Gossamer Superconductor, Mott Insulator, and Resonating Valence Bond State in Correlated Electron Systems

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Gutzwiller variational method is applied to an effective two-dimensional Hubbard model to examine the recently proposed gossamer superconductor by Laughlin (LANL cond-mat/0209269). The ground state at half filled electron density is a gossamer superconductor for smaller intrasite Coulomb repulsion U and a Mott insulator for larger U. The gossamer superconducting state is similar to the resonating valence bond superconducting state, except that the chemical potential is approximately pinned at the mid of the two Hubbard bands away from the half filled.

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Theories for high temperature superconductivity continue to attract much interest in condensed matter physics. Soon after its discovery, Anderson proposed the idea of resonating valence bond (RVB) state for the observed unusual properties in high T_c superconducting Cu-oxides [1]. In the RVB picture, each lattice site is either unoccupied or singly occupied by a spin-up or down electron. The spins are coupled antiferromagnetically without long range order. The charge carriers move in the spin liquid background and condense to a superconducting state [2,3]. The RVB states are oftenly studied using two-dimensional Hubbard or t-J models [1,4]. In this scenario, the undoped cuprate with density one electron per site, or half filled, is a Mott insulator, and the superconductor is viewed as a doped Mott insulator when additional holes or electrons are introduced. A Mott insulator is a special type of insulator casued by electron interaction. It has been established that the ground state of many models in 1-dimensional chain or in ladders at half filled are Mott insulator[5]. In two or higher dimensions, a Mott insulator has a strong tendency toward antiferromagnetic or other types of ordering states breaking translational symmetry.

Very recently, Laughlin has proposed an interesting new notion, the gossamer superconductor, for high temperature superconducting Cu-oxides [6]. In a gossamer superconductor, the superfluid density is very thin, in contrast to the conventional superconductor. Laughlin has proposed an explicit microscopic wave function for the gossamer superconductor, which has the following form,

$$|\Psi_L\rangle = \prod_i (1 - \alpha_0 n_{i\uparrow} n_{i\downarrow}) \,|\Psi_{\rm BCS}\rangle, \tag{1}$$

$$|\Psi_{\rm BCS}\rangle = \prod_{\vec{k}} (u_{\vec{k}} + v_{\vec{k}} c^\dagger_{\vec{k}\uparrow} c^\dagger_{-\vec{k}\downarrow}) \,|0\rangle,$$

where $|\Psi_{\rm BCS}\rangle$ is a BCS superconducting state, and $\Pi_\alpha = \prod_i (1 - \alpha_0 n_{i\uparrow} n_{i\downarrow})$ is a projection operator to partially project out doubly occupied electron states on each lattice site i. $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ is the electron number operator of spin $\sigma = \uparrow, \downarrow$ at site i, and α_0 is a parameter between 0 and 1. If α_0 is close to 1, the projection operator strongly suppresses the superfluid density. In the gossamer superconducting state, the probability to have both spin-up and spin-down electrons occupying the same lattice site is largely reduced but remains to be finite. Because of the partial projection, the state is superconducting even at half filling. This is different from the RVB theory where the electron doubly occupied states are completely projected out, hence the half filled RVB state is a Mott insulator and the superconductivity occurs only away from the half filled. As it has been shown by Laughlin[6], the gossamer superconducting state in Eq. (1) is an exact ground state of a model Hamiltonian given by $H_L = \sum_{\vec{k}\sigma} E_{\vec{k}\sigma} \tilde{b}^\dagger_{\vec{k}\sigma} \tilde{b}_{\vec{k}\sigma}$, where $E_{\vec{k}\sigma} \geq 0$, $\tilde{b}_{\vec{k}\sigma} = \Pi_\alpha b_{\vec{k}\sigma} \Pi_\alpha^{-1}$, and $b_{\vec{k}\sigma}$ is the quasiparticle annihilation operator of the BCS state, $b_{\vec{k}\sigma} \,|\Psi_{\rm BCS}\rangle = 0$. Π_α^{-1} is the inverse of Π_α. Laughlin has also argued that the gossamer superconducting state is related to the large on-site Coulomb repulsion.

It will be interesting to examine the possible gossamer superconducting state in a more realistic model. As it is generally believed that the large Coulomb repulsion may lead to a Mott insulator at half filling, it will also be interesting to examine the possibility of the phase transition from a Mott insulator to a gossamer superconductor as the electron interaction strength decreases. Since a doped Mott insulator can be a RVB superconducting state, it is natural to ask the question of the similarities and the differences between the gossamer and the RVB superconductors.

