispersion of the nodal quasiparticles, above the so-called kink scale (Lanzara *et al.*, 2000), which is found to be dominated by  $\partial\Sigma'/\partial k$  (Randeria *et al.*, 2003).

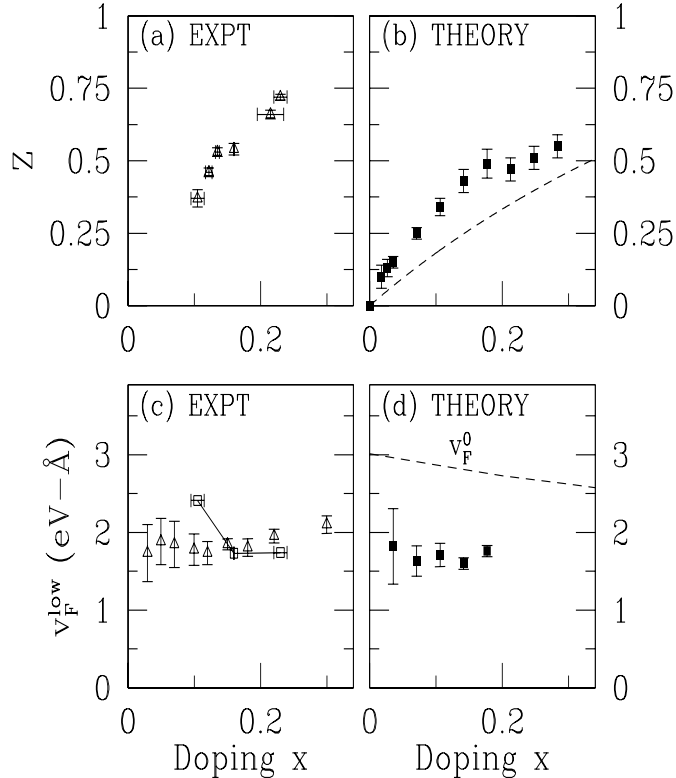


FIG. 3: (a): Doping dependence of the nodal quasiparticle weight  $Z$  in Bi2212 extracted from ARPES data (Johnson *et al.* 2001) with  $x$  calculated from sample  $T_c$  using the empirical formula of Presland *et al.* (1991) with  $T_c^{\text{max}} = 91\text{K}$ . (b):  $Z(x)$  predicted from the variational Monte Carlo calculation of Paramekanti *et al.* (2001). The dashed line is the Gutzwiller approximation result  $Z = 2x/(1+x)$ . (c): The low energy nodal Fermi velocity  $v_F^{\text{low}}$  from ARPES data in Bi2212 (open squares from Johnson *et al.* (2001)) and LSCO (open triangles from Zhou *et al.* (2003)) is nearly doping independent. (d): Predicted renormalized  $v_F^{\text{low}}$  from Paramekanti *et al.* (2001) as a function of  $x$ ; the dashed line is the bare band structure Fermi velocity  $v_F^0$ . This figure is adapted from Randeria *et al.* (2003).

### Transition Temperature

It is also a consequence of our theory that the electromagnetic response function  $\rho_s$  (the phase stiffness, or more conventionally  $1/\lambda^2$ , with  $\lambda$  the penetration depth) renormalizes with  $g_t$ , as does the kinetic energy. In 1997 Lee and Wen (1997) pointed out that the rate of linear decrease of  $\rho_s$  with temperature, which was the earliest experimental evidence for d-wave symmetry (Hardy *et al.*, 1993), maintains its magnitude independently of doping. They argue that the decrease is caused by the thermal excitation of quasiparticles near the

nodes and is an electromagnetic response function of these quasiparticles. In the BCS paper it is pointed out that the electromagnetic response consists of two parts, the diamagnetic current which is the acceleration in the field, and the paramagnetic current, which is a perturbative response of the excited quasiparticles and exactly cancels the diamagnetic term in the normal state (Schrieffer, 1964). The number of these quasiparticles in a d-wave state is only proportional to  $T^2$ , because the density of states is only linear in energy. But the amount of decrease of  $\rho_s$  per quasiparticle is inversely proportional to its energy, canceling one factor of  $T$ . The key to their argument is the assumption that the current carried by each quasiparticle is  $ev_F$ . This is the case in BCS theory, where the quasiparticle does not carry a definite charge because it is a superposition of an electron and hole, but each of the partners carries the same current  $ev_F$ . Later it was pointed out by Millis *et al.* (1998) (see also Paramakanti and Randeria (2002)) that there can be a Fermi liquid renormalization of this current to  $\alpha ev_F$  where  $\alpha$  is a Fermi liquid parameter inherited from the normal state. The slope of  $\rho_s$  vs  $T$  is now proportional to  $\alpha^2$  and we assume that  $\alpha$  is of order unity and relatively insensitive to doping. Thus  $\rho_s$  at  $T = 0$  decreases proportionally to doping, yet its rate of decrease with temperature does not vanish with  $x$ , but instead remains relatively constant. The decrease of  $\rho_s$  to zero is considered by these authors to determine  $T_c$ . At  $T_c$  the system loses phase coherence, but continues to have an energy gap over much of the Fermi surface for small  $x$ . The insensitivity of the linear  $T$  slope in  $\rho_s(T)$  to doping was experimentally demonstrated by Lemberger and co-workers (Boyce *et al.*, 2000; Stajic *et al.*, 2003) and verifies our assumption.

