Magnetic Instability in Strongly Correlated Superconductors

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Recently, a new phenomenological Hamiltonian has been proposed to describe the superconducting cuprates. This so-called Gossamer Hamiltonian is an apt model for a superconductor with strong on-site Coulomb repulsion between the electrons. It is shown that at half-filling the Gossamer superconductor with strong repulsion is unstable toward an antiferromagnetic insulator. The superconducting state undergoes a quantum phase transition to an antiferromagnetic insulator as one increases the on-site Coulomb repulsion. Near the transition the Gossamer superconductor becomes spectroscopically indistinguishable from the insulator.

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The parent materials of the high temperature superconducting cuprates are correlated antiferromagnetic insulators. When they are half-filled, with one hole per copper, they insulate despite having an odd number of electrons in their valence band. The antiferromagnetism and insulation stem from the strong on-site Coulomb repulsion among the copper d electrons. These electron correlations have been postulated to be essential to the superconductivity in the cuprates [1] since its discovery.

We want to suggest that the correlation effects might be seducing us into misidentifying them as the key ingredient for high-T_c superconductivity. In order to study the consequences and viability of such an idea we study a Hamiltonian recently proposed by one of us [2] which has a d-wave superconducting ground state for all dopings up to the half-filled undoped state. This superconductor was baptized the Gossamer superconductor.

The correlation and magnetic effects compete and are, in a sense, detrimental to the superconductivity. In previous work [2] it was estimated that, at strong projection, the spectral function will evolve with decreasing doping toward that of an insulator with two Hubbard bands, a Hubbard gap and an ever fainter redistribution of spectral weight to midgap states [3] corresponding to the collapsing superfluid density.

Thus superconductors with strong on-site repulsion are spectroscopically identical to so-called doped Mott insulators close to half-filling, except for a small amount of conducting fluid corresponding to the dephased superconductor. This naturally accommodates experiments that hint at conduction in the supposedly antiferromagnetic insulating phase [4] and the existence of a d-wave node deep in the underdoped regime [3].

We identify the pseudogap [5] measured in underdoped cuprates with the Cooper pairing gap [6]. In this region the superconducting transition temperature T_c is lower than the pairing temperature because the Gossamer superconductor is becoming ever increasingly unstable to loss of phase coherence due to the small superfluid density [7,8].

In the present Letter we show that the superconducting state with strong on-site repulsion is unstable toward insulation and antiferromagnetism close to half-filling by studying such a half-filling instability in the the Gossamer superconductor. For the Gossamer superconductor the instability is exactly at half-filling while for a different Hamiltonian the instability can occur at nonzero doping. For example, antiferromagnetic or stripe ground states [9] can be stabilized by adding an extra Hubbard U term to the Gossamer Hamiltonian.

The Gossamer superconductor is defined as a superconducting ground state which contains Coulomb correlations. These are introduced by a partial Gutzwiller projection which decreases the probability of having two electrons on the same site:

$$\Pi_{\alpha_0} = \prod_j z_0^{(n_{j\uparrow}+n_{j\downarrow})/2}(1 - \alpha_0 n_{j\uparrow} n_{j\downarrow}). \tag{1}$$

$0 \leq \alpha_0 < 1$ is a measure of how effective the projector is and in a real material it will be related to the Coulomb repulsion. The factor of z_0, the quantum fugacity, in the projector is the extra probability of having an electron at site j after projecting and is necessary in order to keep the total number of particles constant at $(1-\delta)N$ after projecting. The fugacity is given by $z_0 = [\sqrt{1-\alpha(1-\delta^2)} - \delta]/[(1-\alpha)(1-\delta)]$ with $(1-\alpha_0)^2 = 1-\alpha$.

