Microscopic Theories of Cuprate Superconductivity: A Smorgasbord

Before embarking on the main topic of this lecture, let's deal with one question we have so far left unanswered: Are the data compatible with a traditional BCS-like phonon-exchange mechanism? At first sight the "folk-theorems" of the 60's and 70's, which suggest that no such mechanism could produce a T_c much above 40 K, would appear to tell against this; however, the (actually rather few) quantitative calculations done in this context always referred to a bulk 3D situation, and it is conceivable that the special characteristics of a 2D layered system might somehow favor the phonon mechanism to the extent of allowing the maximum T_c to increase by a factor of ~ 4 (to a T_c of approximately half the Debye temperature!). In fact, as we shall see in lecture 13, there is a substantial possibility that superconductivity in the FeAs compounds ($T_c \sim 55$ K) is phonon-mediated.

A more convincing argument has to do with the isotope effect.[1] Originally, the picture here was very confused, but it now seems clear that while the T_c's of the cuprates do sometimes show a substantial isotope effect, with values of a which can actually reach 0.95, these large values always seem to be associated with regions of the phase diagram where T_c is also strongly pressure-dependent, suggesting that the effect principally comes from the effect of the zero-point energy on the lattice structure. If we ignore these "special" regions of the phase diagram (which are only a small portion of the whole), then all existing data seem compatible with the statement that for genuinely high-T_c systems (e.g. YBCO at optimal doping) both the Cu and the O isotope exponents are very small ($\alpha_{\rm Cu} < 0.01,\ \alpha_{\rm O} \sim 0.02-0.05$). For systems with lower T_c, be it "intrinsic" to the material or due to suppression by Zn or magnetic fields, α is larger; e.g. it is typically $0.1 - 0.15$ for LSCO, and for YBCO with T_c suppressed by O deficiency or Zn doping, it gets quite close to the BCS value 0.5 as $T_c \to 0$. What this would tend to suggest is that there is a part of the superconducting condensation energy that is associated with a phonon exchange mechanism, but that it is at best a constant, i.e. does not increase with T_c, and thus is a small part of the whole even in LSCO and almost completely negligible in YBCO (note that the condensation energy of YBCO is of the order of 5 times that of optimally doped LSCO). However, it is very significant that α, while usually small, always appears to be positive, indicating prima facie that the phonon contribution to the condensation energy is positive – something that in the context of a d-wave pairing state is not obvious.

Before leaving the subject of phonons, let's note one curious point about the normal-state ab-plane resistivity $\rho_{ab}(T)$: Whatever other mechanism is contributing to this quantity, one would think at first sight that it ought to be in series with the phonon contribution (i.e. $\rho(T) \sim \rho_{\rm phonon}(T) + \rho_{\rm al}(T)$ where $\rho_{\rm al}$ represents the unknown mechanism: cf. the familiar Matthiessen's rule). This argument would then give an upper limit on the phonon contribution. If we assume that this contribution is described by a simple Drude formula, this gives for the scattering rate $\Gamma_{\rm ph} \equiv \tau_{\rm ph}^{-1}$ due to phonons the

[1] J. P. Franck, Physica C **282**, 198 (1997).

inequality,

$$\Gamma(T)_{\rm ph} \leq \rho_{ab}(T) n_{\rm eff} e^2/m^* \tag{1}$$

where $n_{\rm eff}$ is the effective number of carriers and m^* their effective mass. It is useful to compare this expression with the corresponding expression for (e.g.) Cu at room temperature, where both materials have a resistivity close to linear in temperature: assuming that Cu has one free electron per atom with effective mass equal to the real mass, we get

$$\frac{\Gamma_{\rm ph}(T)}{\Gamma_{\rm Cu}(T)} \leq \frac{\rho_{ab}(T)}{\rho_{\rm Cu}(T)} \frac{n_{\rm eff}}{n_{\rm Cu}} \frac{m}{m^*} \tag{2}$$

The experimentally measured value of the ratio $\rho_{ab}(T)/\rho_{\rm Cu}(T)$ near R.T. is approximately 90, and we may reasonably take $m/m^* \sim 0.25$ from the specific heat data. The value of $n_{\rm eff}/n_{\rm Cu}$ is approximately[2] $0.12 \times p_{\rm eff}$,where $p_{\rm eff}$ is the number of "free carriers" per CuO_2 unit. Consequently, if we take $p_{\rm eff} \sim 1$ (or $1 - 0.16$), we satisfy the inequality comfortably with a $\Gamma_{\rm ph}$ which is comparable to that of Cu; however, if we take $p_{\rm eff} \sim p \sim 0.16$ then the scattering rate by phonons can be at most half of that in Cu.