As the quasiparticles reduce  $\rho_s$ , eventually there will develop thermally generated vortices (in truly two-dimensional systems like LSCO and Bi2212) and the actual phase transition takes place as a Kosterlitz-Thouless (K-T) type of phenomenon (Corson *et al.*; 1999) The notion that a small  $\rho_s$  would lead to strong phase fluctuations which determine  $T_c$  was introduced by Emery and Kivelson (1995) but we must recognize that the  $\rho_s$  which controls the K-T transition is not  $\rho_s(T = 0)$  but the  $\rho_s(T)$  which is greatly reduced by quasiparticle excitations. By combining these effects, the decrease of  $\rho_s(T)$  becomes faster than linear, and eventually infinitely steep. But this happens only quite near to  $T_c$ , because the K-T  $\rho_s$  is relatively low; thus the quasiparticle mechanism gives us a good estimate of  $T_c$ , as was pointed out by Lee and Wen, and fits various empirically proposed relationships (Uemura *et al.*, 1989). In materials such as YBCO which are more three-dimensional, the transition

will be more conventional but is still mediated by phase fluctuations near  $T_c$ , as of course it is in ordinary superconductors but not over as broad a critical range.

The Lee-Wen mechanism of  $T_c$  described above is relevant for the underdoped side of the phase diagram where it offers a natural explanation for  $T_c \sim \rho_s(0)$  and holds all the way up to optimality. On the overdoped side of the phase diagram,  $\rho_s(T)$  continues to be linearly suppressed in temperature due to thermally excited quasiparticles, but now the stiffness corresponding to  $\rho_s(0)$  is much larger than the energy gap. Thus superconductivity is lost by gap collapse and  $T_c$  would be expected to scale like the gap for overdoped systems, as in conventional BCS theory.

## Discussion Of Results

The correspondences between the results of our mean field theory and the very unusual experimental observations on the high  $T_c$  cuprate superconductors are so striking that it is hard to credit that they have had so little general notice, especially considering the fact that many of them constituted predictions made in 1988 before the experimental situation became clear, sometimes many years before. The d-wave nature of the energy gap (Kotliar and Liu 1988; Suzumura *et al.* 1988; Gros 1988; Yokoyama and Shiba, 1988) confirmed only in 1993-94 (Wollmann *et al.*, 1993; Tsuei *et al.*, 1994), is the most striking. The d-wave pairing symmetry was also predicted by the “spin fluctuation theory” based on a more orthodox structure (Bickers, Scalapino and Scalettar, 1987; Monthoux, Balatsky and Pines, 1991). This follows earlier predictions of d-wave superconductivity in models with strong repulsion in connection with the heavy fermions (Hirsch, 1985; Miyake, Schmitt-Rink and Varma, 1986). We emphasize that our theory, though spin-based, is by construction not a spin-fluctuation theory, since the latter is based on Fermi liquid theory. Such a Fermi-liquid based approach may be relevant to the overdoped side of the cuprate phase diagram, but is unable to deal with the unusual properties in the vicinity of the Mott insulator.

A second prediction of the RVB approach is the large energy scale represented by  $\Delta$ , which was first observed as a spin gap by NMR at the end of the eighties (Alloul *et al.* 1989; Walstedt and Warren 1990; Takigawa *et al.* 1991). Its significance was only slowly recognized by the mid-nineties and it has come to be called the pseudogap. It merges with the superconducting gap below  $T_c$ , but is visible in many different kinds of density of states measurements far above  $T_c$  (Ding *et al.* 1996; Loesser *et al.* 1996; Ch. Renner *et*

*al.* 1998). For well underdoped samples it expunges the Fermi surface in the anti-nodal direction (Norman *et al.*, 1998). Its value has been studied in detail by Tallon and Loram (2000), and their numbers are in striking agreement with the calculations of Zhang *et al.* (1988) or Paramakanti *et al.* (2001; 2003), if we leave aside their claim that it falls to zero in the midst of the superconducting range. The pseudogap is often associated roughly with a temperature scale “ $T^*$ ” below which its effects are first felt. Of course, in a rigorous sense our mean field theory is a theory of the superconducting phase at low temperatures, but the pseudogap appears both in the spectra obtained at low temperature as well as in the “mysterious” pseudogap state above  $T_c$ .

