

Quantum dimer model for the pseudogap metal

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We propose a quantum dimer model for the metallic state of the hole-doped cuprates at low hole density, p . The Hilbert space is spanned by spinless, neutral, bosonic dimers and spin $S=1/2$, charge $+e$ fermionic dimers. The model realizes a “fractionalized Fermi liquid” with no symmetry breaking and small hole pocket Fermi surfaces enclosing a total area determined by p . Exact diagonalization, on lattices of sizes up to 8×8 , shows anisotropic quasiparticle residue around the pocket Fermi surfaces. We discuss the relationship to experiments.

spin liquid | Fermi liquid | dimer model | superconductivity

The recent experimental progress in determining the phase diagram of the hole-doped Cu-based high-temperature superconductors has highlighted the unusual and remarkable properties of the pseudogap (PG) metal (Fig. 1). A characterizing feature of this phase is a depletion of the electronic density of states at the Fermi energy (1, 2), anisotropically distributed in momentum space, that persists up to room temperature.

Attempts have been made to explain the pseudogap metal using thermally fluctuating order parameters; we argue below that such approaches are difficult to reconcile with recent transport experiments. Instead, we introduce a new microscopic model that realizes an alternative perspective (3), in which the pseudogap metal is a finite temperature (T) realization of an interesting quantum state: the fractionalized Fermi liquid (FL*). We show that our model is consistent with key features of the pseudogap metal observed by both transport and spectroscopic probes.

The crucial observation that motivates our work is the tension between photoemission and transport experiments. In the cuprates, the hole density p is conventionally measured relative to that of the insulating antiferromagnet (AF), which has one electron per site in the Cu d band. Therefore, the hole density relative to a filled Cu band, with two electrons per site, is actually $1+p$. In fact, photoemission experiments at large hole doping observe a Fermi surface enclosing an area determined by the hole density $1+p$ (4), in agreement with the Luttinger relation. In contrast, in the pseudogap metal, a mysterious “Fermi arc” spectrum is observed (5–7), with no clear evidence of closed Fermi surfaces. However, despite this unusual spectroscopic feature, transport measurements report vanilla Fermi liquid properties, but associated with carrier density p , rather than $1+p$. The carrier density of p was indicated directly in Hall measurements (8), whereas other early experiments indicated suppression of the Drude weight (9–11). Although the latter could be compatible with a carrier density of $1+p$ but with a suppressed kinetic term, the Hall measurements indicate the suppression of the Drude weight is more likely due to a small carrier density. Two recent experiments displaying Fermi liquid behavior at low p are especially notable: (i) the quasiparticle lifetime $\tau(\omega, T)$ determined from optical conductivity experiments (12) has the Fermi liquid-like dependence $1/\tau \propto (\hbar\omega)^2 + (c\pi k_B T)^2$, with c an order unity constant; and (ii) the in-plane magnetoresistance of the pseudogap (13) is proportional to $\tau^{-1}(1+bH^2\tau^2 + \dots)$ in an applied field H , where $\tau \sim T^{-2}$ and b is a T -independent constant; this is Kohler’s rule for a Fermi liquid.

It is difficult to account for the nearly perfect Fermi liquid-like T dependence in transport properties of the pseudogap in a

theory in which a large Fermi surface of size $1+p$ (14) is disrupted by a thermally fluctuating order. In such a theory, we expect that transport should instead reflect the T dependence of the correlation length of the order.

Moreover, a reasonable candidate for the fluctuating order has not yet been identified. The density wave (DW) order present at lower temperature in the pseudogap regime has been identified to have a d -form factor (15–18), and its temperature dependence (19–25) indicates that it is unlikely to be the origin of the pseudogap present at higher temperature. Similar considerations apply to other fluctuating order models (26) based on AF or d -wave superconductor.