From the above considerations it seems that the primary mechanism of superconductivity in the cuprates does not have much to do with phonons,[3] in which case it follows (by exhaustion!) that it must be due to electron-electron interactions. So from now on I will consider only the electrons moving in the field of the *static* lattice.

In the case of the classic superconductors, we have both (a) a conceptually well defined picture of the normal phase, (the Landau-Silin Fermi liquid picture) which, while it does not in itself necessarily permit the calculation of different experimentally observable quantities, at least permits them to be fitted together in an internally consistent way, and (b) an equally conceptually well defined picture of the superconducting phase, which allows us to predict a wide variety of its properties in terms of one or two experimentally determined quantities such as T_c and the normal-state single-particle DOS. A complete theory of cuprate superconductivity would presumably also possess these two properties. In addition, it would allow us to answer questions such as:

- Is the strongly two-dimensional nature of the cuprates essential to high-temperature superconductivity?
- What is the theoretical upper limit (if any) on T_c in systems of this type?
- Why, in the Ca-spaced homologous series, does T_c rise with n up to $n = 3$? (and thereafter fall)?
- Why is the temperature-dependence of the c-axis N-state resistivity so different for the different cuprates?

[2] $N_{\rm Cu} = 8.5 \times 10^{22} {\rm cm}^{-3}$.

[3] This statement may need some qualification in the light of the ARPES results of Lanzara et al. [discuss]. Also Newns & Tsuei ideas (Nature Physics **3**, 184 (2007))

No existing microscopic theory (to my knowledge) answers all of these questions, though some theories claim to answer some of them.

What a priori constraints can we reasonably put on a microscopic theory?

Anderson's "central dogmas" [quote]

1. "All the relevant carriers of both spin and electricity reside in the CuO_2 planes and derive from the hybridized $[O]_{2p}-[Cu]_{d_{x^2-y^2}}$ orbital which dominates the binding in these compounds".

   [agree]

2. "Magnetism and high T_c superconductivity are clearly related, in a very specific sense: i.e. the electrons that exhibit magnetism are the same as the charge carriers".

   [agree, with proviso, that this does not mean that the residual antiferromagnetism is the "cause" of superconductivity].[4]

3. "The dominant interactions are repulsive and their energy scales are large".

   [agree – this in effect simply says that barring very considerable screening of the in-plane interaction by the ion cores, not only the on-site but the nearest-neighbor Coulomb interaction is at least as large as the hopping energy]

4. "The 'normal' metal well above T_c is the solution of the planar one-band problem resulting from Dogma 3 and is not a Fermi liquid".

   [disagree: the evidence for this conclusion is ambiguous][5]

5. "The above state (the Luttinger liquid postulated in Dogma 4) is strictly 2D, and coherent transport in the third dimension is blocked".

   [agree with the second part, but for different reasons].

6. "Interlayer hopping together with the "confinement" of Dogma 5 is either the mechanism of or at least a major contributor to the superconducting condensation energy".

   [strongly disagree, see lecture 12].

I would tend to accept Anderson's dogmas 1-3 and 5, and add a couple more:

A. Phonons are irrelevant, at least for the higher-T_c cuprates.

B. The symmetry of the OP in bulk is $d_{x^2-y^2}$.

[4] So, I would not necessarily agree with Anderson's conclusion that "we must solve the old problem of doping a single Mott-Hubbard band before we can begin the problem of high T_c".

[5] Anderson's argument that the c-axis transport is incoherent [with which I agree] and that since "Fermi liquids cannot localize in one direction and extend in a second" the in-plane state also cannot be FL-like, seems to me to rest on a subtle ambiguity in the concept of "localization".