In this Letter we intend to examine these questions by studying an effective Hubbard model given in Eq. (2) below using Gutzwiller's variational method [7]. In the Gutzwiller's approach, the on-site Coulomb repulsion is treated exactly, while the kinetic energy is studied

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variationally, so that it is suitable to examine some issues in strongly correlated systems. That method was used by Brinkman and Rice [8] to study the phase transition between an insulator and a metallic state described by a partially projected Fermi liquid state. The variational method applied to the effective Hubbard model in two-dimension demonstrates a phase transition from a gossamer superconductor for smaller intra-site Coulomb repulsion U to a Mott insulator for larger U at half filling. The gossamer superconductor is shown similar to the RVB superconducting state of the doped Mott insulator. However, its chemical potential is found to be approximately pinned at the mid of the lower and the higher Hubbard bands, different from the RVB state where the chemical potential is shifted to the lower Hubbard band upon doping.

We study an effective Hubbard Hamiltonian,

$$H = U\sum_i n_{i\uparrow}n_{i\downarrow} - \sum_{\langle ij\rangle\sigma}(t_{ij}c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + \sum_{\langle ij\rangle} J_{ij}\vec{S}_i \cdot \vec{S}_j. \tag{2}$$

In this Hamiltonian, we have introduced an antiferromagnetic spin-spin coupling term ($J_{ij} \geq 0$) to account for the virtual electron double occupancy effect. In the large U limit, $J_{ij} \approx 4t_{ij}^2/U$. This model may be viewed as an effective Hamiltonian of the Hubbard model. The inclusion of the antiferromagnetic spin coupling appears consistent with the weak coupling renormalization group analyses [9], and is appropriate in the variational approach studied here. Although the precise values of J_{ij} are to be determined, that does not alter the qualitative physics we will discuss in this paper. In the limit $U \rightarrow \infty$, the model is reduced to the t-J model.

We consider $|\Psi_L\rangle$ in Eq. (1) as a variational trial wave function to examine the superconductor-insulator transition at half filling, and to compare the gossamer superconducting state with the RVB state away from the half filled. In our theory, $u_{\vec{k}}$, $v_{\vec{k}}$, and α_0 are variational parameters. In the limiting case $u_{\vec{k}}v_{\vec{k}} = 0$, $|\Psi_{\text{BCS}}\rangle$ reduces to the Fermi liquid state. $\alpha_0 = 0$ corresponds to the uncorrelated state, and $\alpha_0 = 1$ corresponds to the limit of no doubly occupied state. $\alpha_0 = 1$ if $U \rightarrow \infty$.

The variational energy $E = \langle H\rangle$ is given by,

$$E = Ud + \langle H_t\rangle + \langle H_J\rangle, \tag{3}$$

where $d = \langle n_{i\uparrow}n_{i\downarrow}\rangle$ is the electron double occupation number, and $0 \leq d \leq 1$. $\langle A\rangle$ is the expectation value (per site) of operator A in the state $|\Psi_L\rangle$. The first term is the intrasite Coulomb interaction energy, while the second and the third terms are the average kinetic and spin-spin correlation energies, respectively. Note that in the Gutzwiller approach and at half filling, d is a measure of the mobile carrier density n_c and proportional to n_c/m^* measured in the a.c. conductivity with m^* the effective mass. At $d = 0$, i.e., $\alpha_0 = 1$, we have $\langle H_t\rangle = 0$, and $E = \langle H_J\rangle$ at the half filling. This state describes a Mott insulator. The case with $d > 0$ or $0 \leq \alpha_0 < 1$ describes Laughlin's gossamer superconducting state.

The variational parameter d is determined by the condition $\partial E(d)/\partial d = 0$, or

$$U + \partial\langle H_t\rangle/\partial d + \partial\langle H_J\rangle/\partial d = 0. \tag{4}$$

At half filling, we expect a transition from the Mott insulator at larger U to the gossamer superconductor at smaller U as U decreases passing through a critical point U_c. To study this phase transition, we follow Brinkman and Rice [8] and compare the energies of the two states with the difference that here we consider the projected BCS state while Brinkman and Rice considered the projected Fermi liquid state. The transition point U_c, assumed to be second type, is given by $U_c = (-\partial\langle H_t\rangle/\partial d - \partial\langle H_J\rangle/\partial d)|_{d=0}$. For $U > U_c$, there is no solution of Eq. (4) for physical values of d, indicating that $d = 0$.

