REVIEWS OF TOPICAL PROBLEMS

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Quasiparticles in strongly correlated electron systems in copper oxides

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<u>Abstract.</u> New experimental and theoretical results on the electronic structure and spectral properties of quasiparticles in copper oxides are reviewed. It is shown that the electronic structure transforms from antiferromagnetic insulators to optimally doped high-temperature superconductors as the doping level is varied. The experimental methods considered are primarily angular resolved photoelectron spectroscopy (ARPES), neutron scattering, and NMR. Two types of electronic structure calculations for data interpretation purposes are considered, namely, exact numerical methods for finite clusters (exact diagonalization and the quantum Monte Carlo method) and approximate schemes for an infinite lattice. As a result, a coherent unified picture emerges, in which magnetic polarons (which are carriers in a weakly doped antiferromagnetic lattice) transform into a system of Fermi quasiparticles dressed in

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Received 24 March 1997, revised 22 April 1997 Uspekhi Fizicheskikh Nauk **167** (10) 1043–1068 (1997) Translated by E G Strel'chenko; edited by S N Gorin short-range antiferromagnetic-type spin fluctuations. In the region of weakly doped metallic compositions, deviations from Fermi-liquid properties are seen, such as the failure of Luttinger's theorem, shadowy photoemission bands, and the spin pseudogap effect in spectral and thermodynamic measurements. The situation in the neighborhood of the insulator – metal concentration transition is noted to be least understood.

1. Introduction

The history of systems with strong electron correlation (SEC) actually stretches back to Ref. [1] which was able to settle the conflict between the insulating properties of 3d-metal oxides, such as Fe₃O₄ and NiO, and the one-electron band-theory prediction of metallic behavior for a partially filled band. The discovery of high-temperature superconductivity (HTSC) [2] caused a resurgence of interest in the SEC because it was very soon realized that conventional band-theoretical methods combined with the local-density-functional approximation lead to a metallic state for undoped insulators such as La₂CuO₄, Nd₂CuO₄, YBa₂Cu₃O₆, Sr₂CuO₂Cl₂, etc. It was widely believed that an understanding of HTSC requires a knowledge of exactly how the doping process transforms the structure of copper oxides, and was impossible to learn without an adequate description of undoped and weakly doped systems with an SEC-determined electronic spectrum and physical properties. That superconductivity may exist in systems near the metal-insulator transition has long been known [3], and consequently a great number of papers on the SEC problem have appeared over the last decade.

Although the electronic structure and superconductivity mechanisms of copper oxides have been reviewed more than once in the literature [4-13], over recent years a number of works of direct relevance to the present subject have appeared. These are, first and foremost, angular resolution photoelectron spectroscopy (ARPES) measurements, from which we know the Fermi surface shapes for a number of superconducting copper oxides [10] and the hole dispersion near the top of the valence band in the insulator $Sr_2CuO_2Cl_2$ [14] with its undoped CuO₂ planes. Furthermore, the ARPES technique enabled the first observations of how the electronic spectrum in Bi-2212 evolves with variation of the hole concentration [15]. It is these results, together with a number of important theoretical predictions for Hubbard's and more complex multiband models, that stimulated the present review.

Some types of single-particle Fermi-like excitations, or quasiparticles, exist even in undoped insulating systems, where the SEC effects are at their strongest and the singleelectron approximation is not applicable. The present review is concerned with two types of approach to these quasiparticles, namely exact numerical methods (exact diagonalization and the quantum Monte Carlo method) for finite clusters, and various approximate methods for an infinite lattice. As it is not within the scope of this review to discuss superconductivity mechanisms, which has already been done in Refs [6, 12] we will only consider the properties of quasiparticles and their effects on the electronic properties of the insulating and normal metallic phases.

The author does not advocate the view that models with SEC are the only ones capable of accounting for HTSC in copper oxides: one surely cannot ignore the successes of ordinary band theory in describing Fermi surfaces [5, 10] and optical properties [16, 17] of superconductors. At the same time, x-ray photoelectron spectroscopy (XPS) and x-ray absorption spectra (XAS) have displayed SEC effects even in metallic compositions [18]. A possible reason why these effects are not observed at the Fermi surface is given in Ref. [19].