We are therefore led to an alternative perspective (3), in which the pseudogap metal represents a new quantum state that could be stable down to very low T , at least for model Hamiltonians not too different from realistic cuprate models. The observed low- T DW order is then presumed to be an instability of the pseudogap metal (27–31). An early discussion (32) of the pseudogap metal proposed a state that was a doped spin liquid with “spinon” and “holon” excitations fractionalizing the spin and charge of an electron: the spinon carries spin $S=1/2$ and is charge neutral, whereas the holon is spinless and carries charge $+e$. However, this state is incompatible with the sharp “Fermi arc” photoemission spectrum (7) around the diagonals of the Brillouin zone: the spin liquid has no sharp excitations with the quantum number of an electron and so will only produce broad multiparticle continua in photoemission.

Instead, we need a quantum state that has long-lived electron-like quasiparticles around a Fermi surface of size p , even though such a Fermi surface would violate the Luttinger relation of a Fermi liquid. The fractionalized Fermi liquid (FL*) (33) fulfills these requirements.

Significance

The most interesting states of the copper oxide compounds are not the superconductors with high critical temperatures. Instead, the novelty lies primarily in the higher temperature metallic “normal” states from which the superconductors descend. Here, we develop a simple, intuitive model for the physics of the metal at low carrier density, in the “pseudogap” regime. This model describes an exotic metal that is similar in many respects to simple metals like silver. However, the simple metallic character coexists with “topological order” and long-range quantum entanglement previously observed only in exotic insulators or fractional quantum Hall states in very high magnetic fields. Our model is compatible with many recent observations, and we discuss more definitive experimental tests.

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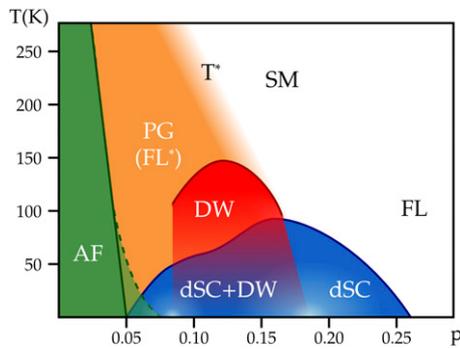


Fig. 1. Schematic phase diagram of hole-doped cuprates (apart from those with La doping) as a function of temperature (T) and hole density (p). The antiferromagnetic (AF) insulator is present near $p=0$, and the d -wave superconductor (dSC) is present below a critical temperature T_c . The pseudogap (PG) is present for $T < T^*$ and acquires density wave (DW) order at low T . The metallic states are the PG metal, the conventional Fermi liquid (FL), and the strange metal (SM). The dimer model of the present paper describes only the PG metal as a fractionalized Fermi liquid (FL*).

Fractionalized Fermi Liquids

The key to understanding the FL* state is the topological nature of the Luttinger relation for the area enclosed by the Fermi surface. For the case of a conventional FL state, Oshikawa (34) provided a nonperturbative proof of the Luttinger relation by placing the system on a torus, and computing the response to a single flux quantum threaded through one of the holes of the torus. His primary assumption about the many-body state was that its only low-energy excitations were fermionic quasiparticles around a Fermi surface. This assumption then points to a route to obtaining a Fermi surface of a different size (35): we need a metal that, in addition to the quasiparticle excitations around the Fermi surface, has global topological excitations nearly degenerate with the ground state, similar to those found in insulating spin liquids (36, 37). In the context of the doped spin liquids noted earlier, we obtain a FL* state when the holon and spinon bind to form a fermionic state with spin $S=1/2$ and charge $+e$ (a possible origin of the binding is the attraction arising from the nearest-neighbor hopping), and there is a Fermi surface with quasiparticle excitations of this bound state (38–40) [other possibilities for the fate of this bound state have also been discussed (41)]. Such a Fermi surface has long-lived electron-like quasiparticles and encloses an area determined by density p , and not $1+p$ (40, 42–44), just as required by observations in the pseudogap metal. Alternatively, a FL* phase can also be obtained from Kondo lattice models (45, 46), but we shall not use this here.

Earlier studies have examined a number of phenomenological and path integral models of FL* theories of the pseudogap (39, 40, 42–44) [and in an ansatz for the pseudogap (47)]. These models contain emergent gauge field excitations, which are needed to provide the global topological states required to violate the Luttinger relation of the FL state. However, they also include spurious auxiliary particle states that are only approximately projected out. The gauge field can undergo a crossover to confinement, but the present models do not keep close track of lattice-scale Berry phases that control the appearance of density wave order in the confining state (48). Here, we propose to overcome these difficulties by a new quantum dimer model that can realize a metallic state that is a FL*. This should open up studies of the photoemission spectrum, density wave instabilities, and crossovers to confinement at low T in the pseudogap metal.