We use the Gutzwiller approximation [7] to carry out the variation and to estimate U_c. In the Gutzwiller approximation, the effect of the partial projection operator on the doubly occupied sites is taken into account by a classical statistical weighting factor which multiplies the quantum coherent result calculated for the unprojected state $|\Psi_{\text{BCS}}\rangle$. A clear description of the method has been given by Vollhardt [10]. The method was used to study the two-dimensional t-J model [11], where the projection operator corresponds to the case of $\alpha = 1$ (the complete projection). In the present model, the hopping and the spin-spin correlation energies in the state $|\Psi_L\rangle$ are related to those in the unprojected state $|\Psi_{\text{BCS}}\rangle$ by the corresponding renormalized constants g_t and g_s:

$$\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle = g_t\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle_0, \qquad \langle\vec{S}_i \cdot \vec{S}_j\rangle = g_s\langle\vec{S}_i \cdot \vec{S}_j\rangle_0, \tag{5}$$

where $\langle A\rangle_0$ is the expectation value of operator A in the state $|\Psi_{\text{BCS}}\rangle$. The renormalization facotrs g_t and g_s are determined by the ratios of the probabilities of the corresponding physical processes in the states $|\Psi_L\rangle$ and $|\Psi_{\text{BCS}}\rangle$. By counting the probabilities [11] we obtain these renormalization constants for the partially projected state (n: electron density),

$$g_t = \frac{(n-2d)(\sqrt{d} + \sqrt{1-n+d})^2}{(1-n/2)n},$$
$$g_s = \left[\frac{(n-2d)}{(1-n/2)n}\right]^2. \tag{6}$$

The value of g_t is the same as that previously obtained for the projected Fermi liquid state [7,10]. At $d = 0$, we have $g_t = 2\delta/(1+\delta)$ and $g_s = 4/(1+\delta)^2$, with $\delta = 1 - n$, recovering the results in Ref. [11]. At half filling, $n = 1$, we have $g_t = 8d(1-2d)$ and $g_s = 4(1-2d)^2$. Using the Gutzwiller approximation, The variational condition for d in Eq. (4) becomes

$$\partial E/\partial d = U + \frac{\partial g_t}{\partial d}\langle H_t\rangle_0 + \frac{\partial g_s}{\partial d}\langle H_J\rangle_0 = 0. \tag{7}$$

We note that $\langle H_t\rangle_0 < 0$, $\langle H_J\rangle_0 < 0$, and that $d \le d_0$ with $d_0 \le n^2/4$ the value at $\alpha_0 = 0$. Using Eqs. (6), we have $\partial^2 E/\partial d^2 = (\partial^2 g_t/\partial d^2)\langle H_t\rangle_0 + (\partial^2 g_s/\partial d^2)\langle H_J\rangle_0 > 0$. Therefore, the solution of Eq. (7) corresponds to a minimum in energy or a saddle point. Since $\partial g_t/\partial d \to +\infty$ at $d \to 0^+$ for $n < 1$, there is always a solution of Eq. (7) away from half filled. At $n = 1$, Eq. (7) has no solution for minimum energy if $U > U_c$, and U_c is the transition point between the Mott insulator and the gossamer superconductor. Note that U_c is generally positive if the kinetic energy term in the uncorrelated state dominates. In the insulating phase, only the spin-spin interaction is nonzero. The problem becomes identical to that in the RVB theory at half filling, and there is a redundancy in the fermion representation of the state due to a local SU(2) symmetry of the spin Hamiltonian [11,12]. The redundancy is removed in the gossamer superconducting state for the kinetic energy term breaks the SU(2) symmetry, similar to the effect of doping in the t-J model. At $d \ll 1$, the symmetry of the gossamer superconductivity is the same as the symmetry of the RVB state. Within the Gutzwiller approximation, the pairing order parameter in the gossamer superconductor is related to the uncorrelated state by a renormalized factor g_t,

$$\langle c_{\vec{k}\uparrow} c_{-\vec{k}\downarrow}\rangle = g_t \langle c_{\vec{k}\uparrow} c_{-\vec{k}\downarrow}\rangle_0. \tag{8}$$

Near the transition point, $g_t = 8d \ll 1$, indicating the smallness of the superfluid density, a quantitative measure of the gossamer superconductivity. It is interesting to note that the pairing order parameter in the RVB state has also the form of Eq. (8) with $g_t = 2\delta$ for $\delta \ll 1$. This comparison indicates that a gossamer superconductor with double occupation d at half filling is similar to the RVB superconductor at doping δ with the correspondance of $\delta = 4d$.

