Ph223c **<u>Problem Set #4</u> (Parts VII, VIII.1&2)** May 28, 2008
(Due: June 6, 2008)

1. The one-band *t-J* model of the cuprates and the slave-boson formalism for pairing in the cuprates

We have described in Part VII.2 the primary assumptions and key steps required to derive a microscopic model Hamiltonian for the strongly correlated cuprates from the Mott insulator limit where no double occupancies at the same site are allowed. Specifically, we may apply the Gutzwiller projection operators P_G to the one-band Hubbard Hamiltonian of the CuO_2 plane so that

$$\tilde{d}^{\dagger}_{i,\sigma} P_G \equiv \tilde{d}^{\dagger}_{i,\sigma}\left(1-n_{i,-\sigma}\right), \qquad \text{(VII.52)}$$

which is only non-trivial if the *i*-th site is not occupied. This procedure effectively reduces the Hilbert space associated with the original Hamiltonian of the Hubbard model to a no-double occupancy Hilbert space of a *t-J* Hamiltonian. Assuming hole doping into the CuO_2 plane so that there is strong *p-d* orbital hybridization and keeping to the lowest order in $(t^2/U) \equiv J$ in the nearly half-filling limit, we want to derive the effective one-band *t-J* Hamiltonian for the CuO_2 plane given by EQ. (VII.51) from the one-band Hubbard model in EQ. (VII.47). That is, we want to show that under the Gutzwiller projection, the one-band Hubbard model in EQ. (VII.47) that consists of a kinetic term $\mathcal{H}_K$ and an interaction term $\mathcal{H}_U$:

$$\mathcal{H} = \sum_{\langle i,j\rangle,\sigma} t_{ij} d^{\dagger}_{i,\sigma} d_{j,\sigma} + U\sum_i n_{i,\uparrow} n_{j,\downarrow} \equiv \mathcal{H}_0 + \mathcal{H}_I \qquad \text{(VII.47)}$$

can be projected out into the one-band *t-J* Hamiltonian given by EQ. (VII.51) (which is reproduced below) in the half-filling limit:

$$\begin{aligned}\mathcal{H} &= -t\sum_{\langle i,j\rangle}\Big[\left(1-n_{i,-\sigma}\right)\tilde{d}^{\dagger}_{i,\sigma}\tilde{d}_{j,\sigma}\left(1-n_{j,-\sigma}\right) + n_{i,-\sigma}\tilde{d}^{\dagger}_{i,\sigma}\tilde{d}_{j,\sigma} n_{j,-\sigma} \\ &\qquad + \left(1-n_{i,-\sigma}\right)\tilde{d}^{\dagger}_{i,\sigma}\tilde{d}_{j,\sigma} n_{j,-\sigma} + n_{i,-\sigma}\tilde{d}^{\dagger}_{i,\sigma}\tilde{d}_{j,\sigma}\left(1-n_{j,-\sigma}\right)\Big] + \frac{U}{2}\sum_{i\sigma} n_{i,\sigma} n_{i,-\sigma} \\ &= -t\sum_{\langle i,j\rangle}\Big[\left(1-n_{i,-\sigma}\right)\tilde{d}^{\dagger}_{i,\sigma}\tilde{d}_{j,\sigma}\left(1-n_{j,-\sigma}\right)\Big] + J\sum_{\langle ij\rangle}\left(\mathbf{S}_i \bullet \mathbf{S}_j - \frac{1}{4} n_{\tilde{d}i} n_{\tilde{d}j}\right) \text{ for no double occupancy.}\end{aligned} \qquad \text{(VII.51)}$$

where the spin operators $\mathbf{S}_i$ are given by $\mathbf{S}_i \equiv \sum_{\mu\nu} \frac{1}{2} d^{\dagger}_{i\mu} \boldsymbol{\sigma}_{\mu\nu} d_{i\nu}$ with $\boldsymbol{\sigma}_{\mu\nu}$ denoting the Pauli matrices, the charge operators are given by $n_{\tilde{d}i} \equiv \sum_{\sigma} \tilde{d}^{\dagger}_{i,\sigma}\tilde{d}_{i,\sigma}$, $\langle i,j\rangle$ refers to sum over nearest neighbors, $U \equiv \varepsilon_p^0 - \varepsilon_d^0$, $t \simeq z t_{pd}^2 \big/ \left(\varepsilon_p^0 - \varepsilon_d^r\right)$, z denotes the hole doping level and t_{pd} is the hopping coefficient in the two-band model, and the cross terms involving $\left(1-n_{i,-\sigma}\right) n_{j,-\sigma}$ and $n_{i,-\sigma}\left(1-n_{j,-\sigma}\right)$ can be removed from the second line of EQ. (VII.51).