Quantum Dimer Models

Quantum dimer models (49–51) have been powerful tools in uncovering the physics of spin liquid phases, and of their instabilities

to conventional confining phases (52–54). Dimer models of doped spin liquids have also been studied (49, 55, 56), but all of these involve doping the insulating models by monomers that carry charge $+e$, but no spin. Here, we introduce an alternative route to doping, in which the dopants are dimers, carrying both charge and spin.

The Hilbert space of our dimer model is spanned by the close-packing coverings of the square lattice with two species of dimers (Fig. 2), with an additional twofold spin degeneracy of the second species. It can be mapped by an appropriate similarity transform (49) to a truncation of the Hilbert space of the t - J model.

The first species of dimers are bosons, D_{ij} , which reside on the link connecting the square lattice site $i \equiv (i_x, i_y)$ to the site $i + \hat{\eta}$, where $\hat{\eta} = \hat{x} \equiv (1, 0)$ or $\hat{y} \equiv (0, 1)$. These are the same as the dimers in the Rokhsar–Kivelson (RK) model (49), to which our model reduces at zero doping. When connecting to the Hilbert space of the t - J model, each boson maps to a pair of electrons in a spin-singlet state:

$$D_{ij}^\dagger |0\rangle \Rightarrow Y_{ij} \left(c_{i\uparrow}^\dagger c_{i+\hat{\eta},\downarrow}^\dagger + c_{i+\hat{\eta},\uparrow}^\dagger c_{i\downarrow}^\dagger \right) |0\rangle / \sqrt{2}, \quad [1]$$

where $c_{i\alpha}$ is the electron annihilation operator on Cu site i with spin $\alpha = \uparrow, \downarrow$, and $|0\rangle$ is the empty state with no dimers or electrons. The phase factors Y_{ij} depend upon a gauge choice: for the choice made by RK, $Y_{ij} = 1$ and $Y_{i\hat{x}} = (-1)^{i_y}$.

The second species of dimers are “fermions,” $F_{i\eta\alpha}$ with $\alpha = \uparrow, \downarrow$, which carry spin $S=1/2$ and charge $+e$ relative to the half-filled insulator, and are present with a density p . Each fermionic dimer maps to a bound state of a holon and a spinon, which we take to reside on a bonding orbital between nearest-neighbor sites:

$$F_{i\eta\alpha}^\dagger |0\rangle \Rightarrow Y_{ij} \left(c_{i\alpha}^\dagger + c_{i+\hat{\eta},\alpha}^\dagger \right) |0\rangle / \sqrt{2}. \quad [2]$$

In a three-band model (57, 58), the state $F_{i\eta\alpha}^\dagger |0\rangle$ can be identified with the $S=1/2$ state of a hole delocalized over a O site and its two Cu neighbors, considered by Emery and Reiter (59, 60).

Let us stress our assumption that spinon and holon bind not because of confinement but because of a short-range attraction. Therefore, the bound state (2) can break up at an energy cost of order the antiferromagnetic exchange, and the holon and spinon appear as gapped, free excitations that would contribute two-particle continuum spectra to photoemission or neutron scattering