I will now try to give an exceedingly brief summary of some of the ideas that are currently actively discussed in the context of cuprate superconductivity. Not all of these exactly qualify as "mechanism"; for example, some leave the nature of the mechanism unspecified and try to explain the peculiar properties of the pseudogap regime. I start with the most conservative:

1. van Hove singularities[6]

The idea, here, is that because of the topological structure of the 2D (or 3D) one-electron bands derived from the hybridized $O_{2p}-Cu_{3d_{x^2-y^2}}$ orbitals, the single-electron density of states $N(0)$ has a singularity at an energy which at optimal doping may coincide with the Fermi energy or at least approach it closely. If T_c is given by something like a BCS formula, namely

$$k_B T_c \sim \epsilon_0 \exp -1/N(0)V_0 \tag{3}$$

and the effective interaction matrix element V_0 and cutoff energy ϵ_0 are relatively insensitive to the position of the Fermi surface, this might explain qualitatively why $k_B T_c$ is so high at optimal doping, and why it falls away relatively rapidly on either side.

The attraction of this idea is that indeed the ARPES data do seem to show some evidence of a rather flat region in the band structure $\epsilon(\mathbf{k})$, which would imply a high DOS. Bok and Bouvier (ref. cit.) claim to explain the phenomena usually associated with the "pseudogap" by the observation that all that the raw data indicates is a large density of states near, but some finite distance away from, the Fermi surface: they also claim to obtain T_c's of the order of the observed ones from a standard BCS-type phonon-induced interaction, and to explain the absence of an appreciable isotope effect.[7] However, they also apparently obtain an s-wave type gap whose minimum value over the Fermi surface is 0.7 $k_B T_c$; they make no suggestion as to how to reconcile this result with (e.g.) the linear T-dependence of $\lambda(T)$ at temperatures $\ll T_c$.

2. Spin fluctuations[8] (and excitons)

If the "most BCS-like" theory, based on a simple Fermi-liquid-like normal state and an attraction generated by exchange of virtual phonons, does not work, then the next simplest hypothesis would seem to be that the normal state is still Fermi-liquid-like, and there is an attraction generated by the exchange of a virtual boson, but the boson is not a phonon but rather some excitation of the locally conserved quantities, namely charge and spin. The shorthand for a mechanism in which it is the exchange of charge fluctuations (plasmon-like objects) which binds the Cooper pairs is "exciton mechanism": in the very early days of high T_c, such mechanisms were quite fashionable in part because

[6] Ref: Bok+Bouvier, Int. J. Mod. Phys B **13**, 3425 (1999).

[7] However, the relevant equation (8) of their ref. (4) would in fact seem to give a substantial isotope effect. ($\alpha \cong 0.8$).

[8] Refs.: D. Pines, in Gap Symmetry ... ed. J. Bok, Plenum 1998; D.J. Scalapino, JLTP **117**, 179 (1999).

of the observation that a MIR peak seemed to be a necessary precondition for high-T_c superconductivity (and, at least in the case of LSCO, its weight scales with T_c), but many of these speculations were dampened by the observation that it is not a sufficient condition (e.g., $La_{2-x}Sr_{1+x}Cu_2O_6$). Nevertheless, some experimental papers (e.g. Holcomb et al.) still try to interpret their data in terms of a phenomenological fermion-exciton coupling treated by the traditional Eliashberg approach.

The other major option is spin fluctuations, and this is the basis inter alia of the "nearly antiferromagnetic Fermi liquid" (NAFL) picture. This has several variants (Scalapino, Moriya, Pines ...) but all have in common that they start from the observation that as one moves at constant T across the phase diagram in the direction of increasing p (hole doping) the system initially displays AF order, and that vestiges of this behavior remain even at optimal doping, in the sense that the spin fluctuation spectrum $\mathrm{Im}\,\chi(\mathbf{q},\omega)$, as observed either directly (in neutron scattering) or indirectly (via the NMR properties, such as Knight shift and nuclear relaxation time T_1) peaks strongly for low frequencies at wave vectors equal or close to the "superlattice" vectors $\mathbf{Q}_i \equiv (\pm\pi/a, \pm\pi/a)$. A phonomenological form that reproduces this peaking and has been widely used by the Pines school is, for $\mathbf{q}$ close to one of the $\mathbf{Q}_i$,

$$\chi_{\mathrm{NAFL}}(\mathbf{q},\omega) = \frac{\chi_{\mathbf{Q}_i}}{1 + (\mathbf{Q}_i - \mathbf{q})^2\xi^2(T) - i\omega/\omega_{\mathrm{SF}}} \tag{4}$$

whereas elsewhere in momentum space the form is more "Fermi-liquid"-like:

$$\chi_{\mathrm{FL}}(\mathbf{q},\omega) = \frac{\chi_{\mathbf{q}}}{1 - i\omega/\Gamma_{\mathbf{q}}} \cong \frac{\chi_0(T)}{1 - i\omega/\Gamma_0} \tag{5}$$