(a) Before making the Gutzwiller projection, let us consider a more general projection procedure for the one- band Hubbard model. For an arbitrary projection operator P_1 that satisfies the condition $P_1^2 = P_1$, if we define a second projection operator $P_2 \equiv 1 - P_1$, we find that $P_2^2 = P_2$ and $P_1P_2 = P_2P_1 = 0$. Next, the eigen-value problem $\mathcal{H}\psi = E\psi$ for the Hamiltonian $\mathcal{H}$ can be rewritten into the following:

$$\mathcal{H}\left(P_1 + P_2\right)\psi = E\left(P_1 + P_2\right)\psi, \qquad (9)$$

$$\Rightarrow \quad P_2\mathcal{H}\left(P_1+P_2\right)\psi = P_2E\left(P_1+P_2\right)\psi \quad \Rightarrow \quad P_2\psi = -\frac{1}{\left(P_2\mathcal{H}P_2-E\right)}P_2\mathcal{H}P_1\psi\ . \tag{10}$$

From $P_1\mathcal{H}\left(P_1+P_2\right)\psi = P_1E\left(P_1+P_2\right)\psi$ and the above expression for $P_2\psi$, show that we can define an effective Hamiltonian $\mathcal{H}_{\text{eff}}$ so that $\mathcal{H}_{\text{eff}}P_1\psi = EP_1\psi$, where

$$\mathcal{H}_{\text{eff}} \equiv P_1\mathcal{H}P_1 - P_1\mathcal{H}\frac{1}{\left(P_2\mathcal{H}P_2-E\right)}P_2\mathcal{H}P_1\,. \tag{11}$$

This effective Hamiltonian $\mathcal{H}_{\text{eff}}$ therefore reduces the Hilbert space of the original Hamiltonian $\mathcal{H}$ into that of the projection operator P_1.

(b) Now if we specify the projection operator P_1 in Part **(a)** as the Gutzwiller projection operator P_G where

$$P_G \equiv \prod_i \left(1-n_{i,\uparrow}n_{i,\downarrow}\right),$$

we find that

$$P_G\mathcal{H}_IP_G = 0 \quad \Rightarrow \quad P_G\mathcal{H}P_G = P_G\mathcal{H}_0P_G\,, \tag{12}$$

$$P_G\mathcal{H}_IP_2 = 0 \quad \Rightarrow \quad P_G\mathcal{H}P_2 = P_G\mathcal{H}_0P_2\,, \tag{13}$$

and

$$P_2\mathcal{H}_IP_G = 0 \quad \Rightarrow \quad P_2\mathcal{H}P_G = P_2\mathcal{H}_0P_G\,. \tag{14}$$

Using the above identities and taking the half-filling limit, show that in the lowest order of (E/U), the effective Hamiltonian becomes

$$\mathcal{H}_{\text{eff}} \simeq P_G\mathcal{H}_0P_G - \left(P_G\mathcal{H}_0P_2\mathcal{H}_0P_G/U\right). \tag{15}$$

(c) Now consider the numerator in the second term of $\mathcal{H}_{\text{eff}}$ and show that it can be expressed as

$$\begin{aligned} P_G\mathcal{H}_0P_2\mathcal{H}_0P_G &= \sum_{i,j,i',j',s,s'} t_{ij}t_{i'j'}P_G\,d^\dagger_{i,s}d_{j,s}\,P_2\,d^\dagger_{j',s'}d_{i',s'}\,P_G \\ &\approx \sum_{\langle i,j\rangle,s,s'} \left|t_{ij}\right|^2 P_G\,d^\dagger_{i,s}d_{j,s}n_{j\uparrow}n_{j\downarrow}d^\dagger_{j,s'}d_{i,s'}P_G \\ &= \sum_{\langle i,j\rangle,s,s'} \left|t_{ij}\right|^2 P_G\,d^\dagger_{i,s}d_{i,s'}d_{j,s}d^\dagger_{j,s'}n_jP_G\ , \end{aligned} \tag{16}$$

where we have used the condition $j = j'$ because of the constraints on P_G and P_2 and have ignored terms with $i \neq i'$.