The Gossamer superconducting ground state is postulated to be $|\Psi\rangle = \Pi_\alpha |\Phi\rangle$. Here $|\Phi\rangle$ is the BCS ground state:

$$|\Phi\rangle = \prod_{\vec{k}}(u_{\vec{k}} + v_{\vec{k}} c^\dagger_{\vec{k}_\uparrow} c^\dagger_{-\vec{k}_\downarrow})|0\rangle, \tag{2}$$

where $u_{\vec{k}}, v_{\vec{k}}$ are the well-known BCS pairing amplitudes given by $u_{\vec{k}} = \sqrt{(E_{\vec{k}} + \epsilon_{\vec{k}} - \mu)/2E_{\vec{k}}}$ and $v_{\vec{k}} = \sqrt{[E_{\vec{k}} - (\epsilon_{\vec{k}} - \mu)]/2E_{\vec{k}}}$ with dispersion $E_{\vec{k}} = \pm\sqrt{(\epsilon_{\vec{k}} - \mu)^2 + \Delta^2_{\vec{k}}}$, where $\epsilon_{\vec{k}}$ is the kinetic energy, μ is

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the chemical potential, and $\Delta_{\vec{k}}$ is the superconducting gap. We take $\epsilon_{\vec{k}} = 2t(\cos(k_x a) + \cos(k_y a))$ for a square lattice with spacing a, and $\Delta_{\vec{k}} = \Delta_o(\cos(k_x a) - \cos(k_y a))$ for a d-wave gap as found for the superconducting cuprates [5]. In superconductors the coherence factors $u_{\vec{k}}$ and $v_{\vec{k}}$ are related to the number of carriers in order to set the value of the chemical potential. For doped cuprates we have $\frac{1}{N}\sum_{\vec{k}} v_{\vec{k}}^2 = 1 - \frac{1}{N}\sum_{\vec{k}} u_{\vec{k}}^2 = (1-\delta)/2$ where δ is the doping level.

Projected ground states like the Gossamer ground state have been previously used in the literature [10,11] to describe high temperature superconductors. We consider only projection away from full projection ($\alpha_0 < 1$) in order for the partial projector to have an inverse,

$$\Pi_\alpha^{-1} = \prod_j z_0^{-(n_{j\uparrow}+n_{j\downarrow})/2}(1 + \beta_0 n_{j\uparrow} n_{j\downarrow}), \qquad (3)$$

with $\beta_0 = \alpha_0/(1-\alpha_0)$. By virtue of this invertibility, the Gossamer ground state is adiabatically continuable to the BCS ground state and its uniqueness follows from the uniqueness of the BCS ground state up to a phase. Therefore the Gossamer superconductor describes the same phase of matter as the BCS superconductor.

The Gossamer ground state is the exact ground state of the Gossamer Hamiltonian,

$$\mathcal{H} = \sum_{\vec{k}\sigma} E_{\vec{k}} B_{\vec{k}\sigma}^\dagger B_{\vec{k}\sigma}, \qquad B_{\vec{k}\sigma}|\Psi\rangle = 0, \qquad (4)$$

where

$$\begin{aligned} B_{\vec{k}\uparrow\{\downarrow\}} &= \Pi_\alpha b_{\vec{k}\uparrow\{\downarrow\}} \Pi_\alpha^{-1} \\ &= \frac{1}{\sqrt{N}} \sum_j^N e^{i\vec{k}\cdot\vec{r}_j}[z_0^{-1/2} u_{\vec{k}}(1 + \beta_0 n_{j\downarrow\{\uparrow\}}) c_{j\uparrow\{\downarrow\}} \\ &\qquad \pm z_0^{1/2} v_{\vec{k}}(1 - \alpha_0 n_{j\uparrow\{\downarrow\}}) c_{j\downarrow\{\uparrow\}}^\dagger], \end{aligned} \qquad (5)$$

with $b_{\vec{k}\uparrow\{\downarrow\}} = u_{\vec{k}} c_{j\uparrow\{\downarrow\}} \pm v_{\vec{k}} c_{j\downarrow\{\uparrow\}}^\dagger$ the Bogoliubov quasiparticle operators. Actually a similar Hamiltonian could be defined and studied for any dispersion $E(k)$ even if the system is not a superconductor. This could be very fruitful in studying the effects on the metallic state as one approaches the Mott regime and points to a certain generality of the methods presented here.

