Doped Spin Liquid: Luttinger Sum Rule and Low Temperature Order

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We analyze a model of two-leg Hubbard ladders weakly coupled by interladder tunneling. At half filling a semimetallic state with small Fermi pockets is induced beyond a threshold tunneling strength. The sign changes in the single electron Green's function relevant for the Luttinger sum rule now take place at surfaces with both zeros and infinities with important consequences for the interpretation of angle-resolved photoemission spectroscopy experiments. Residual interactions between electron and holelike quasiparticles cause a transition to long range order at low temperatures. The theory can be extended to small doping leading to superconducting order.

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While the properties of doped spin liquids in more than one dimension are notoriously difficult to analyze, they are nonetheless highly relevant. In one dimension the two-leg Hubbard ladder at half filling is the spin liquid epitome and as such ladder systems have attracted strong interest [for an early review, see [1]]. Powerful analytic techniques such as bosonization and Bethe ansatz have been applied to single ladders with weak interactions [see [2] and references therein] and have led to comprehensive understanding of both doped and undoped ladders. In this Letter we report the extension of these results to higher dimensions through the introduction of a small long range interladder tunneling in an ensemble of uncoupled half-filled Hubbard ladders. Increasing the tunneling amplitude leads to the formation of closed electron and hole Fermi pockets. The Luttinger sum rule (LSR) now takes on a novel form with the sign changes in the one electron Green's function appearing both as zeros and infinities. This result has strong implications for the interpretation of ARPES results on underdoped cuprates. In the pseudogap phase the experiments interpret infinities as a set of disconnected Fermi arcs [3], but do not (and cannot) observe the zeros. Lastly we analyze possible instabilities of the carriers in the Fermi pockets using interactions derived from the low energy effective field theory for the ladders.

The dynamics of the component half-filled ladders in our ensemble are governed at low energies by an effective field theory. As demonstrated in [4], half-filled ladders with generically repulsive interactions experience under renormalization an enhancement in the symmetry of the bare Hubbard lattice Hamiltonian. With this enhancement, the effective field theory for the ladder is the SO(8) Gross-Neveu model, $H^{\mathrm{SO}(8)}$ [4]. We couple the half-filled ladders together by long range single-particle tunneling. The complete Hamiltonian is then

$$\sum_i H_i^{\mathrm{SO}(8)} + \sum_{\substack{i,i' \\ l,l',n}} t^{\perp}_{ii'll'} \int dx [c^{\dagger}_{nli\sigma}(x) c_{nl'i'\sigma}(x) + \mathrm{H.c.}], \quad (1)$$

where $c^{\dagger}_{nli\sigma}$ creates an electron at the nth site on the lth leg ($l = 1, 2$) of the ith ladder. By making the hopping amplitude long range, we acquire a small parameter, as was done for a similar model of coupled Hubbard chains in [5]. We assume the following hierarchy of energy scales: $W(\text{bandwidth}) \gg \Delta(\text{spectral gap}) \gg t^{\perp}$. The first inequality guarantees that the ladders can be described using the effective field theory. With its renormalization of interactions, this theory is adiabatically disconnected from its noninteracting counterpart.

The Gross-Neveu model is exactly solvable for all semisimple symmetry groups and a great deal is known about its thermodynamics and correlation functions. In the SO(8) case the correlation functions were studied in [6,7]. The spectrum of this model consists of three octets of particles of mass Δ and a multiplet of 29 excitons with mass $\sqrt{3}\Delta$. Two octets consist of quasiparticles of different chirality transforming according to the two irreducible spinor representations of SO(8), while the third octet consists of vector particles. The latter include magnetic excitations as well as the Cooperon (a particle with charge $\pm 2e$). The 16 kink fields, carrying charge, spin, orbit, and parity indices, are direct descendants of the original electron lattice operators on the ladders. According to [6,7], the single electron Green's function is

$$G^{(0)}_a(\omega, k_x) = \left\{ Z_a \frac{[\omega + \epsilon_a(k_x)]}{\omega^2 - \epsilon_a^2(k_x) - \Delta^2} + G_{a,\mathrm{reg}} \right\}, \quad (2)$$

