Metallic conduction and superconductivity in the pseudogap phase

Sanjoy K. Sarker

Department of Physics and Astronomy, The University of Alabama, Tuscaloosa, Alabama 35487, USA (Received 10 December 2007; published 20 February 2008)

A simple theory is developed for the hole-doped antiferromagnet on a square lattice using bosonic spinons and fermionic holons. Spinons form a paired state below a temperature T^* , which evolves out of the Mott phase preserving its symmetry. Metallic conduction and *d*-wave superconductivity result from separate, sublattice-preserving, holon hopping processes. In the metal holons form a spinless Fermi liquid, becoming incoherent (confined) above T^* . In the superconductor holons hop as pairs, reducing kinetic energy. At low doping the theory can account for many features of the cuprate superconductors.

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The normal state of a high-temperature superconductor is not a conventional Fermi liquid. Moreover, a highly unusual "pseudogap" appears below a temperature T^* , superconductivity occurring at $T_c < T^*$.^{1,2} Anderson³ argued that the system is a hole-doped Mott insulator, and proposed a resonating-valence-bond (RVB) state, which is expected to continuously evolve from the insulator, and give rise to anomalous metallic behavior and superconductivity. However, this connection has not been firmly established, and is a key problem in high- T_c theory. The relevant model is the t-J model on a square lattice, which describes holes hopping (with amplitude t) in a spin-1/2 antiferromagnet (with exchange interaction J). The undoped insulator is actually in a mixed phase of a two-sublattice antiferromagnet, and an RVB state. It is well described by a mean-field (MF) theory.^{4,5} The RVB state appears as a condensate of singlets, formed by pairing *bosonic* spin-1/2 neutral "spinons." It has a two-sublattice property of its own (see below)-singlet bonds connect spinons residing on opposite sublattices. A fraction of spinons are unpaired, and they condense independently, giving rise to antiferromagnetic (AF) order.

Moving holes are expected to rapidly destroy AF order, creating a metal. The idea is that the RVB condensate would survive up to $T^*(x)$ (x=hole concentration), accounting for the pseudogap. The electron is represented as a composite object: $c_{i\sigma}^{\dagger} = b_{i\sigma}^{\dagger} h_i$, where $b_{i\sigma}^{\dagger}$ creates a spinon of spin σ at the site *i*, and h_i destroys a spinless fermionic holon, subject to the constraint: $h_i^{\dagger}h_i + \sum_{\sigma} b_{i\sigma}^{\dagger}b_{i\sigma} = 1$, which ensures that no site is doubly occupied. Unfortunately, a MF analysis yields a metallic state with spiral order,⁶ which does not have the expected behavior. Apart from magnetic order, the state is characterized by two other distinct order parameters, which separately break the underlying gauge symetry. The first characterizes the RVB condensate. The other, $D_{ij} = \langle h_i^{\dagger} h_i \rangle$, allows holons to hop coherently onto nearest-neighbor (NN) sites (i.e., on to the opposite sublattice). While many other NN metallic states have been constructed using different representations,^{7,8} their stability relative to the spiral state has not been established.

In this Brief Report we derive a different effective Hamiltonian for small x, constrained by the requirement that the RVB condensate evolves with the same symmetry as in the Mott limit. Our analysis is based on two observations. (i) The spiral state is energetically unstable^{9–11} relative to phase

separation, or insulating domain walls, in the entire range of interest $(t/J \sim 3-4, x < 0.25-0.3)$, and must be abandoned. However, the latter states cost too much kinetic energy, and a uniform metal is expected to appear beyond some small x, which can only happen via higher order hopping processes not included at the MF level. (ii) Hence we consider a uniform state, set the NN (e.g. spiral) order parameter $D_{ii}=0$ self-consistently, and show, via a renormalized perturbation theory, that coupling to the condensate gives rise to two higher order, sublattice-preserving, hopping processes. One allows holons to hop coherently within the same sublattice without additional symmetry breaking. The other, discussed earlier,^{12,13} allows a singlet to hop onto a pair of holons, leading to *d*-wave superconductivity. In the metallic state holons form a (spinless) Fermi liquid and become incoherent above T^* . We find that, for small x, the theory can account for many properties of cuprates.