(d) Given the results in Part **(c)** and the identity for the multiplication rule of the Pauli matrix elements $\sigma^a_{\alpha\beta}\sigma^a_{\mu\nu} = 2\delta_{\alpha\nu}\delta_{\beta\mu} - \delta_{\alpha\beta}\delta_{\mu\nu}$ with a = 1, 2, 3, show that

$$P_G\mathcal{H}_0P_2\mathcal{H}_0P_G = \sum_{\langle i,j\rangle,s,s'} \left|t_{ij}\right|^2 P_G\left(\frac{n_in_j}{2} - 2\mathbf{S}_i\bullet\mathbf{S}_j\right)P_G\ , \tag{17}$$

where we have used the relations

$$d_{i,s}^{\dagger} d_{i,s'} = \frac{1}{2}\delta_{ss'} n_i + S^a \sigma_{ss'}^a \qquad \text{and} \qquad d_{i,s} d_{i,s'}^{\dagger} = \left(1 - \frac{1}{2} n_i\right)\delta_{ss'} - S^a \sigma_{ss'}^a . \tag{18}$$

Finally, verify the validity of EQ. (VII.51) using the results derived from Part **(a)** to Part **(d)**.

(e) In the mean-field limit the exchange interaction term in the one-band *t-J* model can be rewritten by means of the slave-boson formalism into the following form for pseudo fermions $\tilde{d}$ and $\tilde{d}^{\dagger}$:

$$\mathcal{H}_I = J \sum_{\langle i\,j \rangle} \left(\mathbf{S}_i \bullet \mathbf{S}_j - \frac{1}{4} n_{\tilde{d}i} n_{\tilde{d}j} \right) \equiv -\frac{J}{2} \sum_{\langle i\,j \rangle, \sigma} \left(\tilde{d}_{i,\sigma}^{\dagger} \tilde{d}_{j,-\sigma}^{\dagger} \tilde{d}_{i,-\sigma} \tilde{d}_{j,\sigma} + \tilde{d}_{i,\sigma}^{\dagger} \tilde{d}_{j,-\sigma}^{\dagger} \tilde{d}_{j,-\sigma} \tilde{d}_{i,\sigma} \right), \tag{VII.56}$$

The relation given in EQ. (VII.56) is essential for "finding attraction from repulsion" in the CuO_2 plane. That is, the repulsive antiferromagnetic exchange interaction can lead to an effective Cooper pairing due to a special "quantum choreography" of the pseudo fermions imposed by the slave-boson formalism. Prove that EQ. (VII.56) is indeed correct.

2. The staggered flux phase

As discussed in Part VII.2, the staggered flux phase can arises in the limit of half-filling in the CuO_2 plane by considering the one-band *t-J* Hamiltonian under the slave-boson transformation in EQ. (VII.56), which has been reproduced above in Problem 1(e). If we divide the square lattice into a bipartite lattice with sublattices A and B, and perform the transformation

$$\tilde{d}_{\text{B-sublattice}}^{\dagger} \Rightarrow \tilde{d}_{\text{B-sublattice}} ,$$

the antiferromagnetic repulsion ($J > 0$) between nearest-neighbor spins becomes attractive between adjacent pseudo fermions if we define the following definition:

$$\chi_{i\,j} \equiv \sum_{\sigma} \left\langle \tilde{d}_{i,\sigma}^{\dagger} \tilde{d}_{j,\sigma} \right\rangle .$$

(a) Show that the interaction Hamiltonian in EQ. (VII.56) can be rewrittem in terms of the Nambu spinor format $\psi_{\mathbf{k}}^{\dagger} \equiv \left(\tilde{d}_{\mathbf{k}}^{\dagger} \;\; \tilde{d}_{\mathbf{k+Q}}^{\dagger} \right)$ with **Q** denoting the vector (π, π):

$$\mathcal{H}_{\infty} = \sum_{\mathbf{k}'} \psi_{\mathbf{k}'}^{\dagger} \mathcal{H}_{\mathbf{k}'} \psi_{\mathbf{k}'} , \tag{19}$$

where **k′** refers to the k-vectors in the reduced Brillouin zone of the staggered flux phase, and

$$\mathcal{H}_{\mathbf{k}'} = \frac{J}{2} \begin{pmatrix} \left(\cos k_x + \cos k_y\right) & i\left(\cos k_x - \cos k_y\right) \\ -i\left(\cos k_x - \cos k_y\right) & -\left(\cos k_x + \cos k_y\right) \end{pmatrix} = \frac{J}{2}\left[\left(\cos k_x + \cos k_y\right)\tau_3 + \left(\cos k_x - \cos k_y\right)\tau_2 \right], \tag{20}$$

with τ_2 and τ_3 being the Pauli matrices, and we have taken the square lattice constant to be unity.

