Ph223b **<u>Problem Set #4</u> (Parts V.3– V.4)** February 28, 2007
(Due: March 16, 2007)

1. Tunneling spectroscopy of a superconductor with *p*-wave pairing symmetry

In Part V.3 and Part V.4 we have primarily focused on singlet superconductors whose orbital pair wavefunctions are of even angular momentum quantum numbers l = 0, 2, … due to symmetry consideration, and the corresponding pairing symmetries are therefore *s*-wave, *d*-wave, etc. Similar symmetry consideration suggests that for triplet superconductors (such as certain heavy-fermion superconductors discussed in Part V.5) the orbital pair wavefunctions must be associated with odd angular momentum quantum numbers l = 1, 3, … so that the pairing symmetries are *p*-wave, *f*-wave, etc. In this problem, you are asked to derive the quasiparticle tunneling spectrum of certain triplet superconductors by means of numerical analysis.

(a) Using the generalized BTK formalism derived in Part V.3, find the quasiparticle tunneling spectrum (*i.e.*, the tunneling conductance σ_S versus quasiparticle energy E) of a superconductor with a pure *p*-wave pairing potential $\Delta(\mathbf{k}) = \Delta_p \cos\theta_{\mathbf{k}}$, provided that quasiparticles are tunneling along the nodal direction (i.e. the k_y-axis) of the superconductor. Here $\cos\theta_{\mathbf{k}} \equiv \left(k_x / |\mathbf{k}|\right)$, $|\mathbf{k}|^2 = k_x^2 + k_y^2$, and we have assumed a two-dimensional superconductor.

(b) Suppose that the time-reversal symmetry is broken in the *p*-wave superconductor by the presence of a small imaginary component in the pairing potential so that $\Delta(\mathbf{k}) = \Delta_p \left[\cos\theta_{\mathbf{k}} - i\delta \sin\theta_{\mathbf{k}}\right]$ where $\delta < 1$. Find the quasiparticle spectrum of this $(p_x - ip_y)$-wave superconductor for quasiparticles tunneling along the k_y-direction. It is worth mentioning that the quasiparticle wavefunctions associated with the vortex state of a $(p_x - ip_y)$-wave pairing superconductor in fact exhibit non-abelian statistics, and are therefore of interest in the possible construction of qubits for quantum computation.

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

We have described in Part V.4 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

$$\tilde{d}_{i,\sigma}^{\dagger} P_G \equiv \tilde{d}_{i,\sigma}^{\dagger}\left(1 - n_{i,-\sigma}\right), \tag{V.312}$$

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. (V.311) from the one-band Hubbard model in EQ. (V.307). That is, we want to show that under the Gutzwiller projection, the one-band Hubbard model in EQ. (V.307) that consists of a kinetic term $\mathcal{H}_K$ and an interaction term $\mathcal{H}_U$:

$$\mathcal{H} = \sum_{\langle i,j\rangle,\sigma} t_{ij} d_{i,\sigma}^{\dagger} d_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{j,\downarrow} \equiv \mathcal{H}_0 + \mathcal{H}_I \tag{V.307}$$

can be projected out into the one-band *t-J* Hamiltonian given by EQ. (V.311) (which is reproduced below) in the half-filling limit:

$$\mathcal{H} = -t\sum_{\langle i,j\rangle}\Big[\left(1-n_{i,-\sigma}\right)\tilde{d}^{\dagger}_{i,\sigma}\tilde{d}_{j,-\sigma}\left(1-n_{j,-\sigma}\right)+n_{i,-\sigma}\tilde{d}^{\dagger}_{i,\sigma}\tilde{d}_{j,-\sigma}n_{j,-\sigma}$$

$$+\left(1-n_{i,-\sigma}\right)\tilde{d}^{\dagger}_{i,\sigma}\tilde{d}_{j,-\sigma}n_{j,-\sigma}+n_{i,-\sigma}\tilde{d}^{\dagger}_{i,\sigma}\tilde{d}_{j,-\sigma}\left(1-n_{j,-\sigma}\right)\Big]+\frac{U}{2}\sum_{i\sigma}n_{i,\sigma}n_{i,-\sigma}$$