In these formulae χ_0 and $\chi_{\mathbf{Q}_i}$, are respectively the (modest) spin susceptibility at $\mathbf{q} = 0$ and the (much enhanced) one at $\mathbf{q} = \mathbf{Q}_i$, Γ_0 is of the order of the Fermi energy,[9] and the quantities ω_{SF} and $\xi(T)$ (not to be confused with the superconducting coherence length) are respectively a typical frequency and correlation length characterizing the spin fluctuations: it is usually postulated that $\omega_{\mathrm{SF}} \sim \xi^{-2}(T) \sim a + bT$, where the parameters a and b are fitted separately for each cuprate.

In the simplest version of the picture, the system whose spin fluctuations are described by χ_{NAFL} are the same mobile spins that carry the electrical current in the normal state and form Cooper pairs in the superconducting state. Despite this, one can formally treat the spin fluctuations as a sort of boson-like collective excitations which can be thought of as separate from the single fermion excitations and couple to them with some coupling constant g (a similar approach has been quite successful in the case of the "nearly ferromagnetic Fermi liquid" ^{3}He). The question of how to determine the coupling constant g is somewhat controversial, and there have even been suggestions that it may vanish just at the point where it is most needed ($\mathbf{q} = \mathbf{Q}_i$)! If however we assume that g is finite and not too fast varying in the "important" regime close to $\mathbf{Q}_i$, then we can attempt to take over the standard technique of electron-phonon theory, in particular the Eliashberg technique, to discuss the electron-spin fluctuation interaction.

[9] Actually, to ensure local spin conservation $\Gamma_{\mathbf{q}}$ must be $\sim \mathbf{q}\mathbf{v}_{\mathrm{F}}$ for small $\mathbf{q}$, but for $\mathbf{q} \sim \mathbf{Q}$ it is $\sim \epsilon_{\mathrm{F}}$.

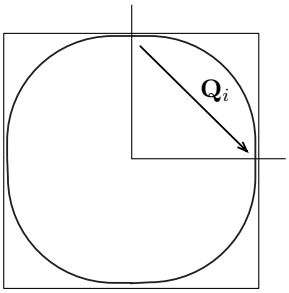
Without going through the details one can see some obvious qualitative features of the results:

If we look at the imaginary part of the spin fluctuation spectrum at the "commensurate" value $\mathbf{Q}_i$ of $\mathbf{q}$, it has the simple form

$$\mathrm{Im}\,\chi(\mathbf{Q}_i,\omega) = \mathrm{const}\ \frac{\omega}{\omega^2+\omega_{\mathrm{SF}}^2} \tag{6}$$

so that it peaks at $\omega = \omega_{\mathrm{SF}}(T)$ which then acts as a sort of "pseudo-Debye" temperature. From our experience with the electron-phonon interaction we would guess that for $k_{\mathrm{B}}T \gg \hbar\omega_{\mathrm{SF}}$ electron-spin fluctuation collisions would give rise to a resistivity that is linear in T as experimentally observed, and that from the coefficient of T one would get out information about the coupling constant g. Detailed calculations confirm this (though caution re N-U distinction!). To obtain agreement with the linear behavior down to T_c for any given cuprate, one evidently needs that ω_{SF} for that compound should be of order T_c or less, and in particular for Bi-2201 one would apparently need $\omega_{\mathrm{SF}} <$ 20K. Presumably, a rather severe test of this model would be its predictions for the low-temperature behavior of the resistivity as a function of doping in LSCO when the superconductivity is suppressed by a magnetic field as in the experiments of Boebinger, but as far as I know no detailed comparison has been made.