(b) From the Hamiltonian given in **(a)**, the eigen-energies of of the staggered flux phase are clearly given by

$$E_{k\pm} = \pm\frac{J}{\sqrt{2}}\sqrt{\left(\cos k_x\right)^2 + \left(\cos k_y\right)^2}\,, \tag{21}$$

which corresponds to a two-dimensional Fermi surface with a pair of points at $(\pi/2, \pm\pi/2)$. In the vicinity of these points the energy bands are cone-shaped if we write $k_x' \equiv k_x - (\pi/2)$ and $k_y' \equiv k_y - (\pm\pi/2)$ so that EQ. (21) becomes $E_{k'\pm} = \pm J\sqrt{[\left(\sin k_x'\right)^2 + \left(\sin k_y'\right)^2]/2}$. Therefore, the pseudo-fermions near $(\pi/2, \pm\pi/2)$ are gapless neutral spin-1/2 Dirac fermions, which we call spinons. Next, we want to investigate the low-energy spinons in the staggered flux phase by considering the continuum limit. Show that the Hamiltonian in the continuum limit acquires the following form:

$$\mathcal{H} = v\sum_{\mathbf{k}'}\psi_{\mathbf{k}'}^{\dagger}\left(k_x'\Gamma_x + k_y'\Gamma_y\right)\psi_{\mathbf{k}'}\,, \tag{22}$$

where $\psi_{\mathbf{k}'}^{\dagger} \equiv \left(\tilde{d}_{\mathbf{k}'}^{\dagger} \;\; \tilde{d}_{\mathbf{k}'+\mathbf{Q}}^{\dagger}\right)$ and $\Gamma_x^2 = \Gamma_y^2 = 1$. Find the explicit expressions for v and $\Gamma_{x,y}$.

(c) In real space, the Lagrangian associated with the Hamiltonian in EQ. (22) is

$$\mathcal{L} = i\psi^{\dagger}\partial_t\psi + v\psi^{\dagger}\left(i\Gamma_x\partial_x + i\Gamma_y\partial_y\right)\psi\,. \tag{23}$$

Show that EQ. (23) can be rewritten into the following form:

$$\mathcal{L} = i\bar{\psi}\left(\gamma^0\partial_t + v\gamma^x\partial_x + v\gamma^y\partial_y\right)\psi\,, \tag{24}$$

where $\bar{\psi} = \psi^{\dagger}\gamma^0$, $\left(\gamma^0\right)^2 = 1$, and $\left(\Gamma_x, \Gamma_y\right) = \left(-\gamma^0\gamma^x, -\gamma^0\gamma^y\right)$. Find the explicit forms of $\gamma^{0,x,y}$.

(d) Verify that $\gamma^{0,x,y}$ in EQ. (24) satisfy the following Dirac algebra in (2+1)-dimensions:

$$\left\{\gamma^{\mu}, \gamma^{\nu}\right\} = \eta^{\mu\nu}\,, \qquad (\mu, \nu = 0, x, y), \tag{25}$$

where $\eta^{\mu\nu}$ is a diagonal matrix with $\eta^{00} = 1$, $\eta^{xx} = \eta^{yy} = -1$.

(e) Find the Lagrangian of the Dirac fermions that is minimally coupled to a $U(1)$ gauge field and is also $U(1)$ gauge invariant.

3. The Chern-Simons term in (D+1)-dimensional space-time

(a) Consider the mass dimensions of the Chern-Simons term and the Maxwell term in (D+1)-dimensional space-time. Prove that at long distances the Maxwell term is irrelevant relative to the Chern-Simons term for D = 2, becomes comparable to the Chern-Simons term for D = 3, and dominates over the Chern-Simons term if D = 4.

(b) In (2+1)-dimensional space-time, calculate the propagator for a $U(1)$-gauge field with the Chern-Simons term. Show that the Chern-Simons term gives rise to a topological mass and examine the behavior of the propagator in the long-wavelength limit.

(c) For a Lagrangian $\mathcal{L}_0$ with a conserved current J^μ in (2+1)-dimensional space-time, we construct a Lagrangian $\mathcal{L}$ that involves the Chern-Simons term $\varepsilon^{\mu\nu\lambda} a_\mu \partial_\nu a_\lambda$:

$$\mathcal{L} = \mathcal{L}_0 - \gamma \varepsilon^{\mu\nu\lambda} a_\mu \partial_\nu a_\lambda + a_\mu J^\mu , \tag{26}$$

where a_μ denotes a gauge potential. Show that with the choice of the Lorentz gauge $\partial_\mu a^\mu = 0$, one can integrate out the gauge potential *a* in EQ. (26) and obtain the following non-local Lagrangian:

$$\mathcal{L}_{\text{Hopf}} = \frac{1}{4\gamma}\left(J_\mu \frac{\varepsilon^{\mu\nu\lambda}\partial_\nu}{\partial^2} J_\lambda \right). \tag{27}$$

The Lagrangian $\mathcal{L}_{\text{Hopf}}$ in EQ. (27) is known as *the Hopf term*, which, in the fractional quantum Hall fluids, is related to the quasiparticle interactions.