where $a = \sigma, j$ with σ spin and $j = \pm$ indexing the bonding-antibonding bands. $\epsilon_a(k_x)$ is the bare band dispersion. There are no off-diagonal Green's functions involving electrons from opposite Fermi points, a result of right and left moving quasiparticles belonging to different irreducible representations of the SO(8) group. As shown in [7], the incoherent part of the Green's function $G_{a,\mathrm{reg}}$ yields a negligible contribution to the spectral weight and so the quasiparticle weight satisfies $Z_a \approx 1$.

RPA analysis.—We will study the properties of our coupled ladders close to the Mott-Hubbard transition, following Ref. [5]. The interladder hopping is diagonal in the

bonding-antibonding indices because of the bands' differing Fermi wave vectors. A random phase approximation (RPA) (diagrammatically pictured in Fig. 1) yields the following expression for the full 2D Green's function:

$$G_a^{\mathrm{RPA}}(k_x, \mathbf{k}_\perp) = \left\{[G_a^{(0)}(k_x)]^{-1} - t_a(\mathbf{k}_\perp)\right\}^{-1}. \quad (3)$$

In our model the interchain tunneling amplitude has strong peaks at $\mathbf{k}_\perp = 0, \mathbf{G}/2$, where $\mathbf{G}$ is the inverse lattice vector in the direction perpendicular to the chains. [The peak at $\mathbf{G}/2$ follows from particle-hole symmetry, i.e., $t^\perp(k) = -t^\perp(k + \mathbf{G}/2)$.] Near these points the following expansion is valid:

$$t_a(\mathbf{k}_\perp + (1 \mp 1)\mathbf{G}/4) = \mp t_{a0}(1 - (\mathbf{k}_\perp)^2/\kappa_0^2 + \cdots), \quad (4)$$

where the dots stand for terms of higher order in $|\mathbf{k}_\perp|/\kappa_0$ and $\kappa_0 \ll G$ is the small parameter of the theory. We note that $t_{+0} > 0$ while $t_{-0} < 0$.

The quasiparticle spectrum is given by

$$\omega - \epsilon_a(k_x) - \Delta^2[\omega + \epsilon_a(k_x)]^{-1} - t_a(\mathbf{k}_\perp) = 0. \quad (5)$$

At this point we note that the RPA Green's function (3) together with (5) bear a remarkable resemblance to the single electron Green's function of underdoped cuprates conjectured in [8] on phenomenological grounds. In both cases the numerator of the self-energy is modified. In contrast, for a conventional superconductor $t_a(\mathbf{k}_\perp)$ would be expected to modify $\epsilon_a(k_x)$.

The dispersion relationships, $E_{a\pm}(\mathbf{k})$, of the quasiparticles are given from Eq. (5) by

$$E_{a\pm}(\mathbf{k}) = t_a(\mathbf{k}_\perp)/2 \pm \sqrt{(\epsilon_a(k_x) + t_a(\mathbf{k}_\perp)/2)^2 + \Delta^2}. \quad (6)$$

The Fermi surfaces (FS) are determined by solving $E_{a\pm} = 0$. Doing so to leading order for $\mathbf{k}_\perp$ near 0 and $\mathbf{G}/2$ yields

$$[2(k_x - k_{Fa})v_F \mp t_{a0}]^2 + 2t_{a0}^2\mathbf{k}_\perp^2/\kappa_0^2 = t_{a0}^2 - 4\Delta^2. \quad (7)$$

Gapless excitations then only emerge when $\max|t_a(\mathbf{k}_\perp)| > 2\Delta$. For $\pm t_{a0} < 0$, the FS pockets are electronlike, while for $\pm t_{a0} > 0$, they are holelike. Now $G^a_{\mathrm{RPA}} = [\omega + \epsilon_a(\mathbf{k})]/[\omega - E_{a+}(\mathbf{k})][\omega - E_{a-}(\mathbf{k})]$. Near the FS of the pockets, $\epsilon_a(k_x) \sim \pm\Delta$ and $E_{a+}(\mathbf{k}) \sim \pm t_{a0}$. The effective quasiparticle weight can then be read off to be $Z_{\mathrm{RPA}} \sim 1/2$. Thus RPA yields well-defined quasiparticles. We note that Ref. [9] found a FS marked by similar pockets.

