PHYS 798C Spring 2022
Lecture 29 Summary

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I. THE CUPRATE MATERIALS

The cuprate superconductors all have one thing in common - the presence of square CuO_2 planes in their crystal structures (see Fig. 1). These materials are all insulating anti-ferromagnetic materials in the un-doped, or parent compound, state. The anti-ferromagnetism is centered in the CuO_2 planes and the Neel temperature is typically near or above room temperature. The insulating state is due in part to the strong on-site Coulomb repulsion created when additional charge carriers try to doubly occupy the Cu d-orbitals. Hence the d-electrons remain localized on each lattice site.

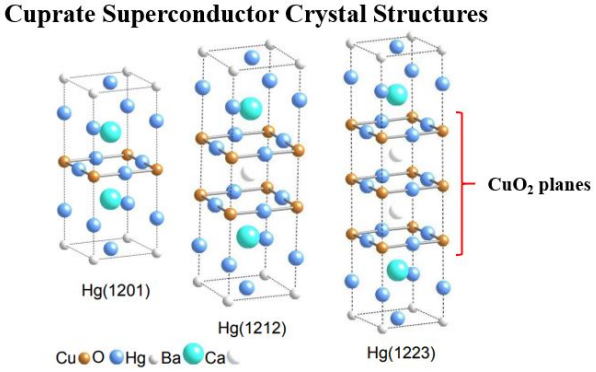

FIG. 1. Crystal structures of the Hg-based cuprate family going from 1-layer to 3-layer structures. The figures in this document come from D. J. Scalapino, "A common thread: The pairing interaction for unconventional superconductors," Rev Mod Phys 84 (4), 1383-1417 (2012); and D. J. Scalapino, "Superconductivity and Spin Fluctuations," J Low Temp Phys 117, 179-188 (1999).

Things change when the CuO_2 planes are doped with carriers, either holes or electrons (see Fig. 2). The Neel temperature drops dramatically with carrier doping, going to zero at a critical doping. Somewhere beyond this doping superconductivity appears, again localized in the CuO_2 planes. The phase diagram of the cuprates shows the temperature-doping plane and includes multiple phases and states. One of the confusing aspects of these materials is that there are many competing effects acting simultaneously, and it is difficult to unambiguously identify the precise mechanism for each observed feature. The un-doped materials can be doped with either holes or electrons, although usually not in a single material.

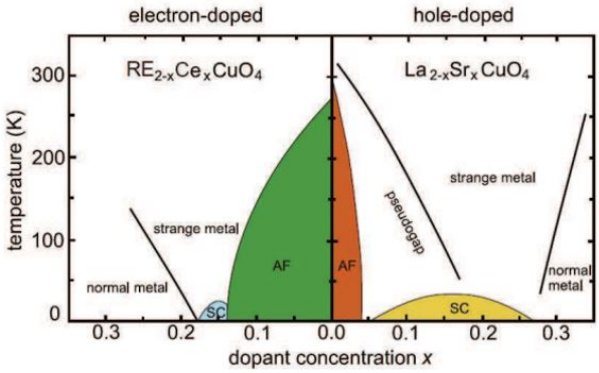

FIG. 2. Phase diagram of the electron-doped and hole-doped cuprate superconductors. Note the superconducting domes as a function of doping, characteristic of materials with competing interactions between superconductivity and other forms of long-range order.

II. SUPERCONDUCTIVITY IN THE CUPRATES

It was demonstrated through flux quantization measurements by Colin Gough that the cuprates have paired charge carriers, giving rise to flux quantization in units of $\Phi_0 = h/2e$. It was also shown that the pairs involve a spin singlet state through measurements of the Knight shift in the superconducting state. The interaction between the electron spin $\vec{S}$ and the nuclear moment $\vec{I}$ is $\mathcal{H}_{int} \sim \vec{S} \cdot \vec{I}$, leading to the Knight shift $K(T)$ that measures the electron spin susceptibility. This is observed to go to zero in the limit of zero temperature, consistent with a spin singlet pairing state.

A number of thermodynamic properties of the cuprates suggest that they have nodes in the superconducting energy gap on the Fermi surface. These include measurements of the magnetic penetration depth temperature dependence. In conventional s-wave superconductors the penetration depth increases from its zero temperature value slowly as a function of temperature, $\lambda(T) - \lambda(0) \sim e^{-\Delta(0)/k_B T}$ for $T < T_c/3$. This activated behavior is due to the fully-gapped nature of the Fermi surface, $\Delta_{\vec{k}} \sim \Delta_0$. Nodal superconductors show a power-law temperature dependence of the penetration depth, $\lambda(T) - \lambda(0) \sim T^n$, with $n = 1$ for the cuprates. This value of n is expected for superconductors with line-nodes of the energy gap on the Fermi surface.