The *t*-*J* Hamiltonian is given by

$$H = -t \sum_{ij,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} - 2J \sum_{ij} A^{\dagger}_{ij} A_{ij}, \qquad (1)$$

where $A_{ij} = \frac{1}{2} [b_{i\uparrow} b_{j\downarrow} - b_{i\downarrow} b_{j\uparrow}]$ destroys a singlet, and *i* and *j* are nearest neighbors. The Hamiltonian has a local gauge symmetry: it preserves the local number of holons plus spinons. It is broken by propagating spinons and holons, and nonlocal pairs.¹⁴ The absence of coherent NN hopping is reminiscent of the results of early single-hole calculations,¹⁵ which led some authors¹⁶ to study an effective sublattice preserving *t'-J* model, without actually deriving it from Eq. (1). We make the same basic assumptions, namely, that incoherent short-range hopping destroys AF order and renormalizes holes. However, the effective Hamiltonian turns out to be different. It corresponds to a short-range valence-bond model,¹⁷ whose structure is determined by the underlying RVB state.

We first examine the symmetry properties in the Mott phase, using the MF solution.⁴ Singlets condense, and is characterized by the order parameter $A_{ij} = \frac{1}{2} \langle [b_{i\uparrow}b_{j\downarrow} - b_{i\downarrow}b_{j\uparrow}] \rangle$. The choice of symmetry

$$A_{ii} = A e^{i(1/2)\mathbf{Q} \cdot (\mathbf{r}_i - \mathbf{r}_j)},\tag{2}$$

with $Q = (\pi, \pi)$, yields the correct state.^{4,5} Equation (2) leads to the spinon "gap" function $\phi(\mathbf{k}) = 4JA(\sin k_x + \sin k_y)$, which determines the properties of the system. Now, since $\phi(\mathbf{k}) = \phi(\mathbf{Q} - \mathbf{k})$, the RVB phase has a two-sublattice property of its own. Consider the pairing function $A_{ij} = \frac{1}{2} \langle [b_{i\uparrow} b_{j\downarrow} - b_{i\downarrow} b_{j\uparrow}] \rangle$ for any two sites *i* and *j*. We find that $A_{ij} = -A_{ij} \cos[\mathbf{Q} \cdot (\mathbf{r}_j - \mathbf{r}_i)]$. We will call this behavior *odd*, i.e., A_{ij} is nonzero only if *i* and *j* are on *opposite* sublattices. Similarly, the hopping function $B_{ij} = \frac{1}{2} \sum_{\sigma} \langle b_{j\sigma}^{\dagger} b_{i\sigma} \rangle$ satisfies $B_{ij} = B_{ij} \cos[\mathbf{Q} \cdot (\mathbf{r}_j - \mathbf{r}_i)]$. Hence, B_{ij} is *even*, i.e., it is nonzero only if *i* and *j* are on the *same* sublattice. These relations hold with or without long-range AF order, and at zero or finite *T*. They are gauge invariant, and have observable consequences. For example, the spin-spin correlation function is given by $S_{sp,ij} = \langle S_i^+ S_j^- \rangle = -|A_{ij}|^2 + |B_{ij}|^2$, which, as expected, alternates in sign.

For x > 0, we consider a uniform state with $(A \neq 0)$, and use a renormalized perturbation expansion to study hopping. To one loop (spinon-holon bubble) order, the theory is similar to that in Refs. 12 and 13 except, now, $\langle h_i^{\dagger} h_i \rangle = 0$, for NN *i* and *j*. If A=0 also, holons (and spinons) can move only a finite distance before returning since gauge symmetry is unbroken. The RVB condensate breaks gauge symmetry, giving rise to additional holon hopping terms, which are derived by integrating out the spinons, and isolating the terms coupled to A_{ii} 's, and setting frequency $\omega = 0.^{12,13}$ For qualtative purposes solving the difficult renormalization problem is not necessary. We simply assume^{13,16} that the incoherent processes disorder the spins, and renormalize the Hamiltonian so that dressed holes hop with an amplitude $t_{eff} \le t$. Destruction of AF order leads to a spinon gap Δ_s , so that A_{ii} and B_{ii} decay as $e^{-r_{ij}/2\xi}$, where $\xi = c_s/2\Delta_s$ is the AF correlation length and c_s is the spinon velocity (see Ref. 5). Then, for small x, we can derive a minimal holon Hamiltonian perturbatively by retaining only the short-range hopping terms (with an appropriate cutoff frequency), as follows. Since holon hopping is accompanied by a spinon backflow, as measured by A_{ij} 's etc., longer-range hopping terms are exponentially suppressed. Hence retaining them should not change the physics qualitatively since they, by continuity, also preserve the underlying symmetry.

