The physics behind high-temperature superconducting cuprates: the 'plain vanilla' version of RVB

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TOPICAL REVIEW

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 wavefunction as an approximate ground state. Recent work by Paramekanti *et al* 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 *et al* 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, is responsible for d-wave superconductivity in the cuprates.

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1. 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 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 favours 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 favour singlet formation rather than the classically ordered Néel state.

In 1986 the high T_c cuprates were discovered (Bednorz and Müller 1986), and it was soon realized (Anderson 1987a) that the operative element in their electronic structures was the square planar CuO_2 lattice. In the 'undoped' condition, where the Cu is stoichiometrically Cu^{2+}, the 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 paired superconducting state; then the spins are paired up in singlet pairs to make a liquid of pair 'bonds'; see figure 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.

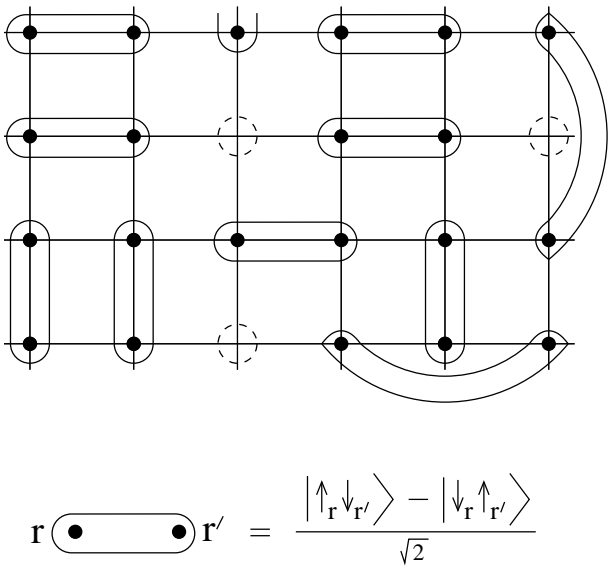

Figure 1. Snapshot of a resonating valence bond (RVB) configuration showing singlet pairs of electrons and, in addition, a fraction x of doped holes. The many-body ground state wavefunction is a linear superposition of such configurations with the spatial dependence of the singlet pairing amplitudes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

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 *et al* (1988) on a simplified model, and using very rough approximation methods. Recently the Gutzwiller-RVB wavefunction approach was revived by Paramekanti *et al* (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 datum, 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 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 *et al*, 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 neighbouring sites as pointed out early on by Gros *et al* (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 *et al* (1987) (see also Anderson 1987b and Zou and Anderson 1988) introduced the ideas of spin–charge separation (see also Kivelson *et al* 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* 1998) have followed this direction, most notably Baskaran (Anderson *et al* 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 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 (Wiegmann 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.

2. The method

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

$$H = T + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{1}$$

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

$$e^{iS} H e^{-iS} = H_{t-J} = PTP + J \sum_{ij} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{2}$$

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 three-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 wavefunction of Hartree–Fock–BCS type, so that

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

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

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

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 figure 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 wavefunctions 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. Similar arguments to those for Koopman's theorem in Hartree–Fock theory tells us that the variational mean field equations will give us approximate single-particle excitation energies.

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 wavefunction. 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 $J/t = 0.3$ (Giamarchi 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 3–5% 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.

3. Mean field theory

In evaluating the energy of these wavefunctions 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 wavefunction $|\Phi\rangle$ 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 zero, one and two 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 wavefunction 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 whether 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 eight 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 wavefunction 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,

$$H_{\rm eff} = g_t T + g_S J \sum \mathbf{S}_i \cdot \mathbf{S}_j. \tag{5}$$

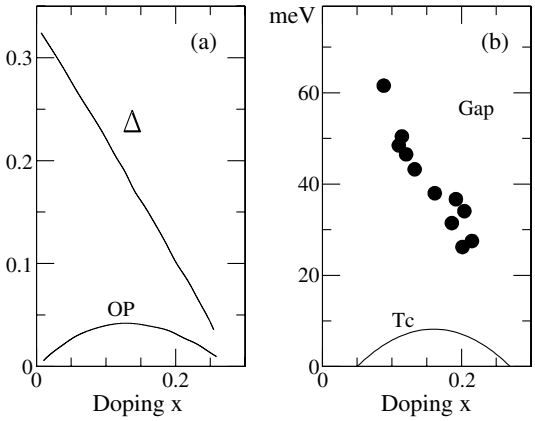

Figure 2. (a) The amplitude of the (dimensionless) d-wave gap Δ (called $\tilde{\Delta}$ in Zhang *et al* (1988)) and the superconducting order parameter (OP) as functions of hole doping x in the t–J model for $J/t = 0.2$ calculated in the renormalized mean field theory of Zhang *et al* (1988). (b) The 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 $T_c^{\max} = 95$ K.