2. New electronic structure data

Of the various techniques currently available for the analysis of electronic structure, ARPES is the most informative one. The photoelectron spectrum is usually considered to be proportional to the single-electron spectral density,

$$A_{+}(p,\omega) = \sum_{n} \left| \left\langle \Phi_{n}^{N+1} | c_{p\sigma}^{+} | \Phi_{0}^{N} \right\rangle \right|^{2} \delta(\omega - E_{n}^{N+1} + E_{0}^{N}), \ \omega > \mu,$$

$$A_{-}(p,\omega) = \sum_{n} \left| \left\langle \Phi_{n}^{N-1} | c_{p\sigma}^{+} | \Phi_{0}^{N} \right\rangle \right|^{2} \delta(\omega - E_{n}^{N-1} + E_{0}^{N}), \ \omega < \mu,$$

(1)

where the functions A_- and A_+ determine the photoemission (PES), and the inverse photoemission (IPES) spectra, respectively, it being implied that the matrix element of the dipole optical transition is merely a constant. That this is not a universally valid assumption may be seen by comparing the ARPES spectra of Sr₂CuO₂Cl₂ taken in nonpolarized and polarized light (see Section 2.1). In a more elaborate analysis,

two-particle correlation functions are introduced for describing the light-induced creation and annihilation of electron – hole pairs. The probability of a light absorption event with a valence electron $c_{p\sigma}^+$ being excited into the photoelectron state $a_{p\sigma}^+$ with energy ε_p is

$$I(p,\omega) = \sum_{\sigma} |M(p,q,\alpha)|^2 \int_{-\infty}^{\infty} \frac{\mathrm{d}t}{2\pi} \\ \times \exp(\mathrm{i}\omega t) \langle c_{p-q}^+(t) \, a_{p\sigma}(t) \, a_{p\sigma}^+ c_{p-q\sigma} \rangle , \qquad (2)$$

where the absorbed photon has a frequency ω , wave vector $q \approx 0$, and polarization α ; and $M(p, q, \alpha)$ is the matrix element of the dipole transition. Neglecting the vertex part responsible for the interaction of photoelectrons with the valence electrons, we have

$$I(p,\omega) = \sum_{\sigma} |M(p,q,\alpha)|^2 \int_{-\infty}^{\infty} \frac{\mathrm{d}t}{2\pi} \\ \times \exp\left[\mathrm{i}(\omega - \varepsilon_{\mathrm{k}} - w_{\mathrm{A}})t\right] \langle c_{p-q,\sigma}^+(t)c_{p-q,\sigma} \rangle \\ = \sum_{\sigma} |M(p,q,\alpha)|^2 \sum_{n} |\langle \Phi_n^{N-1}|c_{p\sigma}|\Phi_0^N \rangle|^2 \\ \times \delta(\omega - \varepsilon_p - w_{\mathrm{A}} - E_n^{N-1} + E_0^N).$$
(3)

Here w_A is the work function. The matrix element is wavevector and polarization dependent and allows for the relevant selection rules. The two-dimensional wave vector p_{II} for an ARPES-detected photoelectron is

$$p_{\rm II} = \left[2m(\omega - w_{\rm A} - E_{n,p}^{N-1} + E_0^N)\right]^{1/2}\sin\theta$$

where θ is the polar angle of emission.

2.1. Electron structure at the top of the valence band in Sr₂CuO₂Cl₂

The oxychloride Sr₂CuO₂Cl₂, having a K₂NiF₄-type structure with CuO_2 layers separated by double Sr-Cl layers, is an analogue of the tetragonal structure La₂CuO₄. The electrical and magnetic properties of Sr2CuO2Cl2 and La2CuO4 are also similar: both are insulators, both — according to band theory - must be half-filled-band metals, and both are antiferromagnets. For single crystals of $Sr_2CuO_2Cl_2$, $T_N = 256$ K [20]. For Sr₂CuO₂Cl₂, no orthorhombic phase is seen down to T = 10 K. Another important difference between Sr₂CuO₂Cl₂ and La₂CuO₄ is that the former cannot be doped [21]; it is believed that Sr₂CuO₂Cl₂ has no charge carriers in its CuO₂ planes. At the same time, its isostructural analogue, $Sr_2CuO_2F_{2+y}$, at large enough y becomes superconducting with $T_c = 46$ K[22]. An experimental study of the hole dispersion at the top of the valence band was carried out using ARPES on single crystals of Sr₂CuO₂Cl₂ [14]. At a spectrum measurement temperature T = 350 K the samples are above the Néel point, in the region of short-range antiferromagnetic order with a correlation length $\zeta_{AFM} \approx 250 \text{ A}$ [23]. For rapid local measurements, this implies that the spectra are sensitive to antiferromagnetic order effects. From two-magnon Raman scattering data [24], the exchange interaction between two nearest neighbors is $J = 125 \pm 6$ meV. ARPES spectra are obtained using a synchronous source with an energy resolution of 75 meV and a wave vector resolution for k_x , k_y of $(1/20)\pi$. The lattice parameter is taken to be unity. The characteristic points of the square-lattice Brillouin zone are denoted $X = \pi(1, 0)$, $Y = \pi(0, 1), M = \pi(1, 1), \overline{M} = \pi(1/2, 1/2)$. Figure 1 shows ARPES data for the direction ΓM in the undoped insulating Sr₂CuO₂Cl₂ and superconducting Bi₂Sr₂CaCuO_{2+y}. From Fig. 1 it is seen that the top of the band is reached at point \overline{M} with energy $E(\overline{M}) = -0.8$ eV as measured from the Fermi level. One further point to be noted is the nonmonotonic behavior of the intensity peak, which has a maximum near \overline{M} and falls off to zero near Γ and M. The total band width is $W = 280 \pm 60$ meV.

