Doped cuprates are characterised by strong electronic correlations which influence substantially excitation spectra and transport properties. Low-energy excitations should describe physics in the low-temperature regime. Models are complex, so only partial and mainly qualitative explanations of experimental data have emerged.

Theoretical Models for High-$T_c$ Superconducting Materials

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Since the discovery in 1986 by Bednorz and Müller of superconductivity with high critical temperatures $T_c$, in the copper oxide-based ceramics, an enormous amount of work has sought a better theoretical understanding of the electronic properties of these materials. We shall discuss some aspects which are nowadays much better understood than they were a few years ago, and others which remain open problems.

Normal State Properties
A theory which will eventually be able to explain superconductivity and to calculate the transition temperatures for the high-$T_c$ materials must be based on sufficient knowledge of the normal state, especially its low-energy excitations. For example, one must know if these excitations are still in an one-to-one correspondence with those of a weakly interacting electron gas, as this is prerequisite for applying Landau's Fermi liquid theory and his concept of quasiparticles. A few examples will show that the low-energy excitations of the normal state are not trivial.

A doped Mott insulator
The quasiparticle concept has been very successful in explaining the physical properties of ordinary metals. However, the high-$T_c$ family of materials has a number of experimental properties which differ strongly from those of conventional metals. Most importantly, $La_2_xSr_xCuO_4$, the parent compound of the high-$T_c$ material, is an antiferromagnetic semiconductor and not a metal. With $La^{3+}$ and $O^{2-}$ one is left with a formal valency of $Cu^{2+}$ implying one hole per unit cell in the Cu 3d shell. One thus expects a half-filled conduction band, and therefore metallic behaviour.

The fact that the material is a semiconductor below and above the magnetic order-

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from both band-structure calculations and the comparisons with photo-emission data. The low-energy excitations of these more refined models corresponded with the excitations of the t-J model.

Three-band Hubbard model

Among the more complex models, the most widely studied is the three-band Hubbard or Emery model. There is evidence that the photo-emission and inverse photo-emission spectra (Fig. 3) obtained by numerical diagonalisation of the Hamiltonian for a \((\text{CuO}_2)_4\) cluster with periodic boundary conditions. The model is a model for a charge carrier (hole) on an O site and a hole on a neighbouring Cu site (see Fig. 1b). Since \(U_d > t_{pd}\), the situation resembles that of a \(\text{H}_2\) molecule in the Hellermann-London limit where the two electrons in \(\text{H}_2\) form a singlet (S) state with an excited triplet (T) state. The same happens here with respect to two holes, whereby one hole occupies a Cu-site \((d^9)\) and the other an orbital which involves four neighbouring O-ligands. Exchange interaction leads to the so-called Zhang-Rice singlet and triplet states. In the electron picture (as opposed to hole) the singlet band is pushed above the non-bonding states and forms the lower edge of the gap (Fig. 3a).

Singlet plus triplet states

This, however, is not the complete answer for the Emery model, as can be seen from the photo-emission and inverse photo-emission spectra (Fig. 3) obtained by numerical diagonalisation of the Hamiltonian for a \((\text{CuO}_2)_4\) cluster with periodic boundary conditions. The model is a model for a charge carrier (hole) on an O site and a hole on a neighbouring Cu site (see Fig. 1b). Since \(U_d > t_{pd}\), the situation resembles that of a \(\text{H}_2\) molecule in the Hellermann-London limit where the two electrons in \(\text{H}_2\) form a singlet (S) state with an excited triplet (T) state. The same happens here with respect to two holes, whereby one hole occupies a Cu-site \((d^9)\) and the other an orbital which involves four neighbouring O-ligands. Exchange interaction leads to the so-called Zhang-Rice singlet and triplet states. In the electron picture (as opposed to hole) the singlet band is pushed above the non-bonding states and forms the lower edge of the gap (Fig. 3a).

Closer inspection reveals that the singlet band separated from the upper Hubbard band by the charge-transfer gap essentially the same physics as a one-band Hubbard model with \(U\) of order \(E_{\text{CT}}\) and \(t\) given by the hopping matrix element for a singlet.