(Again, we ignore the three-site hopping terms.) Zhang *et al* (1988) showed that if we treat this within the 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 $c^\dagger c^\dagger cc$ 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 wavefunction 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:

$$\Delta_{\vec{k}} = \frac{3}{4} g_s J \sum_{\vec{k}} \gamma_{\vec{k}-\vec{k}'} \frac{\Delta_{\vec{k}'}}{2E_{\vec{k}'}} \tag{6}$$

which is an orthodox BCS equation, and

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

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

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

and μ 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 neighbour hopping is allowed, and we reproduce their figure here as figure 2. We see that Δ, 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 by 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 $\langle c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} c_{i+l\uparrow} c_{j+l\downarrow} \rangle$ 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 (Achkir *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 $x \to 0$. 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 figure 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* 2001), which is found to be dominated by $\partial \Sigma'/\partial k$ (Randeria *et al* 2004).

4. Transition temperature

It is also a consequence of our theory that the electromagnetic response function ρ_s (the phase stiffness, or more conventionally $1/\lambda^2$, with λ the penetration depth) renormalizes with g_t, as does the kinetic energy. Lee and Wen (1997) pointed out that the rate of linear decrease of ρ_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 ρ_s per quasiparticle is inversely proportional to its energy, cancelling 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

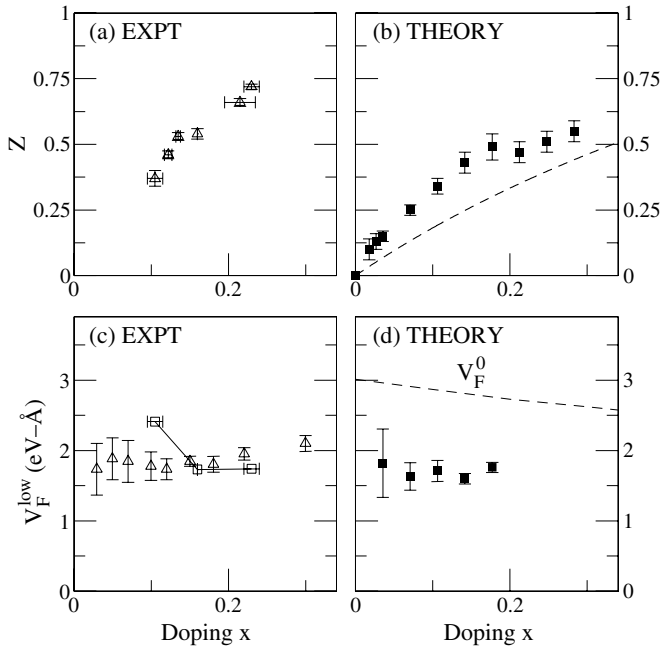

Figure 3. (a) Doping dependence of the nodal quasiparticle weight Z in Bi2212 extracted from ARPES data (Johnson *et al* 2001) with x calculated from sample T_c using the empirical formula of Presland *et al* (1991) with $T_c^{max} = 91$ K. (b) $Z(x)$ predicted from the variational Monte Carlo calculation 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^{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^{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* (2004).

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 Paramekanti and Randeria 2002) that there can be a Fermi liquid renormalization of this current to αev_F where α is a Fermi liquid parameter inherited from the normal state. The slope of ρ_s versus T is now proportional to α^2 and we assume that α is of order unity and relatively insensitive to doping. Thus ρ_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 ρ_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 ρ_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 (KT) type of phenomenon (Corson *et al* 1999). The notion that a small ρ_s would lead to strong phase fluctuations which determine T_c was introduced by Emery and Kivelson (1995) but we must recognize that the ρ_s which controls the KT 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 KT ρ_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.

5. 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 (Wollman *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 *et al* 1987, Monthoux *et al* 1991). This follows earlier predictions of d-wave superconductivity in models with strong repulsion in connection with the heavy fermions (Hirsch 1985, Miyake *et al* 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 Δ, which was first observed as a spin gap by NMR at the end of the 1980s (Alloul *et al* 1989, Walstedt and Warren 1990, Takigawa *et al* 1991). Its significance was only slowly recognized by the mid-1990s 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 state measurement far above T_c (Ding *et al* 1996, Loesser *et al* 1996, 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 Paramekanti *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 and in the 'mysterious' pseudogap state above T_c.

The effects of the renormalization g_t on ρ_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 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 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 ρ_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 wavefunction is the particle–hole asymmetry of the tunnelling conductance as a function of voltage. We will discuss singe-particle excited states and tunnelling asymmetry in a forthcoming paper (Anderson and Ong 2004).

6. 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 on undoped samples which monitor the kinetic energy via the optical sum rule (Molegraaf *et al* 2002).

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 wavefunctions before projection; in fact, as pointed out by Affleck *et al* (1988) (see also Anderson 1987b, 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 wavefunction 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 of 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) and Lee and Wen (2001) 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 a 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 a 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 behaviour in the strange metal. Instead of a smooth crossover, many workers ascribe the anomalous behaviour 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 wavevector 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 transition metal oxides. Even time reversal symmetry is not sacrosanct (see the review on Sr_2RuO_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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