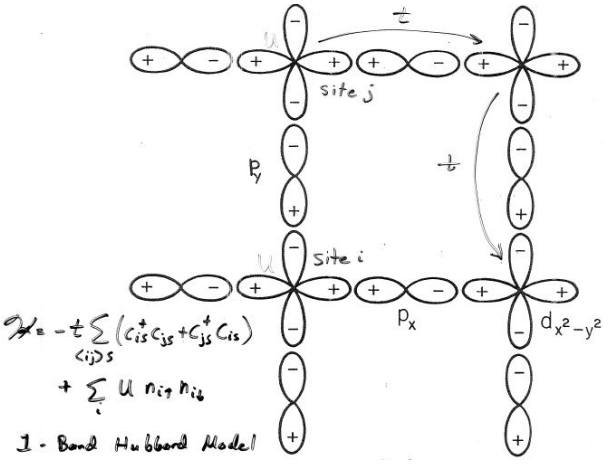

FIG. 3. Diagram of orbitals in a single CuO_2 plane, along with the 1-band Hubbard model.

III. PAIRING MECHANISM IN THE CUPRATES

It is commonly believed that an electronic pairing mechanism, as opposed to an electron-phonon mechanism, is responsible for superconductivity in the cuprates. A simple model of electron transport in the CuO_2 planes is the Hubbard model. In the simple 1-band Hubbard model we treat the Cu $d_{x^2-y^2}$ orbitals as being in a square lattice, with lobes joined to each other through O p_x and p_y orbitals (see Fig. 3). A charge carrier can hop from one Cu to another with transfer energy t. If two charge carriers occupy the same Cu at once, there is a large Coulomb repulsion price $U >> t$. The simple 1-band Hubbard Hamiltonian is,

$$\mathcal{H} = -\sum_{\langle ij \rangle s} t(c_{is}^{+} c_{js} + c_{js}^{+} c_{is}) + \sum_i U n_{i,\uparrow} n_{i,\downarrow}$$

where $n_{is} = c_{i,s}^{+} c_{is}$ is the number operator on site i for spin s, and the notation $\langle ij \rangle$ refers to sites i and j that are nearest neighbors in the square lattice. Here t is the effective one-electron transfer energy, and U is the on-site Coulomb repulsion.

At half-filling of the band there is one electron per Cu site and the ground state shows antiferromagnetic long-range order in a certain range of U/t (see for example arXiv:1505.02290). The nature of this antiferromagnetic ground state is thought by some to be an spin-liquid state, rather than a static ordered array of spins. It is thought by some theorists that away from half-filling, the Hubbard model is unstable to correlations that resemble superconductivity in the low temperature limit.

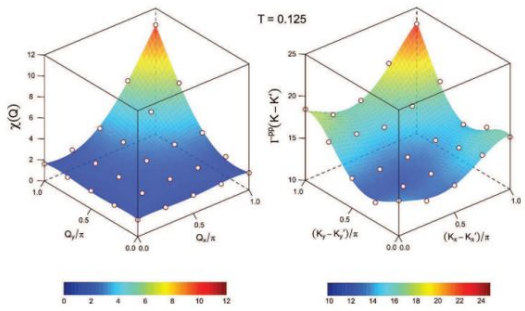

FIG. 4. (Left) Spin susceptibility $\chi(\vec{k},\vec{k}')$ of charge carriers in the CuO_2 plane shown in one quarter of the Brilloiun zone. (Right) Pairing interaction $V(\vec{k}-\vec{k}')$ in a quarter of the Brillouin zone.

How might superconductivity come about in the CuO_2 planes? Berk and Schrieffer (Berk, N. F., and J. R. Schrieffer, Phys. Rev. Lett. 17, 433 (1966)) calculated a pairing interaction associated with anti-ferromagnetic spin fluctuations of the form $V_{\vec{k}\vec{k}'} = \frac{3}{2}U^2\chi(\vec{k}-\vec{k}')$, where $\chi(\vec{k}-\vec{k}')$ is the spin susceptibility at the difference wavenumber. They were interested in understanding why spin fluctuations suppress the T_c of s-wave superconducting materials such as Pd (4d transition metal just below Ni in the periodic table). In the cuprates, calculations show that the spin susceptibility is strongly peaked at the corners of the Brillouin zone, (π,π), $(\pi,-\pi)$, $(-\pi,\pi)$, and $(-\pi,-\pi)$ (see Fig. 4). However, the spin susceptibility, and the resulting pairing interaction, are both strictly positive. This would seem to preclude the possibility of superconductivity. Indeed in the s-wave (zero orbital angular momentum pairing state) with electron momenta $\vec{k}$, $-\vec{k}$ there is no superconductivity.