In the spin-fluctuation theories, the mechanism of formation of Cooper pairs by exchange of virtual spin fluctuations is very similar to the traditional electron-phonon interaction, with one major difference: Whereas the emission of a virtual phonon leaves the electron spin unchanged and changes the momentum by an amount that is essentially random over scales of the order of $\mathbf{k}_{\mathrm{F}}$, the emission of a virtual spin fluctuation flips the spin and, because the spin fluctuation spectrum is strongly peaked around $\mathbf{Q}_i$, changes the momentum by an amount close to one of the $\mathbf{Q}_i$. It therefore favors a structure of the pair order parameter which transforms as nearly as possible into itself under these combined operations. In particular, if the spin structure is a singlet (so that spin flip gives rise to a sign change) then the spatial part of the order parameter must change sign when an electron is scattered from one state on the Fermi surface to another that is connected to it by a commensurate wave vector $\mathbf{Q}_i$. Since for the cuprates close to optimal doping the only parts of the Fermi surface that can be connected in this way are the points along $(\pi,0)$ $(\equiv X)$ and $(0,\pi)$ $(\equiv Y)$ (etc.), it follows that the pair wave function should (a) be large close to the points X and Y and (b) satisfy the condition $\Psi(X) \cong -\Psi(Y)$. The only one of the even parity (spin singlet)irreps realized in C_{4v} symmetry that satisfy both these conditions is the B_{1g} $(d_{x^2-y^2})$ state. Hence, quite generically, spin fluctuation theories predict that the symmetry of the OP should be $d_{x^2-y^2}$.



In addition to this successful prediction (made in advance of most of the relevent experiments), arguments in favor of spin fluctuation models include the fact that one of their main inputs, the form of $\chi(\mathbf{q},\omega)$, can at least in principle be derived directly from

experiment, and the fact that they suggest a natural explanation of the shape of the $T_c(p)$ curve (maximum T_c is, roughly speaking, the point at which the shape and size of the Fermi surface is such that the commensurate vectors exactly connect the points X and Y). Criticisms often leveled at these models include the fact that they need a large number of parameters to be put in by hand (not only is the coupling constant g not known a priori, but one has direct information, from neutron scattering, about the complete form of $\chi(\mathbf{q},\omega)$ only for LSCO and YBCO, neither of which is (arguably) at all typical of the cuprates as a whole).

Pre-formed pairs[10]

The object of the "pre-formed pair" scenario is not so much to explain cuprate superconductivity as such, but to account for the properties of the pseudogap regime in terms of these of the superconducting state. In its purest form (Uemura 1989) the scenario holds that, at least in the UD region of p, there is an effective attraction between electrons so strong that in the N phase the basic entities are tightly bound pairs, with radius $\ll$ the mean inter-electron spacing, and that these can be treated simply as bosons of charge $2e$. The superconducting transition is there nothing more nor less than the onset of Bose condensation (BEC). This proposal has the following attractive consequence: Suppose that we naively estimate the BEC transition temperature from the consideration that the number of single-particle states with energy less than T_c should be of the order of the total number of bosons n (which is presumably proportional to $p/2$ and is measured by the zero-temperature superfluid density $\rho_s \cong n/m^*$). There in 2D we find immediately that $T_c \propto n \propto \rho_s \propto \lambda_{ab}^{-2}$, where λ_{ab} is the in-plane penetration depth. The famous Uemura plot[11] shows that this relation is well obeyed within each individual family of cuprates measured, as p is varied, up to approximately the "optimal" value of p (after which it fails badly, since T_c drops while $\rho_s(\propto \lambda_{ab}^{-2})$ continues to increase). As to the absolute value of T_c, this naive argument predicts

$$k_{\mathrm{B}}T_c = (2\pi\hbar^2/m_{\mathrm{B}}^*)n_{\mathrm{B}} = 2\pi(\hbar^2/ma^2)(m/m_{\mathrm{B}}^*)(p/2) \tag{7}$$

where a is the CuO_2 lattice spacing. Since the quantity $\hbar^2/ma^2$ is approximately 6000K, and since it is presumably reasonable to take $m_{\mathrm{B}}^* = 2m_{\mathrm{el}}^* \cong 8m_{\mathrm{el}}$, this would give at optimal doping ($p = 0.16$) the estimate $T_c \sim 600K$. However, a strictly 2D Bose system will not undergo BEC at any finite temperature, and if we allow for the weak 3D coupling by introducing a mass anisotropy, $\gamma \equiv m_c^*/m_{ab}^*$ the effect is to multiply the above estimate by $\gamma^{-1/2}(a/\overline{d})$ where $\overline{d}$ is the average interlayer spacing. This gives a T_c that is in the right ballpark for YBCO but far too small ($\sim 1K$) for BSCCO. It is possible that one could derive an intermediate scheme that would give a T_c of l00K; but in any case, to the best of my knowledge no concrete mechanism has been proposed that would bind pairs of electrons with the tightness required for the free Bose gas to be a good approximation.