A comparison of the spectra of $Sr_2CuO_2Cl_2$ with data for the metallic compound $Bi_2Sr_2CaCuO_{2+y}$ [25] (Fig. 1b) shows that the peaks in the spectra of the latter are narrower and disappear after crossing the Fermi level near point $\pi(0.45;$ 0.45). The dispersion law below the Fermi level is very similar to the corresponding dispersion for an insulator. Thus, in the region of k from $\pi(0.27; 0.27)$ to $\pi(0.45; 0.45)$, the dispersion in Bi-2212 was 270 ± 30 meV, and in Sr₂CuO₂Cl₂, 240 ± 30 meV. This similarity suggests that the rigid-band model is applicable here, because the doping process simply acts to push the Fermi level into the valence band. This simple dispersion behavior, however, occurs only for the ΓM direction. The absence of peaks in the ΓX direction is inconsistent with the rigid-band picture because doped metallic compositions are known to have a flat band with $\varepsilon_{\rm F}$ near $(\pi, 0)$ [25, 26]. Calculations within the t-J model [7, 27] yield W = 2.2 J over a wide range of values of t/J. Based on the above values of the bandwidth W and the exchange interaction J, $W/J = 2.5 \pm 0.5$, in good agreement with the t-J model. For other Brillouin zone directions there is deviation from the t-J model, which is discussed in more detail in Section 5.2.

In a later work [28], ARPES spectra for single crystals of Sr₂CuO₂Cl₂ were measured for various photon polarizations.



Figure 1. ARPES data for $Sr_2CuO_2Cl_2$ (a) and $Bi_2Sr_2CaCu_2O_{8+y}$ (b) from Ref. [14]. The numbers labeling curves are values of k_x , k_y in units of π . Top: two-dimensional Brillouin zone; closed circles correspond to filled states, the size of a circle indicating the wave vector resolution.

The electron dispersion for the [1, 1] direction was found to be the same as in Ref. [14]. For [1, 0] the spectra were found to be light-polarization dependent, so that the spectral density has no peaks for the electronic states of odd parity for reflections in the plane defined by the normal and [1, 0] direction, whereas even-parity states show a clear quasiparticle peak with a dispersion of 0.2 eV. The difference between the spectra of unpolarized [14] and polarized [28] photons indicates the important role of the matrix elements.

2.2. Shadow bands and antiferromagnetic short-range order in $Bi_2Sr_2CaCu_2O_{8+x}$

That strong antiferromagnetic fluctuations exist not only at a low doping level but also in superconducting compositions is well known from neutron scattering data for $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{7-\nu}$ [30]. The effect of fluctuations on electronic structure is very much under discussion at the present time. Of great importance in this connection are the ARPES data on the electronic structure of $Bi_2Sr_2CaCu_2O_{8+x}$ [31], which directly show the effect of magnetic fluctuations on the Fermi surface. Unlike the standard ARPES procedure, which specifies the direction of the vector $k = (k_x, k_y)$ and in which spectra are generally measured along a limited number of high-symmetry Brillouin zone directions, the authors of Ref. [31] restricted the energy range to $\Delta E = 10$ meV near the Fermi level and mapped the intensities of emitted photoelectrons over the entire Brillouin zone for 6000 discrete values of k, with an angular resolution of better than 0.1° . In Figure 2, which shows the section of the Fermi surface along the plane $k_x k_y$, one clearly sees two distinct types of curves, highintensity X- and Y-centered curves, and low-intensity curves around the center of the zone and the corner points such as M. That the low-intensity curves are obtained from the high intensity ones by shifting by the wave vectors ΓX or ΓY , as