Luttinger sum rule.—The Green's functions (2) and (3) satisfy the Luttinger sum rule (LSR) in the form which, though being well known theoretically, has had limited applications. The LSR relates the electron density to the volume in momentum space in which $G(\omega = 0, \mathbf{k}) > 0$. This volume is bounded by the surface where $G(\omega = 0, \mathbf{k})$ changes sign [10]. The sign change can occur either at an infinity of $G(\omega = 0, \mathbf{k})$ (Fermi surface) or a zero (Luttinger surface). The first possibility is denied for a Mott insulator. For example, the Green's function (2) at $\omega = 0$ vanishes at k_{Fa} where $\epsilon_a(k_{Fa}) = 0$, i.e., at momenta where the noninteracting Green's function had infinities. In this way the LSR is satisfied for this nonperturbative ladder ground state. In the presence of interladder tunneling, the Green's function (3) continues to have zeros at k_{Fa} independent of the $\mathbf{k}_\perp$ component (see Fig. 2). However, when Fermi surface pockets appear, the Green's function additionally changes sign through the newly formed infinities. Electronlike pockets add and holelike pockets subtract from the total electron density, but the LSR remains valid. This example demonstrates, as does the case described in [5], that in doped spin liquids it is generally necessary to determine both the Fermi and Luttinger surfaces in order to obtain the electron density from the LSR. It is important to point out that the Luttinger surface, determined by the zeros of the Green's function, differs dramatically from the surface of minimum gap (see Fig. 2). The latter is often used in ARPES experiments to extrapolate to an underlying Fermi surface. This, however, leads to difficulties in the pseudogap phase of underdoped cuprates where the enclosed area manifestly exceeds one electron per unit cell, inconsistent with hole doping [e.g., see [11]].

Instabilities and doping dependence.—As was demonstrated in [5], the RPA solution may become unstable at low temperatures. The instability is driven by the residual interactions between Fermi quasiparticles and collective modes of the spin liquid. This interaction may receive added strength from nesting of the Fermi surfaces of

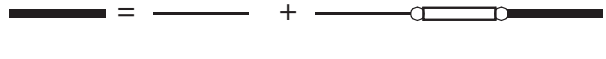

FIG. 1. The RPA equation for single-particle Green's function (thick line), G_a^{RPA}. The double line is the hopping amplitude, t_a, while the thin line is the bare Green's function G_0.

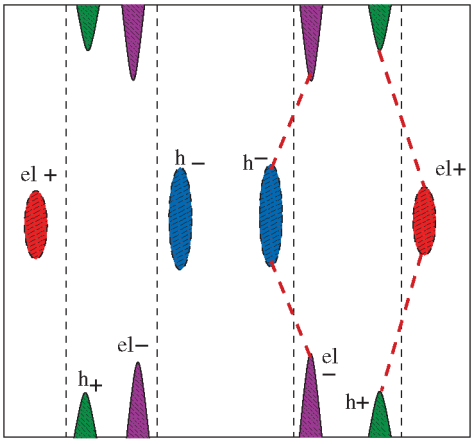

FIG. 2 (color). Electron (red and magenta) and hole (green and blue) pockets. The difference in size between pockets formed from bonding and antibonding orbitals originates from possible difference between the corresponding tunneling amplitudes. The dashed lines represent the Luttinger surfaces $\epsilon_\pm(k) = 0$. The thick dashed red lines are loci of the gap minima, $\epsilon_a(k) = -t_a(\mathbf{k})/2$.