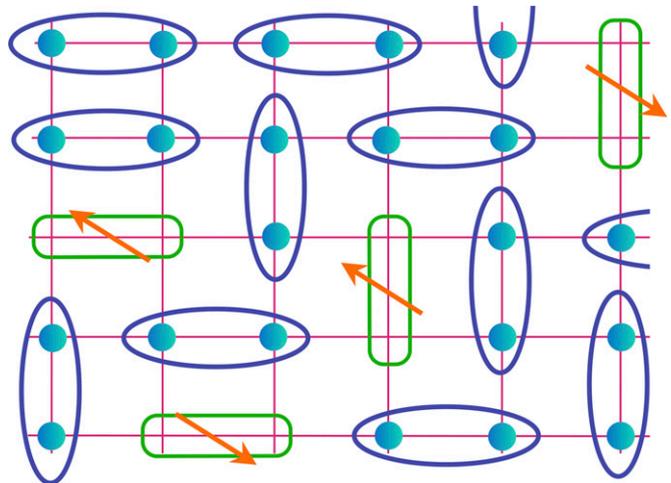


Fig. 2. A typical dimer configuration identifying a state in the Hilbert space. The blue ellipses are the bosons D_{ij} , which are spinless and neutral. The green rectangles are the fermions $F_{i\eta\alpha}$, which carry spin $S=1/2$ and charge $+e$. The density of the $F_{i\eta\alpha}$ dimers is p .

spectra. These fractionalized states can be included in our dimer model by expanding the Hilbert space to include monomers, but we will not do so here because we focus on the lowest energy sector. As a consequence, there is no monomer Fermi surface (42) in the present model of the pseudogap metal.

The states 1 and 2 are precisely those that dominate in the two-site dynamical mean field theory (DMFT) analysis of the Hubbard model by Ferrero et al. (61): they correspond to the S and $1+$ states of ref. 61, respectively, which are shown in figure 15 of this study to be the dominant components of the ground-state wave function at small p (see also ref. 62). The DMFT analysis captures important aspects of pseudogap physics, but with a coarse momentum resolution of the Brillouin zone. In DMFT, the states on the two-site cluster interact with a self-consistent environment in a mean-field way: the equations have so far only been solved at moderate temperatures and the nature of the ultimate ground state at low doping remains unclear. Our dimer model is a route to going beyond DMFT, and to include the nontrivial entanglement between these states on different pairs of sites in a non-mean field manner. The local constraints between different pairs of dimers are accounted for, allowing for the emergence of gauge degrees of freedom.

The original RK model can be mapped to a compact $U(1)$ lattice gauge theory (50, 52, 53). In the doped dimer models studied earlier, the monomers then carry $U(1)$ gauge charges of ± 1 on the two sublattices. By the same reasoning, we see that the $F_{\eta\alpha}$ fermions carry no net gauge charge, but are instead dipoles under the $U(1)$ field.

We can now describe our realization of the pseudogap metal. We envisage a state where the confinement length scale of the compact $U(1)$ gauge field is large, and specifically, larger than the spacing between the $F_{\eta\alpha}$ fermions. Then the $F_{\eta\alpha}$ fermions can move coherently in the presence of a dipolar coupling to the gauge fluctuations (40), and they will form Fermi surfaces enclosing total area p , thus realizing a FL^* state. The confinement scale becomes large near the solvable RK point in the RK model (63, 64), near a Higgs transition to a \mathbb{Z}_2 spin liquid induced by allowing for diagonal dimers (54, 65–67), or more generally near a deconfined critical point (39). Our approach yields a “minimal model” for realizing FL^* (which can be a stable, deconfined state in the \mathbb{Z}_2 spin liquid case), and confinement transitions in metals.

We present results below for the following Hamiltonian, illustrated in Fig. 3, acting on the dimer Hilbert space described above:

$$\begin{aligned}
 H &= H_{\text{RK}} + H_1 + H_2 \\
 H_{\text{RK}} &= \sum_i \left[-J D_{ix}^\dagger D_{i+\hat{y},x}^\dagger D_{iy} D_{i+\hat{x},y} + 1 \text{ term} \right. \\
 &\quad \left. + V D_{ix}^\dagger D_{i+\hat{y},x}^\dagger D_{ix} D_{i+\hat{y},x} + 1 \text{ term} \right] \\
 H_1 &= \sum_i \left[-t_1 D_{ix}^\dagger F_{i+\hat{y},x\alpha}^\dagger F_{ix\alpha} D_{i+\hat{y},x} + 3 \text{ terms} \right. \\
 &\quad - t_2 D_{i+\hat{x},y}^\dagger F_{iy\alpha}^\dagger F_{ix\alpha} D_{i+\hat{y},x} + 7 \text{ terms} \\
 &\quad - t_3 D_{i+\hat{x}+\hat{y},x}^\dagger F_{iy\alpha}^\dagger F_{i+\hat{x}+\hat{y},x\alpha} D_{iy} + 7 \text{ terms} \\
 &\quad \left. - t_3 D_{i+2\hat{y},x}^\dagger F_{iy\alpha}^\dagger F_{i+2\hat{y},x\alpha} D_{iy} + 7 \text{ terms} \right], \quad [3]
 \end{aligned}$$