$$=-t\sum_{\langle i,j\rangle}\Big[\left(1-n_{i,-\sigma}\right)\tilde{d}^{\dagger}_{i,\sigma}\tilde{d}_{j,-\sigma}\left(1-n_{j,-\sigma}\right)+n_{i,-\sigma}\tilde{d}^{\dagger}_{i,\sigma}\tilde{d}_{j,-\sigma}n_{j,-\sigma}\Big]+J\sum_{\langle ij\rangle}\left(\mathbf{S}_i\bullet\mathbf{S}_j-\frac{1}{4}n_{\tilde{d}i}n_{\tilde{d}j}\right), \qquad \text{(V.311)}$$

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, $U \equiv \varepsilon^0_p - \varepsilon^0_d$, $t \simeq zt^2_{pd}\big/\left(\varepsilon^0_p-\varepsilon^r_d\right)$, 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. (V.311).

(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:

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

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

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

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

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
$$P_G\mathcal{H}_IP_G = 0 \quad\Rightarrow\quad P_G\mathcal{H}P_G = P_G\mathcal{H}_0P_G\,,$$
$$P_G\mathcal{H}_IP_2 = 0 \quad\Rightarrow\quad P_G\mathcal{H}P_2 = P_G\mathcal{H}_0P_2\,,$$
and
$$P_2\mathcal{H}_IP_G = 0 \quad\Rightarrow\quad P_2\mathcal{H}P_G = P_2\mathcal{H}_0P_G\,.$$

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

$$\mathcal{H}_{\text{eff}} \simeq P_G \mathcal{H}_0 P_G - \left(P_G \mathcal{H}_0 P_2 \mathcal{H}_0 P_G / U \right).$$

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

$$\begin{aligned} P_G \mathcal{H}_0 P_2 \mathcal{H}_0 P_G &= \sum_{i,j,i',j',s,s'} t_{ij} t_{i'j'} P_G d_{i,s}^\dagger d_{j,s} P_2 d_{i',s'}^\dagger d_{j',s'} P_G \\ &\approx \sum_{\langle i,j \rangle, s,s'} \left| t_{ij} \right|^2 P_G d_{i,s}^\dagger d_{i,s} n_{j\uparrow} n_{j\downarrow} d_{j,s'}^\dagger d_{j,s'} P_G \\ &= \sum_{\langle i,j \rangle, s,s'} \left| t_{ij} \right|^2 P_G d_{i,s}^\dagger d_{i,s'} d_{j,s} d_{j,s'}^\dagger n_j P_G \ , \end{aligned}$$

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 $\sigma_{\alpha\beta}^a \sigma_{\mu\nu}^a = 2\delta_{\alpha\nu}\delta_{\beta\mu} - \delta_{\alpha\beta}\delta_{\mu\nu}$ with a = 1, 2, 3, show that

$$P_G \mathcal{H}_0 P_2 \mathcal{H}_0 P_G = \sum_{\langle i,j \rangle, s,s'} \left| t_{ij} \right|^2 P_G \left(\frac{n_i n_j}{2} - 2\mathbf{S}_i \bullet \mathbf{S}_j \right) P_G \ ,$$

where we have used the relations

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

Finally, verify the validity of EQ. (V.311) 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 $\tilde{d}^\dagger$:

$$\mathcal{H}_I = J \sum_{\langle ij \rangle} \left(\mathbf{S}_i \bullet \mathbf{S}_j - \frac{1}{4} n_{\tilde{d}i} n_{\tilde{d}j} \right) \equiv -\frac{J}{2} \sum_{\langle ij \rangle, \sigma} \left(\tilde{d}_{i,\sigma}^\dagger \tilde{d}_{j,-\sigma}^\dagger \tilde{d}_{j,\sigma} \tilde{d}_{i,-\sigma} + \tilde{d}_{i,\sigma}^\dagger \tilde{d}_{j,-\sigma}^\dagger \tilde{d}_{i,\sigma} \tilde{d}_{j,-\sigma} \right), \qquad \text{(V.316)}$$

The relation given in EQ. (V.316) 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. (V.316) is indeed correct.