Figure 2. (a) Intensity map for photoelectrons from Bi₂Sr₂CaCu₂O_{8+x} in the energy range of 10 meV near the Fermi energy. The logarithmic intensity scale serves to emphasise weak features. The external circumference corresponds to an angle of 90°. (b) Simplified form of (a), indicating points in the Brillouin zone and emphasizing intense (solid curves) and weak (dashed curves) lines. (c) Diagram of extended Brillouin zones showing that when shifted by vector ΓX or ΓY the system of intense lines forms a system of weak lines. (d) Fermi surface of Bi₂Sr₂CaCu₂O₂ computed by the Linearized Augmented Plane Wave (LAPW) method [32]. (After Ref. [31]).

shown in Fig. 2c, indicates the existence of a new periodic 2×2 structure. Since low-energy electron diffraction gives no evidence of atomic structure rearrangement on the surface of a single crystal, the doubling of the period is associated with magnetic fluctuations. The excitation of photoelectrons is a rapid local process whose spatial and temporal scales may be small compared with spin fluctuation correlations, so that the superstructure 2×2 behaves as quasistatic and the weak lines may well be associated with the contraction of the Brillouin zone.

Such states had been predicted earlier [33] and called 'shadow' states. In analyzing the effect of spin fluctuations on the electronic structure, the authors of Ref. [33] used phenomenological arguments to specify the spin susceptibility law and showed that, for sufficiently strong antiferromagnetic correlations the Umklapp processes (the relation between the vectors k and k' with $|k' - k - Q| < 1/\zeta$, where $Q = (\pi, \pi)$ and ζ is the correlation length) lead to the appearance of shadow bands. Their calculations suggest, however, that for the corresponding satellites to be observable in the ARPES spectra, the correlation length ζ must be large enough, $\zeta \approx 20a$, where a is the Cu–Cu separation. Since neutron scattering data indicate that in superconducting Bi-2212 compositions ζ is only a few *a*, this interpretation of the results of Ref. [31] was questioned [34]. However, later microscopic calculations [35, 36] (to be discussed in further detail in 5.3) predict shadow bands at a small correlation length $\zeta = 2.5a$, consistent with neutron scattering data.

Another result of Ref. [31] is that some of the Fermi surface details are consistent with the band-theory predictions of Ref. [32]. These are, for example, $k_{\rm F}$ in the directions to points (1, 0) and (0, 1), and the surface curvature near $k_{\rm F}$ in these directions. However, no small pockets centered at $\overline{M} = (\pi/2, \pi/2)$ and similar points were observed, and, conversely, shadow bands are not predicted by band calculations.

2.3 Band-structure changes with doping

ARPES studies of band structure as a function of hole concentration were performed on two groups of Bi-2212 samples [15]. In the first group, consisting of single crystals of Bi₂Sr₂CaCu₂O_{8+x}, the carrier concentration was varied by annealing in air at T = 600 °C in order to obtain 'overdoped' samples with $T_c = 85$ K, and alternatively in argon at T = 550 °C, to obtain 'underdoped' samples with $T_c = 67$ K; the terms 'under' and 'over' refer to the optimum hole concentration, i.e., T_c -maximizing. The second group were single crystal Bi₂Sr₂Ca_xDy_xCu₂O_{8+x} films grown by molecular-beam epitaxy [37]. For samples with x = 1%, 10%, and 17.5% Dy, T_c was 85 K, 65 K, and 25 K, respectively. For x = 50% Dy, the films were insulating. The spectra were measured in a vacuum at T = 110 K.

The electron dispersion curves are shown in Fig. 3. For all the samples that remain superconducting, the dispersion in the direction [1, 1] does not change significantly, nor do the quantities $k_{\rm F}$. On going to the insulation region, the dispersion in the direction from (0, 0) to $(\pi/2, \pi/2)$ remains similar to the corresponding portion for metallic samples, although the bandwidth decreases. The dispersion near point X shows an entirely different behavior. A transition from optimally doped to underdoped samples results in the disappearance of the Fermi surface cross section on the line XM (Fig. 4). The optimally doped samples $(T_c = 85 \text{ K})$ exhibited large Fermi surface cross sections consistent with



Figure 3. Dispersion relation for samples of varying hole concentration. (a) Films of Bi₂Sr₂Ca_{1-x}Dy_xCu₂O_{8+x}: *1*, 1% Dy, $T_c = 85$ K; *2*, 10% Dy, $T_c = 65$ K; *3*, 17.5% Dy, $T_c = 25$ K, *4*, 50% Dy, insulator. (b) Single crystal of Bi₂Sr₂CaCu₂O_{8+y}: *1*, annealed in air, $T_c = 85$ K; *2*, annealed in argon $T_c = 67$ K. (After Ref. [15]).