[10]Refs: Engelbrecht et al., Phys. Rev. B **57**, 13406 (1998)(and earlier refs. cited therein); Q-J. Chen et al., PRL **85**, 2801(2000).

[11]Y.J. Uemma et al., PRL (1989).

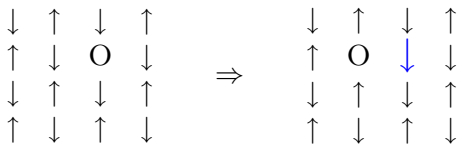
An intermediate scenario is sometimes proposed. If we denote the pair radius schematically as ξ_0, then crudely speaking the "BCS limit" corresponds to $k_F\xi_0 \gg 1$ and the "Bose limit" to $k_F\xi_0 \ll 1$ (where k_F is now defined as the value the Fermi wave vector would have for a free Fermi gas at the same density). Now in fact most estimates of ξ_0 at optimal doping give $\xi_0 \sim 15 - 20$Å, while N-state ARPES measurements of the Fermi surface indicate that $k_F \sim 1$Å^{-1}. If one accepts these values, then $k_F\xi_0$, while appreciably larger than 1, is not obviously large enough to justify all the usual approximations of BCS theory. In particular, one can argue that there may be a regime of temperature where appreciable numbers of Cooper pairs are formed but do not Bose-condense, i.e. they have a COM momentum K different from zero. Such a state would not possess ODLRO and hence would not be superconducting in the usual sense, but if the typical value of K is K_0 then one should be able to define a "local" OP over a length scale $\sim K_0^{-1}$, and hence presumably a "local" energy gap. Various attempts have been make to modify the BCS formalism to describe this situation, the latest being that of Chen et al.[12] One interesting prediction of this version (which it shares with the extreme (Uemura) scenario) is that the "boson-like" branch also contributes a term to the low-T specific heat which in 2D is linear in T (in 3D it would be $T^{3/2}$, cf. the data on the organics).

This general point of view has been further promoted by Emery and Kivelson,[13] who point out that the small value of the superfluid density alone means that phase fluctuations are much more probable than in a classic superconductor. In fact, in their scenario, at optimal doping and in the OD regime the factors that determine T_c are essentially those of BCS theory, while in the UD regime the "BCS" value of T_c corresponds to the pseudogap temperature T^*, and the actual T_c is determined primarily by the destruction of ODLRO by phase fluctuations. Since the energy of a phase transition of a given wave vector $\mathbf{k}$ is proportional to the superfluid density ρ_s, their number is proportional in the classical limit ($k_BT_c \gg \rho_s k^2$) to $kT\rho_s^{-1}$, and since crudely speaking the system goes normal when the total "number" of fluctuations reaches a given threshold, this line of argument suggests that T_c should be proportional to ρ_s, in agreement with the Uemura plot. In one "extreme" version of the scenario, all properties of the UD regime, and in particular the specific heat, are attributed purely to the phase fluctuations and the d-wave nature of the gap is held to be irrelevant. [Relevance of Orenstein et al. experiments]

All the above scenarios start from a model that emphasizes the "band" (delocalized) nature of the electrons. An alternative point of view (enshrined in Anderson's "dogma 2") starts as it were from the other end, from the recognition that the parent compound is a Mott insulator, and that at least for small enough p the excitations are most naturally described as holes in this background. So one often starts by considering the motion of one, two or a few holes in a Mott insulator (even though it is experimentally clear that AF and S phases do not overlap in the phase diagram). One interesting point

[12] Q-J. Chen et al., ref. cit.
[13] Nature **374**, 434 (1995).

was appreciated from very early on: if a single hole moves in an AF without any spin-flip processes, the AF superlattice is disrupted (e.g. in the figure, the crosses mark "disadvantageous" nearest-neighbor arrangements). In fact, as the hole moves it leaves behind it a "string" of wrongly oriented spins, and thus an energy proportional to the length of the string.



However, it is clear that a second hole following in the path of the first will restore the original spin configuration and cancel out the unwanted energy. Consequently, one gets an effective potential between any two holes, which is proportional to the length of the "uncancelled" string, that is to the distance between them (cf. QCD!), and for nearest-neighbor separation is of order the AF coupling constant J (see below). This then provides a mechanism for binding of holes even for $p \to 0$. While this argument is very suggestive, it clearly cannot be the whole truth for the cuprates, since the AF order goes away with increasing p before SC kicks in.