particles and holes. To describe the instability one needs to move beyond RPA. We follow here Ref. [5] and write down an effective action for quasiparticles interacting with collective excitations. The interaction comes from the diagram depicted on the left-hand side of Fig. 3. This four-point function can be approximated as shown on the right-hand side of this same figure, leading to the following effective action [$p = (\omega, \mathbf{k})$]:

$$S = \frac{1}{2}\sum_{p,j} A_j(-p)[\omega^2 - (v_F k_x)^2 - \Delta^2]A_j(p) + \sum_{p,\alpha} \psi_{\pm}^{\bar{\alpha}}(-p) G_{\mathrm{RPA}}^{-1}(p)\psi_{\pm}^{\alpha}(p) + \sum_{q,k} \Gamma\left(\frac{q}{\Delta}, \frac{k}{\Delta}\right) A_j(q)\psi_{+}^{\alpha}(k)(C\gamma^j)_{\alpha\beta}\psi_{-}^{\beta}(-k-q), \quad (8)$$

where all fields are real and $\bar{\alpha}$ is the charge conjugate of α. A_j is the bosonic field transforming according to the vector representation of the SO(8) group, $\psi_{\pm}^{\alpha}$ are spinor fields of right and left chirality, and γ^j are gamma matrices of the SO(8) group. In principle, there is an interaction within each particle multiplet, but we neglect it by accepting the approximation of Fig. 3. Such interactions lead to the creation of bound states with spectral gap $\sqrt{3}\Delta$. We, however, treat these as high energy processes. From general considerations, supported by the calculation that follows, we conclude that $\Gamma \sim \sqrt{v_F}\Delta$.

In coupling the ladders together, the SO(8) symmetry is reduced to SO(6) (provided $|t_{+0}| = t_{-0}$). The quasiparticles that transformed in an 8 dim. representation under SO(8) now are arranged into 4 dim. spinors. These spinors are precisely the same that appear in the SO(5) theory of superconductivity [12]. We thus expect the same phenomenology present in SO(5) models to be present here. At half filling the coupling of the ladders will lead to a spontaneous breaking of the SO(6) symmetry. Possible ordered states include superconductivity (SC), antiferromagnetism (AFM), and a staggered flux phase (SFP). The physics of explicit SO(6) breaking terms will be studied in later work.

Moving away from half filling introduces a nonzero chemical potential μ, and the SO(6) symmetry is reduced down to SU(2) × U(1). The chemical potential acts on the vector bosons as a ''magnetic field'' moving the Cooperon down in energy. At the same time it partially removes the nesting such that the electron and hole pockets become unequal in size and pockets of one type may even disappear. In this case SC becomes the leading instability.

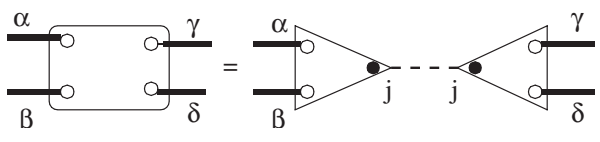

FIG. 3. Approximation of the four-quasiparticle interaction by the emission of an intermediate vector boson.

We are able to provide an estimate of the superconducting ordering temperature, T_c. The RPA result remains valid at $\mu < \Delta/2$ so that the Cooperon has not yet condensed and the ground state of the single ladder remains unchanged. [For $\Delta \approx 2\mu$ where Cooperons do condense, a more sophisticated approach similar to [13] is required.] The dispersion relations are modified to

$$E_a(\mathbf{k}) \approx \frac{(k_x - p_0)^2}{2m_{\|}} + \frac{\mathbf{k}_{\perp}^2}{2m_{\perp}} - \epsilon_F - \mu; \qquad E_a(\mathbf{k} + \mathbf{G}/2) \approx -\frac{(k_x - p_{\mathbf{G}/2})^2}{2m_{\|}} - \frac{\mathbf{k}_{\perp}^2}{2m_{\perp}} + \epsilon_F - \mu, \quad (9)$$

where $\epsilon_F = t_{a0}/4 - \Delta^2/t_{a0}$, $p_{(1\mp1)\mathbf{G}/4} = k_{Fa} \pm t_{a0}/2v_F$, $m_{\perp} = \kappa_0^2/t_{a0}$, and $m_{\|} = t_{a0}/2v_F^2$. In two dimensions the density of states on the Fermi surface is $\rho_F = \frac{\sqrt{m_{\|}m_{\perp}}}{\pi} = \frac{\kappa_0}{\sqrt{2}\pi v_F}$. The pairing susceptibility is

$$\chi^{-1} = [(\omega + 2\mu)^2 - (v_F q_x)^2 - \Delta^2] + \Gamma^2 \Pi(\omega, \mathbf{q}). \quad (10)$$