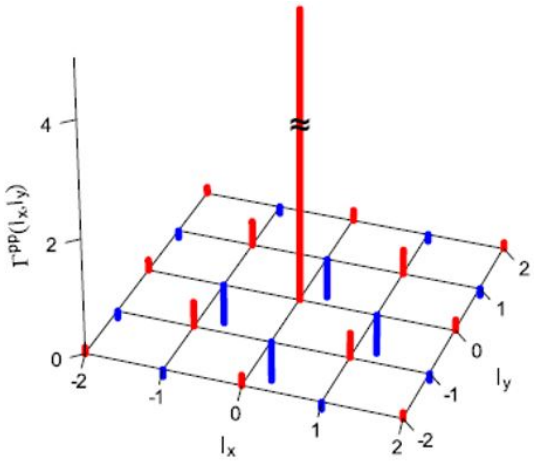

FIG. 5. Fourier transform of anti-ferromagnetic spin fluctuation pairing interaction $V(\vec{r})$ into real space (l_x, l_y). Note the large positive spike at $(l_x, l_y) = (0, 0)$

To understand how superconductivity comes about, it is useful to Fourier transform the pairing interaction into real space, $V(\vec{r}) = \int e^{i\vec{q}\cdot\vec{r}}V(\vec{q})d^3q$. Figure 5 shows a very strong on-site repulsion, signified by the large positive value of $V(l_x = l_y = 0)$. On the other hand, there are negative values (blue) for the pairing interaction in real space, at the nearest neighbor locations in the l_x and l_y directions. This suggests that the charge carriers will avoid double occupation of a site, and preferentially choose nearest neighbor sites that are in the directions of the oxygen atoms in the CuO_2 planes. This can be accomplished if the Cooper pairs go into an $\ell > 0$ orbital angular momentum state.

Now look at the BCS gap equation, $\Delta_{\vec{k}} = -\sum_{\vec{k}'} V_{\vec{k},\vec{k}'} \frac{\Delta_{\vec{k}'}}{2\sqrt{\xi^2_{\vec{k}'}+\Delta^2_{\vec{k}'}}}$. Recall that $V_{\vec{k},\vec{k}'}$ is large and positive and peaked in value at the corners of the Brilloiun zone. To take advantage of the large values, the system has to change the sign of the gap $\Delta_{\vec{k}}$ for regions on opposite sides of the Fermi surface that differ in momentum by $(\pm\pi,\pm\pi)$ (see Fig. 6). A gap function with $d_{x^2-y^2}$ symmetry gives a self-consistent solution to the gap equation, and has the form $\Delta_{\vec{k}} = \Delta_{Max}(\cos(k_x a) - \cos(k_y a))$, where a is the lattice parameter of the CuO_2 planes. In this case the two charge carriers avoid the strong on-site repulsion and go into an $\ell = 2$ orbital angular momentum state. The nodes (or zeros) of this gap function point in the

diagonal directions in real space where the short range $V(\vec{r})$ is positive. There is experimental evidence from angular resolved photoemission spectroscopy, and from several types of tunneling experiments, that this order parameter symmetry is dominant in the cuprate superconductors.

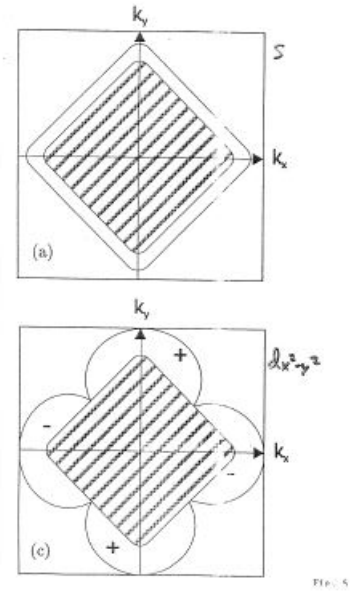

FIG. 6. Gap functions on the Fermi surface of a cuprate superconductor. (a) Upper plot shows an isotropic s-wave gap. (c) Lower plot shows the $d_{x^2-y^2}$ gap function over the Fermi surface.