A superconductor with strong on-site Coulomb repulsion is described by the Gossamer Hamiltonian with nearly full projection, i.e., $\alpha_0 \to 1^-$. The strong projector collapses the superfluid density with doping according to $\sim\delta$ [2], with corrections of order δ^2 and $(1-\alpha_0)\delta$, and introduces correlations intrinsic to an antiferromagnetic insulator.

In order to determine the correlations arising in the different limits of the Gossamer Hamiltonian, Eq. (4), we will expand the Hamiltonian and analyze its terms. After some manipulation, we can bring the Hamiltonian in the form of a sum of three physically distinct terms:

$$\mathcal{H} = \sum_{\vec{k}\sigma} E_{\vec{k}} B_{\vec{k}\sigma}^\dagger B_{\vec{k}\sigma} = \mathcal{A} + \mathcal{B} + C, \qquad (6)$$

where $\mathcal{A}, \mathcal{B}, C$ are, explicitly,

$$\mathcal{A} = \sum_{\vec{k}} \frac{E_{\vec{k}}}{N} \sum_{i,j}^N e^{-i\vec{k}\cdot(\vec{r}_i - \vec{r}_j)}\{z_0^{-1} u_{\vec{k}}^2 (1 + \beta_0 n_{i\downarrow})(1 + \beta_0 n_{j\downarrow}) c_{i\uparrow}^\dagger c_{j\uparrow} + z_0 v_{\vec{k}}^2 (1 - \alpha_0 n_{i\downarrow})(1 - \alpha_0 n_{j\downarrow}) c_{i\uparrow} c_{j\uparrow}^\dagger\} + \{\uparrow \rightleftarrows \downarrow\}, \qquad (7)$$

$$\mathcal{B} = \sum_{\vec{k}} \frac{E_{\vec{k}}}{N} \sum_{i,j}^N e^{-i\vec{k}\cdot(\vec{r}_i - \vec{r}_j)} u_{\vec{k}} v_{\vec{k}} \{(1 + \beta_0 n_{i\downarrow})(1 - \alpha_0 n_{j\uparrow}) c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger - (1 + \beta_0 n_{j\downarrow})(1 - \alpha_0 n_{i\uparrow}) c_{i\downarrow} c_{j\uparrow}\} - \{\uparrow \rightleftarrows \downarrow\}, \qquad (8)$$

$$C = \sum_{\vec{k}} \frac{E_{\vec{k}}}{N} \sum_j^N u_{\vec{k}} v_{\vec{k}} \{\alpha_0 (1 + \beta_0 n_{j\downarrow}) c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger + \beta_0 (1 - \alpha_0 n_{j\uparrow}) c_{j\downarrow} c_{j\uparrow}\} - \{\uparrow \rightleftarrows \downarrow\}. \qquad (9)$$

The last term C vanishes by use of the identity $E_{\vec{k}} u_{\vec{k}} v_{\vec{k}} = \frac{\Delta_{\vec{k}}}{2}$ as well as the relation

$$\sum_{\vec{k}} e^{-i\vec{k}\cdot(\vec{r}_i - \vec{r}_j)} \Delta_{\vec{k}} = \begin{cases} 0, & \vec{r}_i \neq \vec{r}_j + \vec{a}, \\ \Delta_0, & \vec{a} \parallel \hat{x}, \\ -\Delta_0, & \vec{a} \parallel \hat{y} \end{cases} \qquad (10)$$

(true for a d-wave gap), where $\vec{a}$ is a vector pointing toward a nearest neighbor in the lattice. The $\mathcal{A}$ term is responsible for the chemical potential, kinetic energy, as well as a Hubbard U term. $\mathcal{B}$ is responsible for the superconducting part of the Gossamer Hamiltonian. The d-wave form of the gap makes $\mathcal{B}$ have no on-site contributions. $\mathcal{A}$ contains on-site and off-site contributions.