The effects of the renormalization  $g_t$  on  $\rho_s$  and on the Drude weight, which was shown by Sawatzky and coworkers (Eskes *et al.*, 1991; Tajima *et al.*, 1990) to be renormalized with precisely the factor  $2x$ , is a natural consequence of the RVB based theories, including the mean field theory described here.

One important observation also postdated the original paper: that the Green’s function of the quasiparticles in the superconducting state contains a sharp “coherence peak” at the quasiparticle energy on top of a very broad incoherent spectrum, and ARPES experiments (Feng *et al.*, 2000; Ding *et al.*, 2001) have estimated that the amplitude of that peak is proportional to  $2x$ .

One result has not been previously mentioned in the literature. The renormalization  $g_t$  applies to any term in the Hamiltonian which is a one-electron energy. Therefore matrix elements for ordinary time-reverse invariant scattering are reduced by a factor of about  $2x$ , and their squares, which enter into such physical effects as the predicted reduction in  $T_c$ , or into resistivity, are reduced by more than an order of magnitude. At the same time the effects of magnetic scattering are relatively enhanced. Thus the effects of impurities on high  $T_c$  superconductivity – the notorious contrast of the effects of Zn or Ni substitutions in the plane relative to non-magnetic doping impurities which lie off the plane, (Fukuzumi *et al.*, 1996) – are explained without having any mysterious spin-charge separation in the formal sense. The same reduction will, on the whole, apply to the effects of electron-phonon scattering which, like ordinary impurity scattering, seem to have little influence on the resistivity. The electron-phonon interaction, which enters into ordinary BCS superconductivity, is renormalized relative to the spin interaction by the factor  $g_t^2/g_S \sim x^2$  and seems unlikely to play a role.

Finally, a word as to the Nernst effect experiments of Ong and coworkers (Xu *et al.*, 2000; Ong and Wang, 2003) which measure the electric field transverse to an applied thermal gradient in the presence of a perpendicular magnetic field. The Nernst signal is expected to be dominated by the motion of vortices, and the results on two dimensional materials are very consistent with expectations for a generalization of the Kosterlitz-Thouless type of transition. What is seen is a Nernst signal at and below  $T_c$  varying at low magnetic field  $B$  as  $B \ln B$  (Ong and Wang, 2003) indicating that the underlying  $\rho_s$  of the effective Ginsburg-Landau free energy does not vanish at  $T_c$ ; the  $\ln B$  variation, giving an infinite slope, follows from thermal proliferation of large vortices whose energies vary as  $\rho_s \ln B$ . As  $B$  is increased, however, the signal does not drop to zero until a very large  $B$  is reached, indicating a retention of phase stiffness at short length scales long after superconducting long-range order has disappeared. We believe that this is a natural and probably calculable effect. But with increasing temperature the Nernst effect disappears well below  $T^*$ , at least for low fields. In this region we are well out of the region of applicability of mean field theory, and expect very large fluctuation effects for which we have no controlled theory.

An additional experimental phenomenon which, we think, supports the essential validity of a projected wave function is the particle-hole asymmetry of the tunneling conductance as a function of voltage. We will discuss single-particle excited states and tunneling asymmetry in a forthcoming paper (Anderson *et al.*, 2003)

## Conclusion

In broad outline, our basic assumptions as to the physics of the cuprates, together with a mean field theory which is little less manageable than BCS theory, seem to give a remarkably complete picture of the unusual nature of the superconducting state. The RVB state is still a pairing state between electrons. It has its genesis in the BCS state and is smoothly connected to it, a fact which is made clear in the recent studies of a partially projected BCS state (Laughlin, 2002; Zhang, 2003). Furthermore, its low lying excitations are well defined quasiparticles which dominate the low temperature physics. Thus the RVB state is in some ways rather conventional. What is unusual is the reduction of the superfluid density and the quasiparticle spectral weight. With increasing degrees of projection, the state evolves from pairing of quasiparticles to one which is better understood as a spin singlet formation with coherent hole motion. This evolution has the following dramatic consequence. The BCS



pairing is driven by a gain in the attractive potential at the expense of kinetic energy, since the energy gap smears out the Fermi occupation  $n(\vec{k})$ . With projection,  $n(\vec{k})$  is already strongly smeared in the non-Fermi liquid normal state, and superconductivity is instead stabilized by a gain in kinetic energy due to coherent hole motion. This picture has been verified by experiments which monitor the kinetic energy via the optical sum rule (van der Marel *et al.*, 2003)