Since the interaction decays at high energies at the scale Δ, we can take it as the high energy cutoff in the polarization operator. At $\omega, q = 0$ we have $\chi^{-1}(0,0) \approx -\Delta^2 + 4\mu^2 + (v_F\rho_F\Gamma^2/\Delta)\ln[\sqrt{(\epsilon_F + \mu)\Delta}/T]$ which determines the mean field temperature of the transition to a superconductor with a stiffness determined by the dopant density:

$$T_c \approx \sqrt{[\epsilon_F(t_{a0}) + \mu]\Delta}\exp\left[-\frac{1 - (2\mu/\Delta)^2}{\mathrm{const} \times (\kappa_0 v_F/\Delta)}\right]. \quad (11)$$

This expression is valid only when t_{a0} exceeds 2Δ. As μ increases so does T_c. The T_c of other possible instabilities (AFM and SFP) is found approximately (ignoring the consequences of the destruction of a (π, π) nesting) by setting $\mu = 0$ in Eq. (11). These instabilities are thus exponentially disfavored.

While the expression for T_c is not valid if $\mu > \Delta/2$, we can still ask what happens to the Fermi surface for temperatures above any putative T_c. Upon increasing $\mu > \Delta/2$, the single-particle gap *on the ladder* decreases but never vanishes [6] and so the ladder Green's function retains its zeros. It is these zeros that prevent the RPA electron pockets from merging together (see Fig. 2). We thus do not expect, within the validity of the model, a transition to a large Fermi surface for some μ_c.

To provide an estimate of Γ entering the expression for T_c, we calculate the three-point correlation function in the SO(8) Gross-Neveu model using the form factor approach. To evaluate this correlator, we insert a resolution of the identity between fields, reducing the correlation function to a sum over matrix elements. Keeping only matrix elements involving single-particle states we find upon Fourier transformation,

$$\frac{1}{v_F^2}D^a_{\alpha\beta}(p_1,p_2)=\frac{\langle a,-p_1|A^a|0\rangle}{E_1(E_1+\omega_1)}\left[\frac{\langle 0|\psi^\alpha_+|\bar\alpha,-p_2\rangle\langle\bar\alpha,-p_2|\psi^\beta_-|a,-p_1\rangle}{E_2(\omega_2-E_2)}+\frac{\langle 0|\psi^\beta_-|\bar\beta,-p_1-p_2\rangle\langle\bar\beta,-p_1-p_2|\psi^\alpha_+|a,-p_1\rangle}{E_{12}(\omega_1+\omega_2+E_{12})}\right]$$
$$-\frac{\langle 0|A^a|a,p_1\rangle}{E_1(\omega_1-E_1)}\left[-\frac{\langle a,p_1|\psi^\beta_-|\bar\beta,-p_2\rangle\langle\bar\beta,-p_2|\psi^\alpha_+|0\rangle}{E_2(\omega_2+E_2)}+\frac{\langle a,p_1|\psi^\alpha_+|\beta,p_1+p_2\rangle\langle\beta,p_1+p_2|\psi^\beta_-|0\rangle}{E_{12})(\omega_1+\omega_2-E_{12})}\right]$$
$$-\frac{\langle 0|\psi^\alpha_+|\bar\alpha,p_2\rangle\langle\bar\alpha,p_2|A^a|\beta,p_1+p_2\rangle\langle\beta,p_1+p_2|\psi^\beta_-|0\rangle}{E_{12}E_2(\omega_2-E_2)(\omega_1+\omega_2-E_{12})}$$
$$+\frac{\langle 0|\psi^\beta_-|\bar\beta,-p_1-p_2\rangle\langle\bar\beta,-p_1-p_2|A^a|\bar\alpha,-p_2\rangle\langle\bar\alpha,-p_2|\psi^\alpha_+|0\rangle}{E_{12}E_2(\omega_2+E_2)(\omega_1+\omega_2+E_{12})}. \tag{12}$$