We can write $\mathcal{A}$ as a sum between on-site and off-site contributions $\mathcal{A} = \mathcal{A}_{\text{on-site}} + \mathcal{A}_{\text{off-site}}$, where the two contributions read

$$\begin{aligned} \mathcal{A}_{\text{on-site}} = \sum_{\vec{k}} \frac{E_{\vec{k}}}{N} \sum_j^N \{ & z_0^{-1} u_{\vec{k}}^2 (1 + \beta_0 n_{j\downarrow})^2 c_{j\uparrow}^\dagger c_{j\uparrow} \\ & + z_0 v_{\vec{k}}^2 (1 - \alpha_0 n_{j\downarrow})^2 c_{j\uparrow} c_{j\uparrow}^\dagger\} + \{\uparrow \rightleftarrows \downarrow\}, \end{aligned} \qquad (11)$$

$$\mathcal{A}_{\text{off-site}} = \sum_{\vec{k}} \frac{E_{\vec{k}}}{N} \sum_{i\neq j}^{N} e^{-i\vec{k}\cdot(\vec{r}_i-\vec{r}_j)}\{z_0^{-1}u_{\vec{k}}^2(1+\beta_0 n_{i\downarrow})(1+\beta_0 n_{j\downarrow})c_{i\uparrow}^\dagger c_{j\uparrow} + z_0 v_{\vec{k}}^2(1-\alpha_0 n_{i\downarrow})(1-\alpha_0 n_{j\downarrow})c_{j\uparrow}^\dagger c_{i\uparrow}\} + \{\uparrow\rightleftarrows\downarrow\}. \tag{12}$$

The Hubbard U term will arise out of the on-site contribution, $\mathcal{A}_{\text{on-site}}$. After some operator algebra the term can be transformed into

$$\mathcal{A}_{\text{on-site}} = \sum_{\vec{k}} \frac{E_{\vec{k}}}{N} \sum_{j}^{N} \{2z_0 v_{\vec{k}}^2 + [z_0^{-1}u_{\vec{k}}^2 - z_0 v_{\vec{k}}^2 - 2\alpha_0 z_0 v_{\vec{k}}^2 + \alpha_0^2 z_0 v_{\vec{k}}^2](n_{j\uparrow}+n_{j\downarrow}) + [z_0^{-1}u_{\vec{k}}^2(4\beta_0+2\beta_0^2) + z_0 v_{\vec{k}}^2(4\alpha_0 - 2\alpha_0^2)]n_{j\uparrow}n_{j\downarrow}\}. \tag{13}$$

The first term is a zero-point energy, the second term is a chemical potential, and, most interestingly, the third term is the Hubbard U term ($\sum_j^N U n_{j\uparrow}n_{j\downarrow}$) with

$$U = \sum_{\vec{k}} \frac{E_{\vec{k}}}{N}[z_0^{-1}u_{\vec{k}}^2(4\beta_0+2\beta_0^2) + z_0 v_{\vec{k}}^2(4\alpha_0-2\alpha_0^2)]. \tag{14}$$

Thus the Gossamer Hamiltonian has a Hubbard U term.

The Gossamer Hamiltonian is constructed such that its ground state is superconducting for all nonzero dopings. It will be most susceptible to antiferromagnetism at zero doping under almost full projection where the superfluid density is arbitrarily close to zero (vanishing in the limit of full projection.) We thus concentrate on half-filling $\delta = 0$, where U becomes

$$U|_{\delta=0} = \sum_{\vec{k}} \frac{2E_{\vec{k}}}{N}\frac{\alpha_0(2-\alpha_0)}{1-\alpha_0}. \tag{15}$$

As we can see, at almost full projection $\alpha_0 \rightarrow 1^-$, U becomes very large.