Why then is the subject so controversial? Aside from purely socio-political reasons, there is a real difficulty: the proliferation of nearby alternative states of different symmetry. Here we mention a number of possibilities that are actively being considered. One important issue is the evolution to the antiferromagnet at very low doping. On general principles (Baskaran, 2000; Anderson and Baskaran, 2001), mesoscopically inhomogeneous states (“stripes”) are likely to be stable at low doping on some scale. They show up in some numerical calculations (White and Scalapino, 1999) and a few of the cuprates show indications of them as static (Tranquada *et al.*, 1995) or dynamical excitations (see Stock *et al.*, 2004). While static stripes are undoubtedly detrimental to superconductivity, there have been arguments that dynamical stripes may be the source of pairing (see Carlson *et al.*, 2004). We note that in this scenario, the pairing originates from the ladder structure of the hole-free part of the stripe which also has its origin in RVB physics. Given the success of the uniform projected wavefunction, we find these more complex scenarios neither necessary nor sufficient for the intermediate doping range.

A second class of competing states has its origin in the  $SU(2)$  gauge symmetry first identified for the projected wavefunction at half-filling. The states of an undoped RVB, or in fact any state of the Mott insulator, can be represented by an enormous number of wave functions before projection; in fact, as pointed out by Affleck *et al.* (1988) (see also Anderson (1987b) and Zhang *et al.* (1988)), it has an  $SU(2)$  gauge symmetry. In the undoped state, with exactly one electron per site, the presence of an up spin is equivalent to the absence of a down spin and vice versa, thus permitting independent  $SU(2)$  rotations at each site. This degeneracy in the representation of the wave function does not imply any true degeneracy, it is merely the consequence of our using an underdetermined representation.

When we add holes, this gauge freedom gradually becomes physical, which we experience as the development of a stiffness to phase fluctuations which grows from zero proportionally to  $x$ . The fluctuations can actually take place in a larger space of gauge degrees of freedom

which we can represent in terms of staggered flux phases, etc. (Affleck and Marston, 1988) as possible Hartree-Fock states, but we expect that these are higher energy than the superconducting state for the interesting values of  $x$ . However, the energy difference is small for small  $x$ , and Wen and Lee (1996) have proposed that in the underdoped region  $SU(2)$  rotations which connect fluctuations of staggered flux states and  $d$ -wave superconductivity may play a role in explaining the pseudogap phenomenon. Remarkably, orbital current correlations which decay rather slowly as power law have been seen in projected  $d$ -wave wavefunctions (Ivanov *et al.*, 2000). These fluctuations are very natural in the  $SU(2)$  gauge theory but are otherwise unexpected. In a related development, a static orbital current state, called  $d$ -density wave, has been proposed to describe the pseudogap on phenomenological grounds (Chakravarty *et al.*, 2001).

In this review we have focused our attention on the ground state and low-lying excitations in the underdoped region. Due to the multitude of competing states mentioned above, much work remains before a full understanding of the pseudogap is achieved. The situation becomes even worse for doping to the right of the  $T^*$  crossover line, commonly called the “strange metal” phase. Here one sees highly anomalous transport properties such as the linear resistivity which played such an important role in early thinking. While the RVB theory leads naturally to a crossover from pseudogap to strange metal and to Fermi liquid as one increases the doping at a temperature above the optimal  $T_c$ , the ideas presented here are no help in understanding the breakdown of Fermi liquid behavior in the strange metal. Instead of a smooth crossover, many workers ascribe the anomalous behavior to a quantum critical point which lies in the middle of the superconducting dome (Varma, 1997; Tallon and Loram, 2000; Varma, 2003). We simply remark that the quantum critical point, if it exists, is different from any previous examples in that there is no sign of a diverging correlation length scale in any physical observable, and it is difficult to draw lessons from past experience even phenomenologically.

Finally, what about phonons? Of course there is some coupling to optical phonons, which will influence both the phonons themselves – an influence which will change sign with the phonon wave vector  $Q$ , because of coherence factors – and the dispersion of quasiparticles. But as remarked, the net effect of an optical phonon on  $d$ -wave superconductivity will tend to cancel out over the Brillouin zone. It certainly will not play a controlling role in a system so dominated by Coulomb repulsion. In any case, phonon effects on electron self-energies

will tend to be renormalized downwards by the square of  $g_t$ , as we pointed out before.

We close by remarking that great strides have been made in the discovery of unconventional superconductors since 1986. Today, non- $s$ -wave pairing states are almost commonplace in heavy fermions, organic superconductors, and in transition metal oxides. Even time reversal symmetry is not sacrosanct (see the review on  $\text{Sr}_2\text{RuO}_4$  by MacKenzie and Maeno, 2003). The discovery of high  $T_c$  has opened our eyes to the possibility that superconductivity is an excellent choice as the ground state of a strongly correlated system. This may be the most important message to be learned from this remarkable discovery.

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