The most appealing experimental evidence supporting this picture comes from x-ray absorption spectroscopy. An important prediction of the Hubbard model is that the number of states in the upper Hubbard band should decrease as hole doping increases. This is precisely what the experiments indicate (Fig. 4). These results are in striking contrast to the behaviour of conventional semiconductors where the number of states in the conduction band is independent of the number of atoms, and is independent of the number of holes in the valence band.

The Fermi Surface Problem

Consider \(\text{La}_2\text{CuO}_4\) doped with a few holes. Leaving aside the possibility that the holes might be trapped at impurity centres, we are dealing with the problem of hole motion in a quasi-two dimensional Heisenberg antiferromagnet. This topic has attracted many theorists. A moving hole generates a chain of overturned spins if the ground state is approximated by a Neel state with antiferromagnetic correlations.

The spin-2 spin model may be meaningful even in the paramagnetic phase because short-range antiferromagnetic order still persists. The spin-2 spin model may be meaningful even in the paramagnetic phase because short-range antiferromagnetic order still persists. The bag can be considered as a number of locally excited spin waves, implying that the excitation spectrum has a large incoherent part. An equivalent statement is that the Green's function

\[
G(k;\omega) = \frac{a(k)}{\omega - E(k) + i\delta} + G_{\text{unc}}(k;\omega) \tag{3}
\]

has a quasiparticle pole with a small residue \(a(k)/\delta\) and hence a large incoherent contribution \(G_{\text{unc}}(k;\omega)\). The dispersion \(E(k)\) is determined by the energy scale \(J\) rather than by \(t\).

As more holes are doped into the system, they fill the lowest energy states \(E(k)\) of the hole band which are around the points \((\pm x/2, \pm y/2)\) of the Brillouin zone. A "small" hole Fermi surface is established with an enclosed volume given by the doping concentration. Antiferromagnetic long-range or-
The scattering rate is proportional to the doping concentration of donors (which are viewed as comprising the real part of the conductivity), a feature typical of a Drude-like conductivity.

Drude peak and mid-infrared absorption

The considerations above strongly suggest that the high-$T_c$ superconducting materials are close to a Mott-Hubbard type insulator-to-metal transition [1]. Much data on the electronic response to various external perturbations support this picture. One interesting example is the frequency-dependent conductivity $\sigma(\omega)$. When La$_{2-x}$Sr$_x$CuO$_4$, for example, is doped with holes one finds for the real part of the conductivity a Drude-like peak near the Fermi level, with a well-defined Drude peak and mid-infrared absorption in the Drude peak and mid-infrared absorption spectrum of La$_{2-x}$Sr$_x$CuO$_4$. This absorption is interpreted as the upper Hubbard band, which also grows in proportion to the number of holes. The remaining gap at low energy is probably due to finite-size effects.

A "marginal" Fermi liquid

An interesting phenomenological approach to the electronic response has been suggested under the name "marginal" Fermi liquid theory [6]. This approach is based on the observation that a number of the anomalous effects observed in the resistivity, Raman scattering intensity, nuclear relaxation rate, and other quantities can be qualitatively explained by simply assuming a high density of low-energy excitations, with the property that only the temperature appears as an energy scale. One immediate consequence is that the scattering rate, equivalent to the inverse lifetime of the electronic excitations, is given by

$$\frac{1}{\tau} = \text{max.} \{\text{Im} \chi(\omega)\} \approx \frac{1}{T+\delta},$$

(4)

This is in contrast to ordinary Fermi liquid theory where $1/\tau = \text{max.} \{\omega^2, T^2\}$.

No microscopic justification for Eq. (4) has been provided up to now. But the qualitative agreement with some of the experiments is striking. Note the agreement of Eq. 4 with the findings for $\sigma(\omega)$ discussed above. One consequence of Eq. 4 is that there are no well-defined quasiparticles near the Fermi energy owing to the short lifetimes. There is also no longer a jump in the momentum distribution $n(p)$ at $|p| = p_F$, the Fermi momentum, a hallmark of Fermi liquid theory.