When a hole hops from sublattice a to b it breaks a singlet and creates two spinons, costing, say, an energy Ω . There are three ways to remove the energy. First, the hole can hop back, which is confining. The other two lead to coherent motion, as shown below.

(A) One-hole process: Metallic state. The hole hops to another site on sublattice *a*, and the singlet is reconstructed on a different link (Fig. 1). This yields an effective hopping term

$$-\frac{2t_{eff}^2}{\Omega}\sum_{ijl}A_{jl}^*A_{ij}h_l^\dagger h_i(1-h_j^\dagger h_j), \qquad (3)$$

where h^{\dagger} creates a *renormalized* holon. We can replace the gauge invariant density $(1-h_j^{\dagger}h_j)$ by its average value ~ 1 –*x*. Using Eq. (2) for A_{ij} , we obtain the Hamiltonian

$$H_h = \sum_{ij} t_{h,ij} h_j^{\dagger} h_i, \qquad (4)$$

which describes coherent holon propagation within the same



FIG. 1. One hole process. A hole hops from l to j, breaking the singlet (ij) denoted by the solid line. Here i and l are on sublattice a and j is on sublattice b. The hole then hops to i, and the singlet is reconstituted at (jl).

sublattice, the sublattices are connected by a backflow of *singlets*. Here $t_{h,ij} = \pm t_h$ for *i*, *j* next-nearest neighbors along $(1, \pm 1)$; $t_{h,ij} = -t_h/2$ for next-next-nearest neighbors, and $t_h = 4t_{eff}^2 A^2(1-x)/\Omega$. Then the holon energy is

$$\boldsymbol{\epsilon}_h(\mathbf{k}) = -2t_h + 2t_h(\sin k_x + \sin k_y)^2. \tag{5}$$

The holon band (hence, metallic conduction) appears as soon as $A \neq 0$ without additional symmetry breaking. Note, ours is not the usual Fermi liquid since, in the absence of magnetic order, the spinon-holon bubble (electron Green's function) does not have a pole (unlike the case with bosonic holons). In our case, an electron "quasiparticle" can appear only through a collective process,¹³ which may occur at larger x. Also, since A=0 above T^* , neither holons nor electrons are coherent.

Let us consider correlation functions for renormalized particles, which clearly preserve the two-sublattice property. Using $\epsilon_h(\mathbf{k}) = \epsilon_h(\mathbf{Q} - \mathbf{k})$, we find $D_{ii} = \langle h_i^{\dagger} h_i \rangle = D_{ii} \cos[\mathbf{Q} \cdot (\mathbf{r}_i)]$ $-\mathbf{r}_i$], (even). This leads to following results. (1) The magnetic correlation function has the same symmetry as in the Mott phase. (2) The electron hopping amplitude $P_{ii,\sigma}$ $=\langle c_{i\sigma}^{\dagger}c_{i\sigma}\rangle = -B_{ij}D_{ij}$. Hence it is even, and decays exponentially, reflecting the non-Fermi liquid behavior of the electron. Then the momentum distribution function satisfies $n_c(\mathbf{k}) = n_c(\mathbf{Q} - \mathbf{k})$. (3) Let $\rho_i = h_i^{\dagger} h_i - \langle h_i^{\dagger} h_i \rangle$. Then the charge structure factor is given by $S_{ch,ij} = \langle \rho_i \rho_j \rangle = -|D_{ij}|^2$, for $i \neq j$, and $S_{ch,ii} = x(1-x)$. Hence, it is even, and has the long-range oscillatory structure of a metal. In **k** space we find $S_{ch}(\mathbf{k})$ $=S_{ch}(\mathbf{Q}-\mathbf{k})$. In contrast, $S_{ch}(\mathbf{k})$ of an ordinary metal increases from zero at k=0 and becomes a constant for k $> 2k_F$. In our case, an image of the behavior near k=0 appears near k=Q. These properties are mostly hidden since the experiments probe the correlators of bare particles, which are dominated by incoherent processes that do not preserve the two-sublattice property. The best candidate is $S_{ch}(\mathbf{k})$ since holon motion is coherent. The experimental (bare) $S_{ch}(\mathbf{k})$ would not vanish at **Q**, but there will be a dip.