We therefore need some description that will allow us to deal with both the AF phase and the nonmagnetic metal (and possibly also the S phase). The simplest candidate is the famous Hubbard model:

$$\hat{H}_{\rm Hub} = -t \sum_{\langle ij\sigma \rangle} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{8}$$

This is often regarded as a reasonable description of a "tight-binding" band, where the electronic states i are strongly localized on atoms, the hopping is only between nearest-neighbor sites and described by a TB matrix element t, and the on-site interaction U between opposite spins is repulsive.[14] Despite its apparent simplicity, the Hubbard model in more than 1D has resisted analytical solution for general values of the ratio U/t; however, it is known that in the "strong-coupling" limit ($U/t \to \infty$) the groundstate at half filling (one electron per site) corresponds to a Mott insulator (i.e. the electrons are localized on lattice sites and have alternating spins). In the opposite limit, $U/t \to 0$, the system should be well described by band theory with U treated as a perturbation.

By treating the hopping terms as a perturbation, one derives from the Hubbard model the equally famous "$t-J$ model":

$$\hat{H}_{t-J} = -t \sum_{\langle ij\sigma \rangle} c^{\dagger}_{i\sigma} c_{j\sigma} + J \sum_{i} \mathbf{S}_i \cdot \mathbf{S}_j, \quad \mathbf{S}_i \equiv \sum_{\alpha\beta} c^{\dagger}_{i\sigma} \boldsymbol{\sigma}_{\alpha\beta} c_{i\beta} \tag{9}$$

plus an explicit prohibition of double occupation. Here the AF exchange coupling constant J is given by $J = t^2/U$, and determines the spin-wave excitation spectrum. By

[14] If there is only one relevant orbital on each atomic site, double occupation of the i spin state (etc.) is forbidden by the Pauli principle.

measuring the latter by inelastic neutron scattering, one deduces that at half filling (i.e., in the "parent" compound, $YBa_2Cu_3O_6$, etc.) the value of J is approximately 1500K (0.13 eV), and since TB band structure calculations give a value of t of the order of 0.5eV, this would imply that the on-site Coulomb repulsive is $\sim 2eV$, which for a pair of hybridized $2p-3d_{x^2-y^2}$ orbitals is probably not unreasonable. The $t-J$ Hamiltonian has been used as the starting point for many calculations on the cuprates. However, one should be worried that it (along with its parent, the Hubbard model) leaves out at least one effect that may be important, namely the long-range part of the Coulomb interaction.[15]

Spin-charge separation[16]

One of the main attractions of the $t-J$ model in the context of a theory of the (N and S states of the) cuprates is that it doesn't assume a priori that the ground state of the system is anything like a traditional Fermi liquid. Indeed, currently there is a major industry of postulating various kinds of exotic groundstate (usually with one or more symmetries other than $U(1)$ spontaneous broken) and exploring their properties. A very persistent theme in this context is the notion of spin-charge separation. In many 1D models this idea is almost trivial. For example, consider a 1D chain of fermions with exactly one fermion per site. Suppose initially the spins are oriented in some particular configuration. Then if there is any spin-spin coupling (irrespective of sign) neighboring spins can flip and this will result in transfer of spin: e.g.

$$\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow \longrightarrow \uparrow\uparrow\uparrow\downarrow\uparrow\downarrow\downarrow\downarrow \longrightarrow \uparrow\uparrow\downarrow\uparrow\uparrow\downarrow\downarrow\downarrow \ldots$$

Evidently, a "down" spin moves from R to L without any charge transfer. If now we introduce a hole, then if the lattice is initially disordered it will propagate without (on average) spin transfer:

$$\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow \text{ O } \uparrow \longrightarrow \uparrow\downarrow\downarrow\uparrow\uparrow \text{ O } \downarrow\uparrow \longrightarrow \uparrow\downarrow\downarrow\uparrow \text{ O } \uparrow\downarrow\uparrow \ldots$$

In the case of 2 or more dimensions, the generalization of this idea is not so clear. What is usually done is the following: one splits the electron creation operator $c^\dagger_{i\sigma}$ for site i and spin σ into a "spinon" and a "holon" operator, $f^\dagger_{i\sigma}$ and $b^\dagger_i$ respectively:

$$c^\dagger_{i\sigma} = f^\dagger_{i\sigma} b_i \tag{10}$$

The operator $f^\dagger_{i\sigma}$ obeys Fermi statistics and $b^\dagger_i$ obeys Bose statistics. The constraint of no double occupancy is replaced by the condition

$$f^\dagger_{i\sigma} f_{i\sigma} + b^\dagger_i b_i = 1, \tag{11}$$

which is enforced by introducing an appropriate Lagrange multiplier.