Magnetic response

Of particular interest is the magnetic response when the systems are perturbed by neutron scattering or time varying magnetic fields (nuclear magnetic resonance or NMR). Neutron-scattering experiments established early on that spin correlations incommensurate with the lattice structure persist at hole concentrations at which magnetic long-range order no longer exists. For example, in La$_{1-x}$Sr$_x$CuO$_4$, the antiferromagnetic Bragg peak at $q_0 = (\pi, \pi)$ in the undoped system splits into four quasi-elastic peaks at $q = \pm (\pi, \pi) \pm \delta q$ on moderate doping. The relative sharpness of these peaks in the neutron scattering cross-section (i.e., in $\text{Im} \chi(\omega)$) where $\chi$ is the magnetic susceptibility) implies a magnetic coherence length $\xi_m \approx 4.5 \AA$ at low temperatures (10 K), where $\delta q$ is the Cu-Cu distance in the plane.

There still exist well-defined magnetic excitations in these strongly doped superconducting systems. Just such a splitting of the Bragg peak at $(\pi, \pi)$ was expected from earlier quantum Monte Carlo calculations on small clusters for the Hubbard model [7]. Conventional band-structure computations of the magnetic susceptibility seem to give a splitting of the Bragg peak along the $(\pi, \pi)$ direction instead. At higher temperatures, the magnetic coherence length decreases, reaching $\sim 2\delta q$ at 100 K.

NMR provides another important experimental tool. A temperature-dependent coherence length of the form $\xi(T) = 1/(T+\delta)$ is required for $T \geq T_c$ to account for the Cu relaxation rates. Since this technique is a local probe it measures a momentum space average of $\text{Im} \chi(\omega)$ for $\omega \rightarrow 0$. A consensus concerning the results of these two techniques has not yet been reached, one reason being the lack of precise calculations of the magnetic susceptibility.

Superconductivity

The ultimate aim of all theoretical efforts with regard to the high-$T_c$ materials is to explain why the superconducting transition temperatures are so high. Two burning questions are: which interactions lead to the formation of the superconducting state, and what is the form of that state? Owing to the complexity of the materials, progress towards answering both questions has been rather limited. There is unambiguous evidence, however, that the superconducting state is a pair state, i.e., one in which electrons form pairs [8]. Furthermore, experiments show clearly that in the superconducting state there is a weak Josephson-type coupling between the Cu-O planes.

Although most theoretical studies focus on the properties of a single Cu-O plane, the coupling between planes is also important. A key parameter in superconductivity is the coherence length $\xi_L$, which is found to be as small as $\xi_L = 20 \AA$ within the Cu-O planes and $\xi_L \approx 5 \AA$ perpendicular to them. The length $\xi_L$ is of the same order as the distance between the doped holes, in contrast to conventional superconductors where $\xi_L$ is 2 to 4 orders of magnitude larger than the
distance between charge carriers. The high-
$T_c$ materials therefore lie between two limiting
cases. A large number of pairs overlap in the case of large $\xi$, as in the Bardeen-Cooper-Schrieffer (BCS) theory for super-
conductivity, which is described using a pair wave function of a single pair. The other limit is that of well-
separated pairs (bipolarons) which form well above the superconducting transition tempera-
ture. Below $T_c$, these bosonic electron-pairs become superfluid [9].

Numerous experiments suggest that one is really dealing with an extended BCS case rather than with a convention Bose condensate. Experiments also show that unlike in ordinary metals, the ratio between $T_c$ and the Fermi temperature $T_F$ (related by Boltzmann's constant to the Fermi energy, i.e., $T_c/T_F$) is no longer small. The ratio is therefore no longer a good expansion parameter, and corrections for strong coupling are expected to be large. But strong coupling effects cannot be directly calculated or easily esti-
mat ed. This shows why it is unrealistic to expect a quantitative microscopic theory of $T_c$ in the near future.

**Symmetry of the order parameter**

Still uncertain are the symmetries which are broken at the superconducting transition. Gauge symmetry is broken in the BCS ground state due to the establishment of off-diagonal long-range order at $T_c$. The order parameter consisting of the Cooper-pair amplitude $\psi_{ab}$ is added to the ground state if a phase $\alpha$ is added to all one-electron states. Symmetries of the lattice may also be broken at $T_c$, as in p- or d-wave pairing, where the order parameter has a lower symmetry than, for example, the Fermi surface. There is growing experimental evidence that the order parameter vanishes along lines in momentum space. There have even been suggestions that parity and time-reversal symmetries are broken by a radially differe-
tent mechanism of superconductivity, pos-
sibly only in two dimensions (anyon super-
conductivity). Experiments rule out this form of symmetry breaking so we shall not dis-

cuss this interesting superconducting state.