(B) *Two-hole process: Superconductivity.* The system can also relax if a second hole hops from sublattice *b* to *a*, and the singlet is reconstituted (Fig. 2). This yields a term $-t_s \Sigma_{ij:lm} A^*_{ml} A_{ij} h^{\dagger}_i h^{\dagger}_j h_l h_m$, where $t_s = 4t_{eff}^2 / \Omega$, which describes hopping by a singlet, accompanied by the backflow of a holon pair. This is the small *x* form of the interaction derived earlier,¹² but here the normal state is different. Using Eq. (2), we obtain



FIG. 2. Two hole process. A hole hops from l to j, breaking the singlet (ij), a second hole hops from m to i, and the singlet is reconstructed at (ml).

$$H_{h,int} = -t_0 \sum_{ij;lm} F_{ij}^{\dagger} F_{ml}, \qquad (6)$$

where $t_0 = t_s A^2$, and $F_{ij}^{\dagger} = h_i^{\dagger} h_j^{\dagger}$ creates a holon pair on the link *ij*. The order of the indices is important, and follows from the symmetry of A_{ij} . Evidently kinetic energy is lowered if two holons hop as a pair. Pairs, being bosonic, will condense, leading to $F_{ij} = \langle F_{ij} \rangle \neq 0$. Let $C_{ij} = \langle (c_{j\downarrow} c_{i\uparrow} - c_{j\uparrow} c_{i\downarrow})/2 \rangle$ denote the pairing order parameter for electrons. Then, $C_{ij} = -A_{ij} F_{ij}^* \neq 0$, giving rise to superconductivity below $T_c \leq T^*$.

Solution of the resulting mean-field problem depends on the symmetry of F_{ij} . Now, $F_{ij}=-F_{ji}$ (Fermi statistics). For a uniform system, $|F_{ij}|=F_0$, but the phases along x and y can be different. We can choose $F_{ij}=\pm iF_0$ along $\pm x$ and F_{ij} $=\pm i\alpha F_0$ along $\pm y$ direction, with $\alpha = e^{i\theta}$. Then, $\Delta_h(\mathbf{k})$ $=2t_0F(\mathbf{k})$ is the holon gap function, where

$$F(\mathbf{k}) = 2F_0(\sin k_x + \alpha \sin k_y). \tag{7}$$

The choice of $\alpha = \pm 1$ leads to $C_x = \pm C_y$, corresponding to *s*-wave (*d*-wave) symmetry for the electron pair wave function. A numerical solution shows that $\alpha = -1$, (i.e., *d* wave) yields the largest F_0 , and hence the largest condensation energy. The origin of this result can be seen from the gap equation itself, which for real α and T=0 is given by

$$\frac{1}{t_0} = \frac{1}{N} \sum_{\mathbf{k}} W(\mathbf{k}) \frac{(\sin k_x + \alpha \sin k_y)^2}{E_{\mathbf{k}}},\tag{8}$$

where $E_{\mathbf{k}} = [(\epsilon_h(\mathbf{k}) - \mu_h)^2 + \Delta_h^2(\mathbf{k})]^{1/2}$ is the quasiholon energy, μ_h is the chemical potential, and $W(\mathbf{k})$ is a suitably chosen cut-off function. The dominant contribution to the sum comes from the region where $|\epsilon_h(\mathbf{k}) - \mu_h|$ is small, and the symmetry factor $|\sin k_x + \alpha \sin k_y|$ is large. As shown in Fig. 3, the holon Fermi surface is in the second and fourth quadrants, exactly where $|\sin k_x + \alpha \sin k_y|$ has maxima for $\alpha = -1$ (*d* wave) and vanishes for $\alpha = 1$ (*s* wave). Hence, *d*-wave always wins. Thus the symmetry is determined by the twosublattice property of the normal and Mott phases.

Since $F(\mathbf{k})=F(\mathbf{Q}-\mathbf{k})$, the two-sublattice property is preserved. The holon pairing function for any two *i* and *j* satisfies $F_{ij}=-F_{ij}\cos\mathbf{Q}\cdot(\mathbf{r}_i-\mathbf{r}_j)$. Hence the electron pairing function C_{ij} is odd. The symmetries of $n_c(\mathbf{k})$ and spin-spin correlation function remain unchanged. The charge structure factor, however, picks up an additional contribution: $S_{ch,ij}$ $=|F_{ij}|^2-|D_{ij}|^2$, and is no longer restricted to the same sublattice; however, like the spin-spin correlation function, it oscillates in sign.