The off-site contributions of $\mathcal{A}$ give a hopping (kinetic) term in the Hamiltonian. Prior to the partial Gutzwiller projection ($\alpha_0 = 0, z_0 = 1$) this term is just the kinetic energy or hopping term of the Hamiltonian $\sum_{\vec{k}\sigma}(\epsilon_{\vec{k}} - \mu)c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma}$. Including the partial projection, particularizing to zero doping and imposing the mean field values $\langle n_{i\uparrow}\rangle = \langle n_{i\downarrow}\rangle = 1/2$, the off-site, after some manipulation, becomes

$$\mathcal{A}_{\text{off-site}} = \frac{1}{4}\frac{(2-\alpha_0)^2}{(1-\alpha_0)}\sum_{\vec{k}\sigma}(\epsilon_{\vec{k}}-\mu)c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma}. \tag{16}$$

At half-filling, the effect of the partial projection on the kinetic term in the Gossamer Hamiltonian is, surprisingly, just a renormalization. Upon strong projection, the physically relevant ratio, U/t, approaches a number of order unity or greater which provides the right physics for the appearance of strong antiferromagnetic correlations and insulation [12].

The superconducting part of the Gossamer Hamiltonian, $\mathcal{B}$, given in Eq. (8) is, when unprojected, just the pair attraction term $\sum_{\vec{k}}\Delta_{\vec{k}}[c_{\vec{k}\uparrow}^\dagger c_{-\vec{k}\downarrow}^\dagger + c_{-\vec{k}\downarrow}c_{\vec{k}\uparrow}]$ from the mean field d-wave superconducting Hamiltonian. Concentrating on half-filling, we estimate $\mathcal{B}$ by imposing the mean field condition $\langle n_{i\uparrow}\rangle = \langle n_{i\downarrow}\rangle = 1/2$, and keeping in mind that $E_{\vec{k}}$ and $\Delta_{\vec{k}}$ are even in $\vec{k}$. We thus obtain

$$\mathcal{B} = \frac{1}{4}\frac{(2-\alpha_0)^2}{1-\alpha_0}\sum_{\vec{k}}\Delta_{\vec{k}}(c_{\vec{k}\uparrow}^\dagger c_{-\vec{k}\downarrow}^\dagger + c_{-\vec{k}\downarrow}c_{\vec{k}\uparrow}). \tag{17}$$

The new superconducting gap, at half-filling, upon projection is still d wave, and is renormalized by the same constant as the kinetic energy. Upon strong projection, the physically relevant ratio, U/Δ_0, is a number of order unity or greater, the right physics for antiferromagnetism and insulation. It is very interesting that the gap survives along with the Hubbard U term at half-filling where the superfluid density can be arbitrarily close to zero upon strong projection.

We have thus shown that at half-filling and under strong projection the Gossamer superconductor Hamiltonian is a Hubbard Hamiltonian with a d-wave pairing interaction added to it. If we define the spinors,

$$\Psi_{\vec{k}} \equiv \begin{bmatrix} c_{\vec{k}\uparrow} \\ c_{-\vec{k}\downarrow}^\dagger \end{bmatrix}, \tag{18}$$

the noninteracting part of the Gossamer Hamiltonian, the part with the U term disregarded, is

$$\mathcal{H} = \frac{1}{4}\frac{(2-\alpha_0)^2}{1-\alpha_0}\begin{bmatrix} \epsilon_{\vec{k}} & \Delta_{\vec{k}} \\ \Delta_{\vec{k}} & -\epsilon_{\vec{k}} \end{bmatrix}, \tag{19}$$

where μ has been omitted because we are at half-filling. The bare Green function, $G_{\vec{k}}(E) = 1/(E - \mathcal{H})$ is then given by

$$G_{\vec{k}} = \frac{1}{E^2 - \gamma^2(\epsilon_{\vec{k}}^2 + \Delta_{\vec{k}}^2)}\begin{bmatrix} E+\gamma\epsilon_{\vec{k}} & \Delta_{\vec{k}} \\ -\gamma\Delta_{\vec{k}} & E-\gamma\epsilon_{\vec{k}} \end{bmatrix}, \tag{20}$$

with $\gamma \equiv (2-\alpha_0)^2/4(1-\alpha_0)$.