where the undisplayed terms are generated by operations of the square lattice point group on the terms above. The first term, H_{RK} , coincides with the RK model for the undoped dimer model at $p=0$. Single fermion hopping terms are contained in H_1 , with hoppings t_i , which are expected to be larger than J . A perturbative estimate of the dimer hopping amplitudes t_i in terms

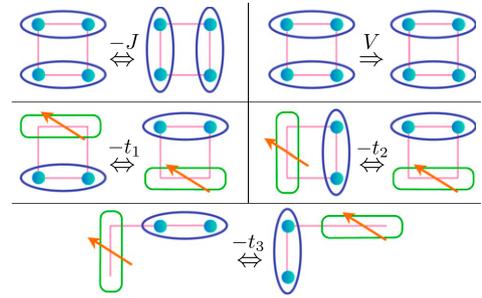


Fig. 3. Terms in the Hamiltonian $H_{\text{RK}} + H_1$.

of electron-hopping parameters can be found in *SI Appendix*. Note that all such terms must preserve the dimer close-packing constraint on every site, and we have chosen three terms with short-range hopping; longer-range hopping terms for the fermionic dimers are also possible, but expected to decay with distance, and are omitted for simplicity. Finally, H_2 allows for interactions between the fermionic dimers, with terms of the following form:

$$H_2 \sim \sum_i \left(F_{ix\beta}^\dagger F_{i+\hat{y},x\alpha}^\dagger - F_{ix\alpha}^\dagger F_{i+\hat{y},x\beta}^\dagger \right) F_{iy\beta} F_{i+\hat{x},y\alpha} + \dots, \quad [4]$$

which preserve the dimer constraint and spin rotation invariance. Purely fermionic dimer models with similar dimer hopping terms have been considered by Pollmann et al. (68).

Results

We now present results for the dispersion and quasiparticle residue of a single fermion described by $H_{\text{RK}} + H_1$; the interaction terms in H_2 play no role here. At a small p , the interactions between the fermionic dimers can be treated by a dilute gas expansion in p , whereas the dominant contributions to the quasiparticle dispersion and residue arise from the interaction between a single fermion and the close-packed sea of bosonic dimers. We computed the latter effects by exactly diagonalizing the single fermion Hamiltonian on lattice sizes up to 8×8 with periodic boundary conditions, with the largest matrix of linear size 76,861,458. The RK model has two conserved winding numbers in a torus geometry, and these conservation laws also hold for our model: all results presented here are for the case of zero winding numbers. We extend these results to nonzero fermion density by interpolation in *SI Appendix*.

Our numerical study explored the dispersion of a single fermion over a range of values of the hopping parameters. We show in Fig. 4 the dispersion $\varepsilon(\mathbf{k})$ for a single $F_{\eta\alpha}$ fermion for hopping parameters obtained by a perturbative connection on a t - J model appropriate for the cuprates at the RK point $V=J=1$. *SI Appendix* has similar results for additional parameter values.

The minima of the fermion dispersion were found at different points in the Brillouin zone, but there was a wide regime with minima near momenta $\mathbf{k} = (\pm \pi/2, \pm \pi/2)$. In fact, for the momentum points allowed on a 8×8 lattice, the global minimum of the dispersion in Fig. 4 is exactly at $(\pi/2, \pi/2)$. However, it is also clear from the figure that the dispersion is not symmetric about the antiferromagnetic Brillouin zone boundary, and that any interpolating function will actually have a minimum at (k_m, k_m) with $k_m < \pi/2$. A dispersion with these properties is of experimental interest because it will lead to formation of hole pockets near the minima for the dimer model with a nonzero density of $F_{\eta\alpha}$ fermions. Fig. 5 shows that changes to the dispersion from a 6×6 lattice are smaller than 5%.