(C) Two dimensions vs three dimensions. A key question in high- T_c superconductivity is as follows: Why is the nor-



FIG. 3. (Color online) Origin of *d*-wave symmetry. Upper panel: Holon Fermi surface. Holons live within the crossing strips centered at $\frac{1}{2}(\pi, -\pi)$ and $\frac{1}{2}(-\pi, \pi)$. Lower panel: the symmetry factor $|\sin k_x + \alpha \sin k_y|$. It has broad maxima in the hole-rich region for $\alpha = -1$, resulting in maximum condensation energy. In contrast, the symmetry factor vanishes in this region for $\alpha = 1$ (*s*-wave). Under a gauge transformation both the Fermi surface and the symmetry factor move together to preserve these results.

mal state two dimensional, whereas superconductivity is not? This is easily resolved. Consider interlayer hopping of amplitude $t_z < t$. The corresponding exchange interaction J_z $=(t_z/t)^2 J \ll J$. Hence singlets form only within the plane. Now, suppose a hole hops on to another layer (or, an electron hops back, by breaking a singlet). The effect is to create two unpaired spinons—one in each layer—at a cost of Ω . Now there is no one-hole process for the system to relax, except by sending the hole back to the original plane. Hence the normal state is two dimensional. However, superconductivity is three dimensional since it involves hopping of a singlet (or a pair of holons). This also explains the enhancement of T_c due to interlayer hopping. Note that pair hopping between layers in the interlayer pair tunneling model¹⁸ is nominally similar, but the physics is different, as the normal-state spinon spectrum is gapless. Also, electrons hop, not holons, and pair-hopping amplitude is diagonal in k_{xy} , i.e., long ranged in the plane.

Other implications. For small x, the theory has many implications for cuprates. Some have been observed (as cited below), and others can be taken as predictions. Here we list a few. Above T^* , the system is predicted to be in the confine-

ment phase: holons are localized due to gauge symmetry. There is no coherent charge carriers and, consequently, no Drude peak—only an incoherent background, with dc resistivity ρ far exceeding the Mott limit.¹⁹ Below T^* holons become coherent, and form a "Fermi liquid" of concentration x, and an effective mass determined by the bandwidth $8t_h < 8t_h$, leading to a small plasma frequency. However, holon Fermi surface is not gauge invariant and thus not observable. For this system, (i) ρ decreases rapidly below T^* ,²⁰ and becomes metallic (i.e., $<\rho_{Mott}$) at low T, so that $\rho = a + bT^2$, with the T^2 term coming from fermion-fermion scattering. This is consistent with experiments; however, actual power of T has not been precisely determined, and may have contributions from other sources of scattering. (ii) The optical conductivity $\sigma(\omega)$ has a Drude component, with an integrated area (spectral weight) $\propto x$ and a small plasma frequency.²¹ It broadens by scattering as T increases, and merges into the incoherent background above $T^{*,19,22}$ (iii) The Hall coefficient is positive and $\propto 1/x$, and independent of T at low T.²³ (iv) The holons contribute a T-linear term to heat capacity. (v) The pseudogap is due to spinon pairing, and causes a rapid downturn in paramagnetic susceptibility (χ_{para}) below T^* .²⁴ In addition, there is a true spinon gap Δ_s , so that χ_{para} vanishes as $T \rightarrow 0$ in the normal state. Hence, total normal-state χ becomes more diamagnetic²⁵ at low T due to the holon contribution. (vi) A finite Δ_s would also lead to a gap in the electron Green's function ("bubble").²⁶ (vii) Since both terms in

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the effective Hamiltonian arise from hopping, condensation energy $\propto -t_s^2/t_h$, hence kinetic energy is reduced, as observed,²⁷ unlike conventional superconductors in which kinetic energy increases. (viii) In the superconductive state holons acquire a gap which has zeroe along the (1,1) direction, and would lead to the usual power law behavior, e.g., of heat capacity.

The renormalized parameters are hard to compute, but can be estimated for x not too close the AF critical point. Roughly, $\Omega \sim J$ since it is the singlet breaking energy. Interestingly, for t > J we expect $t_{eff} \sim J$ from one-hole calculations, so that the coherent bandwidth $\sim t_h \sim J$.^{15,16} There will be additional weak dependence on t/J and x. For larger x, physical electrons will have to be taken into consideration.¹² Our results do not change qualitatively if a small intrasublattice hopping (t') term is included in the orginal model. A more elaborate method is required to describe gauge fluctuations and collective excitations, such as nodal quasiparticles.

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