Each state is labeled by its isotopic index and momentum, p. Momentum and energy are parametrized in terms of rapidities, θ_i via $p_i=\Delta\sinh(\theta_i)/v_F$, $E_i=\Delta\cosh(\theta_i)$, and $E_{12}=\sqrt{v_F^2(p_1+p_2)^2+\Delta^2}$. The matrix elements of the Fermi operators are given by [6]:

$$\langle 0|\psi^\alpha_\pm|\rho,\theta\rangle=Ae^{\pm i\pi/4}C_{\alpha\rho}e^{\pm\theta/2};\qquad \langle\rho,\theta_1|\psi^\beta_\pm|a,\theta_2\rangle=(C\gamma^aC)_{\alpha\rho}e^{\pm(\theta_1+\theta_2)/4}g(\theta_1-\theta_2);$$
$$g(\theta)=\frac{B}{1/2-\cosh\theta}\exp\left\{\int_0^\infty\frac{dx\sin^2(x\theta/2\pi)}{x\sinh x\cosh(x/2)}[2\cosh(x/6)+e^{-7x/6}]\right\}, \tag{13}$$

where C is the charge conjugation matrix. A and B are related constants on the order of $\sim\sqrt{\Delta/v_F}$. For the Bose operators we have $\langle 0|A^a|b,\theta\rangle=\langle b,\theta|A^a|0\rangle=A_B\delta_{ab}$, $\langle\rho|A^a|\eta\rangle=0$, where A_B is $\mathcal{O}(v_F^{-1/2})$. The vertex is then given in terms of the three-point function via $\Gamma^a_{\alpha\beta}=2\pi G_a^{-1}(p_1)G_\alpha^{-1}(p_2)G_\beta^{-1}(-p_1-p_2)D^a_{\alpha\beta}(p_1,p_2)$, where

$$D^a_{\alpha\beta}(p_1,p_2)=\frac{A_BA(C\gamma^a)_{\alpha\beta}e^{-\theta_{12}/4}g(\theta_{12})}{E_1E_2}\left[\frac{e^{-i\pi/4}}{(\omega_1-E_1)(\omega_2+E_2)}-\frac{e^{i\pi/4}}{(\omega_1+E_1)(\omega_2-E_2)}\right]$$
$$-[(p_1,p_2,\omega_1,\omega_2)\to(-p_1,p_1+p_2,-\omega_1,-\omega_1-\omega_2)], \tag{14}$$

where $p_{1,2}=\Delta/v_F\sinh\theta_{1,2}$ and the G's are the corresponding noninteracting propagators. We also note that $g(x)\sim-Be^{-|x|/4}$ for $|x|\gg1$. As we see, the vertex is a smooth function of momenta and frequencies changing with a characteristic scale Δ as written in (9). This derivation justifies Eq. (11).

In conclusion, we have constructed a toy model of a doped spin liquid. This model possesses a number of interesting features. *Vis-à-vis* ARPES measurements, it offers an alternative framework in which to understand the observed arcs in underdoped cuprates [3,11]: such arcs may be Fermi pockets unresolved by ARPES due to disorder and limited experimental accuracy. It further suggests using an observed line of minimal gap will lead to overestimate of the number of electrons present in a band. Beyond implications for ARPES, the model (at half filling) possesses an SO(6) symmetry and so encompasses the same phenomenology as SO(5) models of superconductivity including a π resonance at energy 2μ. Away from half filling superconductivity is preferred and the model is under sufficient control to provide an estimate for the superconducting T_c. Finally we point out above T_c the model predicts the existence of a low lying Cooperon excitation.

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