ELECTRONIC STRUCTURE AND FERMIOLOGY OF HIGH TEMPERATURE SUPERCONDUCTORS: THEORETICAL SUMMARY

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ABSTRACT- A summary of theoretical issues raised at the conference on Electronic Structure and Fermiology of High Temperature Superconductors in the context of the more general question of the role of electron correlations.

From a theoretical point of view, it is quite natural that a conference such as this should be a celebration of the successes of electronic band structure calculations; and they are indeed impressive. We have been provided with remarkably accurate predictions of the location of the "Fermi surface" of high temperature superconductors and an identification of the atomic states which are relevant for an understanding of low-energy phenomena. Recent examples of this kind of calculation are to be found in the talks of Oguchi on $YBa_2Cu_4O_8$ and Oshiyama on C_{60} . Moreover frozen phonon calculations, such as the ones described by Pickett, have enhanced our understanding of the strength of the electron-phonon interaction and the possible role of phonons in determining the physical properties of these materials.

But, as in all areas of condensed matter physics, this is only the first step; we must also consider the importance of electron correlations and whether they modify the predictions of band theory in a significant way. Fermiology experiments might contribute to this goal by, for example, measuring the imaginary part of the self energy, which is an important test of the suggestion that high temperature superconductors are not Fermi liquids and that quasiparticle excitations are ill-defined. Of course, transport and magnetic measurements have a very direct bearing on the question of electron correlations, and talks on these subjects have been a very important part of this conference and its predecessor.

It frequently happens that, on a semi-phenomenological level, many experiments do not really distinguish between the strong-correlation and weak-correlation pictures, and it is useful to try to identify so-called "smoking gun" experiments, the ones that are difficult or impossible to explain from one point of view or the other. The fact that the undoped parent compounds of the high temperature superconductors are antiferromagnetic insulators, in contrast to the predictions of band theory, already shows that electron correlations are important: the magnitude of the staggered magnetization as well as the very large contribution of Cu^{2+} to the magnetic form factor indicate that the correlations are strong. For superconducting materials the situation is more complicated because there are two distinct points of view which must be resolved before the precise significance of electron correlations can be understood. The issues may be appreciated by considering the different attitudes to the changes in physical properties as a function of doping. The common description of these effects as the evolution from underdoped through optimally-doped to overdoped materials, mentioned repeatedly at this conference, has been interpreted in two diametrically opposite ways:

- 1) The main task is to understand the optimally-doped materials: underdoped and overdoped materials are, in some way, imperfect. The fact that the undoped parent materials are antiferromagnetic insulators is irrelevant.
- 2) The unusual normal state and the existence of high temperature superconductivity itself are properties of a doped antiferromagnetic insulator: the various regions of the phase diagram are all to be understood as different manifestations of this fact.

Both points of view have been expressed in the theoretical contributions to this conference. The first was adopted by Pickett and by Ueda in considering the consequences of the scattering of

electrons from phonons and spin fluctuations respectively. It is also implicit in the marginal Fermi liquid phenomenology, which has been mentioned at various points of the discussion. Its advocates think of the crossover from insulating to metallic behavior as a transition between two distinct phases, and they place emphasis on the increase in T_c with doping away from the insulating phase, as well as the "cleanliness" of the physical properties of optimally-doped materials. The second approach was taken by Nagaosa and by Emery and Kivelson. Here, an important issue, which was also emphasized at the first fermiology conference, is "the large versus the small Fermi surface" or, in other words, the fact that the carrier concentration is given by the doped holes, whereas the Fermi surface measured by the fermiology experiments is essentially in agreement with the predictions of band structure calculations. But there are other ways in which metallic samples display their memory of the insulating state. Takigawa's talk showed that, according to NMR and neutron scattering experiments on $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ antiferromagnetic correlations in metallic samples peak at the same wave vector as in the insulator, rather than at a nesting vector of the Fermi surface. In the same spirit, Tanner's analysis of the optical conductivity relied on a mid-infrared peak which is present for all levels of doping and appears to be a reflection of localized charges. It is important to note that these effects do not disappear in optimally-doped materials.

In either approach, it may turn out that the normal state of high temperature superconductors is not a Fermi liquid which, in itself, is an important consequence of electron correlations, although it does not *necessarily* require a particularly strong interaction but may simply indicate a breakdown of perturbation theory. The doped-insulator description is stronger, since it makes use of electron correlations in an essential way. The one-dimensional electron gas is an oft-quoted paradigm of this kind of behavior; it is a non-Fermi liquid with a "Luttinger" Fermi surface and a clear region in which the proximity to the insulating state is evident in the optical conductivity. These properties are, in some respects, similar to those of high temperature superconductors, but the details are different and we do not yet know how much may be carried over to two dimensions.