In what follows we take an example and consider the effective Hamiltonian in a 2-dimensional square lattice with only the nearest neighbour hopping $t_{ij} = t$ and the nearest neighbor spin coupling $J_{ij} = J$ and consider the case $n \le 1$. For any given value of d, the Coulomb interaction term in the present theory contributes a constant Ud to the variational energy, and the variational procedure for other parameters ($u_{\vec{k}}$ and $v_{\vec{k}}$) is almost the same as that in study of the t-J model carried out in Ref. [11] except that the renormalization constants g_t and g_s here depend also on the double occupation d.

We introduce two correlation functions ($\tau = x, y$), $\Delta_\tau = \sum_\sigma \sigma \langle c_{i\sigma} c_{i+\tau,-\sigma}\rangle_0$, $\chi_\tau = \sum_\sigma \langle c^\dagger_{i\sigma} c_{i+\tau,\sigma}\rangle_0$. The variational solution is then given by the coupled gap equations,

$$\Delta_\tau = \sum_{\vec{k}} \cos k_\tau\, \Delta_{\vec{k}}/E_{\vec{k}}, \qquad \chi_\tau = -\sum_{\vec{k}} \cos k_\tau\, \chi_{\vec{k}}/E_{\vec{k}},$$

where $\Delta_{\vec{k}} = \sum_\tau \Delta_\tau \cos k_\tau$, $\chi_{\vec{k}} = \tilde{\epsilon}_{\vec{k}} - \sum_\tau \chi_\tau \cos k_\tau$. In the above equations, $E_{\vec{k}} = \sqrt{|\Delta_{\vec{k}}|^2 + \chi^2_{\vec{k}}}$, $\tilde{\epsilon}_{\vec{k}} = [-2g_t t(\cos k_x + \cos k_y) - \tilde{\mu}]/(3g_s J/4)$, and $\tilde{\mu}$ is related to the chemical potential μ by

$$\mu = \tilde{\mu} + \frac{\partial g_t}{\partial n}\langle H_t\rangle_0 + \frac{\partial g_s}{\partial n}\langle H_J\rangle_0. \tag{9}$$

In Eq. (9), the second and the third terms originate from the n dependences of g_t and g_s in the variational procedure [11], which will be important in calculation of the chemical potential of the state. These gap equations must be solved simultaneously with Eq. (7) for d and the electron number equation given by $\delta = \sum_{\vec{k}} \chi_{\vec{k}}/E_{\vec{k}}$.

We first discuss the half filled case. The ground state of the insulating phase ($d = 0$) is the same as that of the Heisenberg model. In the metallic phase ($0 < d \ll 1$), the kinetic energy breaks the local SU(2) symmetry and favors the d-wave superconducting state with $\Delta_x = -\Delta_y$. The symmetry is the same as the symmetry studied in the t-J model slightly away from the half filled [11,13,14]. At the superconductor-insulator transition point, we have $\langle H_t\rangle_0 = -2\sqrt{2}tC$ and $\langle H_J\rangle_0 = -(3/4)JC^2$, with $C = \frac{1}{2}\sum_{\vec{k}} \sqrt{\cos^2 k_x + \cos^2 k_y} = 0.479$. We estimate from these values that $U_c = 10.8t - 2.75J$ for large J/t. While for small J/t, $U_c = 128t/\pi^2 = 13t$.

We now discuss the slightly less than half filled case. We expect that the variational parameter d is a smooth function of the electron density around the half filled. The gossamer superconducting state essentially remains unchanged in the regime $\delta \ll d$, and the superconducting order parameter is mainly controlled by d, weakly depending on δ as we can see from the expression for g_t. The chemical potential μ can be calculated by using Eq. (9). In the limit $\delta \to 0^+$, $\tilde{\mu} \to 0$, and we have $\mu \to -4(1 - 4d)\langle H_t\rangle_0 + 8(1 - 2d)\langle H_J\rangle_0 = U/2$. In the last step of the above calculations, we have used variational equation (7) to relate the kinetic and spin coupling energies to the Coulomb energy. Since $\mu = U/2$ at the half filled by electron-hole symmetry of the model, we conclude that in the gossamer superconducting state the chemical potential is continuous at the half filled, and is pinned at the middle of the lower and the higher Hubbard bands. This result is reasonable because the gossamer superconducting state is a metallic state and the chemical potential is expected to be continuous [6]. This feature is in contrast to the RVB state discussed below.