**Strong electron correlations**

The form of the order parameter is inti-
mately connected with the type of interac-
tion which leads to the formation of electron pairs. Leaving aside for the moment the electron-phonon interactions, one would like to know whether or not the $t$-$J$ model, for example, can have a superconducting ground state.

The question of hole-hole interactions within the model has been studied by numerical diagonalisation as well as analyti-
cally by the method of string states [10]. The latter calculations accurately reproduce the former; they also specify when numerical results suffer from the use of clusters that are too small. It is generally found that two holes attract each other with a binding energy $\Delta J/T_c$. One contribu-
tion to the attraction is the energy gain due to a reduced number of broken bonds $S_i S_j$ when the holes sit next to each other. In this case this number is $7$, while it is 8 when the holes are well separated. Additional contribu-
tions arise from changes in the spin cor-

**Table 1 — Experiments on high-$T_c$ superconductors that indicate a strong coupling between phonons and those electrons which become superconducting.**

- Raman (infrared active) phonons show frequency shifts at $T_c$ or at the upper critical field which are much larger than in ordinary superconductors [13].
- Heat conduction, to which phonons contribute predominantly, shows a strong increase as drops below $T_c$. This results from an increase in the phonon mean-free path due to a freezing out of electronic excitations; it allows the phonon transport coupling constant $\nu$ to be estimated.
- There are pronounced isotope shifts of $T_c$ in many high-$T_c$ superconducting compounds below and above optimal doping concentrations. Isotope shifts are a classical indicator for identifying lattice vibrations as source of attraction in ordinary superconductors, although one cannot rule out this mechanism from the absence of a shift. However, it appears to be a gene-
teral trend that at optimal doping (corresponding to the highest $T_c$ in a given class of materials) the isotope shift is practically zero. This suggests that a mechanism not involving phonons is responsible for the high $T_c$.
- Small changes in lattice structure lead in some systems to a complete disappearance of superconductivity.
- Raman spectroscopy of the superconducting density-of-states multiplied by the coupling constant squared, have been observed in tunneling measurements. This is a clear signature of phonon-mediated contributions to electron attractions.

**Electron-phonon interaction**

This leads us to a discussion of the role played by the electron-phonon interaction. It appears to be widely accepted that electron-phonon interactions cannot alone explain the high $T_c$ temperatures [11]. Nevertheless, several experiments (some are listed in Table 1) give direct evidence for a strong coupling between phonons and those electrons which become superconducting.

Studies of the phonon frequency-shifts and of the heat conductivity based on the standard Migdal-Eliashberg theory of the interplay of phonons and superconducting electrons lead to an electron-phonon cou-
pling constant $\lambda = 2\nu$. This is in rough agreement with values of $\lambda \approx 1-1.5$, derived from conventional band-structure theory and from frozen phonon calculations in which the strong electronic correlations are left out. Values of 2-3 would be sufficient to explain the high $T_c$ values. Using such large values of $\lambda$, it was shown that the linear dependence of $\rho_{ab}$ on $T$ can at least be explained in the 100-400 K temperature range; the $T_c^2$ behaviour observed in overdoped La$_{2-x}$Sr$_x$CuO$_4$ remains unexplained.

What is asked for is a unified description of both, namely of the strong electron-phonon interac-
tions and strong electron correla-
tions. Such a theory is presently not in sight.

**Conclusions**

It has become obvious that the doped cuprates are not simply conventional, aniso-
tropic metals. They are instead characte-

rised by strong electronic correlations which change substantially excitation spectra and transport properties. We have discussed models for low-energy excitations and presented arguments why they are expected to correctly describe the physics of these systems in the low-energy regime. Yet the models are still complex enough that so far only partial and mainly qualitative explanations of the various experimental results could be provided. This is why the fields of high-$T_c$ superconducting materials and strongly correlation electrons remain a challenge for both experimentalists and theorists.