In order to show the magnetic ordering properties of the Gossamer Hamiltonian at half-filling, we will compute the magnetic susceptibility and tune it through the transition. The bare susceptibility is given by

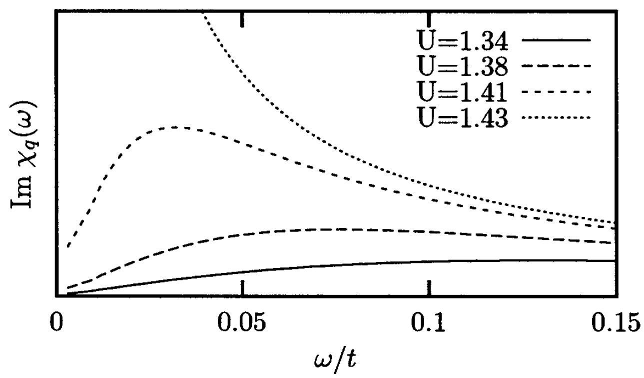

FIG. 1. Dependence of the imaginary part of the spin susceptibility in RPA approximation on the energy in units of t. The specific curves plotted here are for $\Delta_0 = 0.4t$ and $q = (\pi, \pi)$. Upon increasing the Hubbard U toward the critical value $U = 1.43t$ we notice the divergence of the susceptibility, a sign that magnetic order is about to set in.

$$\chi_q^0(\omega) = \frac{1}{(2\pi)^3} \iint \mathrm{Tr}[G_k(E) G_{k+q}(E + \omega)] dE dk. \quad (21)$$

We calculate the effects of U by the ladder approximation for the spin susceptibility $\chi_q(\omega) = \chi_q^0(\omega)/[1 + U\chi_q^0(\omega)]$. The numerical evaluation of the spin susceptibility is shown in Fig. 1. We see that beyond at critical value for U of order of t and/or Δ_0, the system goes to the critical point becoming infinitely susceptible to going over into an antiferromagnetic insulator as signaled by the diverging susceptibility at the critical value.

The ladder technique will not provide the right critical value of U, nor will it provide the correct critical exponents. It will, however, provide a faithful qualitative picture of the transition of the divergence of the spin susceptibility at the critical point for the development of antiferromagnetic order.

In the present Letter we demonstrated that, when extremely strongly projected, the Gossamer superconductor is arbitrarily close to a continuous zero temperature phase transition into an antiferromagnetic insulator. The critical point is at half-filling when fully projected and it is the Anderson resonating valence bond ground state [1]. Since the Gossamer superconductor is adiabatically continuable to a completely regular BCS superconductor our correlation effects are generic to the superconducting state.

Under strong projection, the Gossamer superconductor has a superfluid density that collapses with doping and projection. This collapsing superfluid density leads to a temperature order parameter phase instability [7]consistent with the transition out of the superconducting state in underdoped cuprates [5]. Even without the development of antiferromagnetism, such a superconductor would be insulating since it would dephase due to the small superfluid density [8].

The proximity to the antiferromagnetic transition found here under strong projection will make the spectroscopic properties of the material be very much like those of an antiferromagnetic insulator near half-filling. The superfluid density will be so low that it would be almost impossible to tell that the system is not an insulator except at extremely long wavelengths or low energy scales.

An antiferromagnet with a small interpenetrating density of dephased superfluid provides a possible explanation for the recent measurements of metallic transport below the Néel temperature in underdoped LaSrCuO [4]. That the charge mobility in these measurements is equal to that in the optimally doped material [13] suggests a common origin, possibly the dephased Gossamer superconductor. Moreover, adding by hand an extra Hubbard term, an insulating static stripe phase would be stabilized with a possible coexistence of dephased superfluid. Coupling of the coexisting dephased superfluid to the stripe phase would lead to anisotropic copper-oxygen plane charge transport [14].

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