If $U > U_c$ with U_c defined as the critical U at half filling, the state changes dramatically from an insulator to a RVB superconducting state as the electron density varies away from the half filled. At $U \gg U_c$, d changes very little from zero [15], the physics is essentially the same as that given by the t-J model. While the RVB state is similar to the gossamer superconducting state in the sense that they have the same pairing symmetries and small pairing order parameters, the chemical potential in the RVB state is very different from that in the gossamer superconductor. To see this explicitly, we consider the limit $\delta \to 0^+$, so that we have $\tilde{\mu} \to 0$, and $\partial g_t/\partial n = -2$, $\partial g_J/\partial n = 8$. From these values, we obtain $\mu \to -2\langle H_t\rangle_0 + 8\langle H_J\rangle_0 \approx 2.7t - 1.38J$, which is about $U_c/4$

for $J \ll t$, and is much smaller than the chemical potential $U/2$ at the exact half filled. We conclude that the chemical potential in the RVB state is discontinuous at the half filled, and it is shifted from $U/2$ at the half filled to the lower Hubbard band away from the half filled. The difference in the chemical potentials in the gossamer and the RVB states can in principle be distinguished in spectroscopic experiments, although other symmetry broken states not included in the variational theory and the inhomogeneity will complicate the analyses.

The metal or insulator nature of the variational gossamer superconducting states we considered here are insensitive to the electron band structure. Some other broken symmetry states such as antiferromagnetism, which we do not include in the theory, are more sensitive to the band structure. For instance, the Hubbard model with nearest neighbor hopping integral in a square lattice has perfect nesting at half filling, and any small value of U leads to an antiferromagnetic or spin density wave ground state. Therefore, the present theory may be more applicable to systems with general electron band structure. Furthermore, the phase transition and the similarities and the differences between the gossamer and the RVB superconductors should be relevant to the systems away from half filled. It is interesting to note that the half filled superconducting state may be stabilized against the antiferromagnetism in the presence of an explicit pair hopping term in the Hubbard model as studied by Assaad *et al.* [16]. The gossamer superconductor should also be relevant to the frustrated magnetic systems where the anitferromagnetism is suppressed. For instance, there have been numerical studies of the antiferromagnetic Heisenberg spin model with nearest and next nearest neighbor couplings to show evidence for a spin liquid ground state [17]. There have been numerical studies of the Hubbard model at half filling with nearest and next nearest hoppings to demonstrate a paramagnetic insulating phase with a transition to a metallic phase at zero temperature as U decreases [18]. It will be interesting to examine the possible gossamer superconductivity in that metallic phase.

In summary, we have used the Gutzwiller variational method to study an effective Hubbard model. The calculation based on the Gutzwiller approximation supports Laughlin's recent proposal of gossamer superconductor at relatively smaller intrasite electron Coulomb repulsion U, and predicts a phase transition from the gossamer superconductor to the Mott insulator as U increases at density one electron per site. The gossamer superconductor is similar to the RVB superconducting state with the major difference on the positions of their chemical potentials. The Gutzwiller approximation we used in this Letter has been previously tested against variational Monte Carlo method [19] with quite good agreement [11]. The variational parameter d in the Gutzwiller method has one-to-one correspondance with the parameter α_0 in Laughlin's theory. As α_0 varies from 0 to 1, d varies monototically from the uncorrelated value d_0 to 0. The explicit relation between d and α_0 is given by $g_t \approx g^2$, with g_t given by Eq. (6) in the present Letter and g^2 by Eq. (19) in Ref. [6]. In the limit $\alpha_0 \to 1$, $d = (1 - \alpha_0)/2$. The variational calculation can be in principle extended to include also an antiferromagnetic order parameter. We speculate that the ground state at half filling can be an antiferromagnetic insulator at large U and a gossamer superconductor possibly coexisting with the antiferromagnetism at small U.

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