There is common agreement that an explanation of the unusual normal state properties of high temperature superconductors requires the existence of some kind of low-energy excitations in the system. As emphasized by Dzyaloshinsky, this follows immediately from the fluctuation-dissipation theorem and the existence of a T-linear resistivity. Obviously, it is desirable that high temperature superconductivity should emerge in a natural way from any description of the normal state, without having to introduce new physics specifically for that purpose. The simplest possibility is that the same low-energy excitations are responsible for the pairing of electrons, although other suggestions have been advanced. Consequently, in more than the usual sense, a successful interpretation of experiments in both the superconducting and the normal states will add credence to any given picture. This is a fortunate state of affairs, since it is not easy to find unequivocal evidence for a particular mechanism of superconductivity, especially an unconventional one. In this conference several candidates have been proposed as the crucial low-energy modes; specifically phonons (Pickett), antiferromagnetic spin fluctuations (Ueda), gauge fields (Nagaosa), and local collective modes associated with fluctuating electronic phase separation (Emery and Kivelson). Of these, it arguably is most important to support or refute the phonon mechanism for, although many of us find it difficult to believe that phonons can account for the properties of high temperature superconductors, it is nevertheless the venerable and tested mechanism of superconductivity and, if it fails, new physics must be involved. Pickett showed to us that, contrary to earlier beliefs, it is quite usual for the electron-phonon interaction to give a T-linear electrical resistivity. But then it is also necessary to explain why the scattering rate obtained from the dc resistivity or the optical conductivity a) is linear in frequency for optimally-doped materials; b) is not precisely T-linear for under- and overdoped materials; c) is T-linear down to 10K in Bi(2201) ; and d) drops rapidly below T_c . In particular, c) can only be explained if there is an exceptionally low-energy phonon mode and d) would require that the onset of superconductivity has an unexpectedly large effect on electron-phonon scattering.

An electronic mechanism has to explain all of these features and is also faced with the questions:

1) Where does the momentum go? (if phonons are ineffective, impurities are ignored, and there is no umklapp scattering); and 2) Why do the phonons not contribute? (since the resistivity is T-linear up to 1000K, with constant slope. If there were a T-linear contribution from phonons above some temperature T^* , then the slope should be different above and below T^*). Electronic mechanisms may have an easier time with points a) through d), but there has been rather little consideration of the problems presented by questions 1) and 2).

Evidently a resolution of all of these effects imposes rather severe constraints on proposed theories of the normal and superconducting states, as does an explanation of the Hall coefficient, whose behavior was described by Iye and Hamada. Plainly there is no shortage of "smoking-gun" indicators of the effects of electron correlations in high temperature superconductors, and we must go beyond band theory if we are to find a satisfactory explanation of what is going on.

There was relatively little discussion of the specific properties of the superconducting state at this conference. Ueda considered the symmetry of the order parameter implied by spin-fluctuation exchange. Abrahams described a new form of pairing in which the order parameter is spin-singlet but has odd parity. Conventional singlet pairing has an even-parity order parameter in order to satisfy Fermi statistics. But in general spin-singlet odd-parity pairing is permitted if the order parameter is also odd in frequency or, equivalently, odd in time. Emery and Kivelson pointed out that pairing correlations of this type are enhanced in the two-channel Kondo problem which, in their picture of high temperature superconductors, is a model of the scattering of mobile holes from the low-frequency collective modes that give rise to the anomalous normal state properties and to high temperature superconductivity. The point is that the ground state of the two-channel Kondo problem consists of a pairing resonance involving two mobile holes and a collective mode (or the impurity spin). This state is the generalization of the one-particle singlet resonance of the usual (one-channel) Kondo problem. In this realization, the two holes are in a singlet state of true spin and have even parity, but the total state carries the odd parity of the operator of the collective mode. An equivalent representation for the pairing resonance is given by the time derivative of an operator which creates a pair of holes in a spin-singlet odd-parity state. This is odd in time, and is a realization of the pairing discussed by Abrahams. Consequently there is the possibility that this novel kind of pairing may occur in high temperature superconductors. The challenge is to find experiments that are capable of distinguishing it from various other forms of pairing that have been proposed to account for the properties of the superconducting state.

What can the traditional fermiology experiments say about all of this? They will continue to give us improved information about the location of the "Fermi surface," which, at the very least, is the place in the zone where "the action is." They will continue to give us important parameters, such as the effective mass at the Fermi surface and the frequency dependence of the imaginary part of the self energy. In the future they may give some limits on the magnitude of the quasiparticle renormalization. As shown to us by Bansil, there is yet more information to be obtained from the use of polarized incident light in an ARPES experiment. More immediately, ARPES will continue to contribute to the debate on the existence and magnitude of the energy gap and, as Shen proposed, may be able to tell us something about the symmetry of the order parameter. In this regard, the current experiments are instructive but less than unequivocal. However if there are zeros of the gap, and they could be located by ARPES, this would be a most significant contribution.

In conclusion, I should like to express our gratitude to Takashi Takahashi, Arun Bansil and Hiroshi Katayama-Yoshida, for putting together a stimulating meeting in which the growing sophistication and continuing challenge of the experiments was so much in evidence. We all look forward to Fermiology III.

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