[15] The arguments given in the literature as to why this omission is legitimate seem mainly to refer to the 3D case. There may be an important difference in the 2D case, see lecture 12

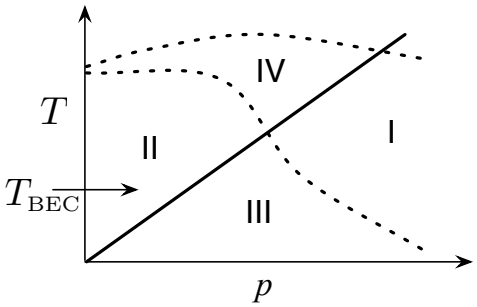
[16] Ref: P.A. Lee, Physica C **317**, 194 (2000).

While it is almost trivial to write the electron operators in terms of spinon and holon operators, it is not at all obvious how to invert the process and express the spinons and holons in terms of real electrons. Thus it is not altogether clear (at least to me) that the procedure described by (10) is well defined. Nevertheless, let us see what consequences follow.

The most obvious guess is that the holons, which obey Bose statistics with (presumably) conserved particle number, undergo BEC[17] at a temperature $T_{\rm BEC} = 2\pi xt$ (where $x \equiv p$ is the doping). On the other hand, the exchange term can be written in terms of the spinor operators alone:

$$J\,\mathbf{S}_i \cdot \mathbf{S}_j = -J|f^\dagger_{i\alpha} f_{j\alpha}|^2 =$$
$$= J\big(f^\dagger_{i\uparrow} f^\dagger_{j\downarrow} - f^\dagger_{i\downarrow} f^\dagger_{j\uparrow}\big)\big(f_{i\downarrow} f_{j\uparrow} - f_{i\uparrow} f_{j\downarrow}\big)$$

The last expression is an identity, but it suggests making various mean-field types of decoupling. First, it is natural to suppose that at low temperatures $\langle f^\dagger_i f_j\rangle \neq 0$, which when Fourier transformed implies the existence of an energy band and a Fermi surface. Secondly, it is tempting to suppose that at sufficiently low temperature the quantity $f^\dagger_{i\uparrow} f^\dagger_{j\downarrow} - f^\dagger_{i\downarrow} f^\dagger_{j\uparrow}$ also acquires are expectation value (in the usual BCS sense):



$$\langle f^\dagger_{i\uparrow}\, f^\dagger_{j\downarrow} - f^\dagger_{i\downarrow}\, f^\dagger_{j\uparrow}\rangle = \Delta_{ij} \qquad (12)$$

Since the sites i and j involved here are different, the "gap" Δ_{ij} cannot have s-wave symmetry,[18] and since it is confined (prima facie at least) to nearest neighbors and is a spin singlet, the only possibility is d-wave (in fact, in a square lattice with only n.n. pairing, $d_{x^2-y^2}$).

The resulting phase diagram is predicted to look as follows: To the right of the solid line we have BEC of the holes, and below the lower dashed line $\Delta_{ij} \neq 0$ for the spinors. Superconductivity, that is a finite $\langle c^\dagger_{i\sigma} c^\dagger_{j-\sigma}\rangle$ where the c_i's are true electron operators, requires simultaneous BEC and pairing ($\Delta_{ij} \neq 0$), thus it corresponds to region III. Region I is a FL-like phase (despite the BEC of holons!), region II is the "spin-gap" (pseudogap) phase and region IV is said to be a "strange- metal" phase. For further discussion, see Lee, ref. cit.

[other theoretical ideas: marginal Fermi liquid, stripes, quantum critical point, SO(5).]

Refs: Orenstein + Millis, Science **288**, 468; Sachdev, *ibid*, 475.]

[17] Actually, in strictly 2D BEC is impossible, but for $T < T_{\rm BEC}$ these will be a crossover to a phase which at least locally "looks" Bose-condensed.

[18] Or at least this does not look very "natural".