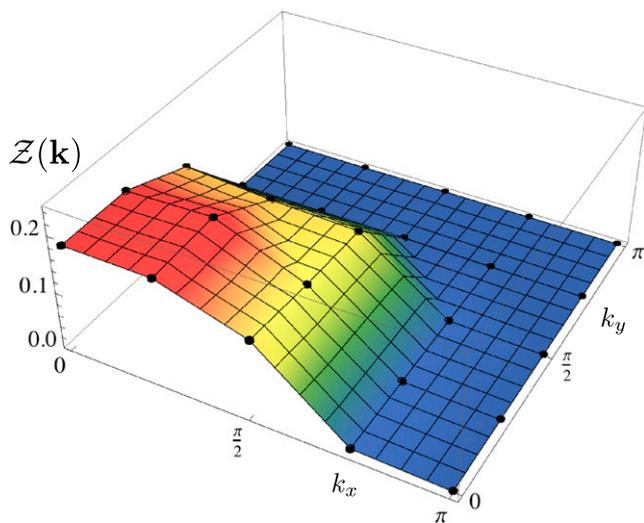


Fig. 6. Quasiparticle residue of a charge $+e$ fermion computed from Eq. 6 for the parameters in Fig. 4, for a 8×8 lattice. The symmetry of the wave function yields $Z(\mathbf{k})=0$ for all points between (π, π) and $(\pi, 0)$. Line cuts of $Z(\mathbf{k})$ are in Fig. 5.

an area distinct from the Luttinger value in a conventional Fermi liquid.

The undoped RK model on the square lattice features a deconfined spin liquid ground state only at the special RK point $J=V$, whereas the ground state breaks lattice symmetries away from this point. Consequently, our numerical results of a single fermionic dimer coupled to the background of bosonic dimers focused at the RK point to uncover properties of the FL* state. At finite densities of fermionic dimers, we expect that our model (3) features a FL* phase in an extended parameter range. However, similar to the RK model, we also expect a wide parameter regime where our model has a ground state with broken lattice symmetries. We leave the computation of the phase diagram of our model for future study.

The main implication of our model of the pseudogap metal (in zero applied magnetic field and at moderate T below T^*) is that there are four well-formed pockets of charge $+e$ fermions carrying spin $S=1/2$ in the vicinity of (but not exactly centered at) momentum $(\pi/2, \pi/2)$. The total area enclosed by these pockets is $2\pi^2p$. Clearly, such pockets can immediately explain the Fermi liquid-like transport observed in recent optical (12) and

magnetoresistance (13) measurements. We also note that the hopping of electrons between CuO_2 layers requires to break either fermionic or bosonic dimers in our model, which naturally accounts for the observed gap in c -axis optical conductivity.

Experiments that involve removing one electron from the system (such as photoemission) have difficulty observing the back sides of the pockets because of the small (but nonzero) quasiparticle residue $Z(\mathbf{k})$ noted above (Fig. 6). We propose this feature as an explanation for the photoemission observation of ref. 7 in the pseudogap metal. For further studies of these pockets, it would be useful to use experimental probes of the Fermi surface that keep the electrons within the sample (70): possibilities include ultrasound attenuation, optical Hall, and Friedel oscillations.

Our theory can be loosely summarized by “the electron becomes a dimer in the pseudogap metal,” as in Eq. 5: with a spin-liquid background present, there can be no single-site state representing an electron, and a dimer is the simplest possibility.

The main advantage of our quantum dimer model over previous treatments (39, 40, 42–44) of fractionalized Fermi liquids (FL*) is that it properly captures lattice-scale dispersions, quasiparticle residues, and Berry phases: all of these are expected to play crucial roles in the crossovers to confinement and associated symmetry breaking at low T (48, 52, 53). Given the elongated dimer and dipolar nature of the electron, Ising-nematic order (71) is a likely possibility; the d -form factor density wave (15, 16) is then a plausible instability of such a nematic metal. The interplay between the monopole-induced crossovers to confinement (52, 53) and the density wave instabilities of the hole pockets (30, 31) can also be examined in such dimer models. The onset of superconductivity will likely require additional states, such as a spinless, charge $+2e$ boson consisting of a pair of empty sites.

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