Figure 4. Cross sections of the Fermi surface of Bi-2212 superconductors for various hole concentrations (From Ref. [15]). Note the opening of a gap on the line $(\pi, 0) - (\pi, \pi)$ with decreasing hole concentration.

Luttinger's theorem [10]. If the rigid-band model were valid, then decreasing the hole concentration would only reduce the area but not the shape of the cross section (as shown by a dashed line in Fig. 4), and the Fermi surface would remain intersected by the line XM — which disagrees with experiment which shows an energy gap opening along this line at the Fermi surface. The authors of Ref. [15] suggest three ways of explaining their results. The first is that quasiparticles may pair with no pair coherence above T_c . This pairing would be able to open a gap without giving rise to a coherent superconducting state. Quasiparticle pairing above T_c was treated in terms of the extended Ginzburg-Landau theory for d-type superconductivity in Refs [38-40]. The pairing of d-type spinons [41, 42] within the theory of resonant valence bonds (RVB) [43] was also discussed for temperatures above T_c . For either type of pairing, the shift in photoelectron energy near X is treated as the appearance of a gap of symmetry $d_{x^2-y^2}$,

which is greatest at X and zero along ΓM . The amplitude of the gap can be estimated from the shift in the binding energy for point X, which varies between 20 and 30 meV.

The second interpretation involves the formation of a superstructure, due either to antiferromagnetic ordering or an atomic ordering rearrangement. In this case points Γ and M become equivalent in the new Brillouin zone, and shadow bands appear on the side of M. The mixing of the original and shadow bands opens a gap near X in exactly the same way as in the theory of spin density waves (SDW) [44]. The section of the Fermi surface by a shadow band in this case is shown by a dash-dot line in Fig. 4. The third approach, finally, also involves the d-pairing of spinons, but assumes SU(2) symmetry to be conserved in doping [45]. Comparing the data of Refs [15, 31] with theoretical predictions [7-9, 33, 35, 35]36] indicates that the band structure is partially rearranged, with the density of states at the Fermi surface being modified by spin fluctuations. In this case the reconstruction of the Fermi surface with decreasing hole concentration is due to a change in its topology. Comparing the dispersion curves in Figs 1 and 3 allows an important conclusion to be drawn about the transformation of the electronic structure, namely that in an undoped sample the top of the valence band is reached at point $\overline{M} = (\pi/2, \pi/2)$. Doping gives rise to in-gap impurity states with deep levels [46-50]. A detailed understanding of the effect of doping on the electronic structure near the metal-insulator transition is still lacking. In an underdoped metallic phase, new states appear near X, which form a flat band. The assumption that these states arise from the in-gap states of the insulating phase in a very natural way explains the fact that they have no dispersion. As the hole concentration is increased to its optimum value, these states form a band with a saddle point near X and a maximum at M.

2.4 Band structure of Sr₂RuO₄

The role of CuO₂ layers remains a central question for the understanding of the mechanism of superconductivity. Could other, copper-free, layered perovskites be superconducting? The recent discovery of Sr₂RuO₄ superconducting compounds with $T_c = 0.93$ K [51] allows an interesting comparison to be made with copper oxides. Crystals of Sr₂RuO₄ have a body-centered tetragonal K₂NiF₄ type lattice with a = b = 3.8694 A, and c = 12.764 A at room temperature [52]. The differences between Sr₂RuO₄ and layered cuprates are as follows: (a) superconductivity already exists in undoped samples; (b) for the ion $Ru^{4+}(4d^4)$ in the low-spin state, S = 1; (c) the process of p-d hybridization in Sr₂RuO₄ involves t_{2g} (d_{xy} , d_{xz} , and d_{yz}) orbitals. The ARPES spectra for Sr₂RuO₄ were measured at 10 K in vacuum with an energy resolution of 22 meV and an_angular resolution of 1°, which corresponds to $\Delta k = 0.06 \,\mathrm{A}$ [53]. Analogous to the cuprates, the dispersion curve near $(\pi, 0)$ has a saddle point that produces a Van Hove singularity (Fig. 5). Comparing these results with local density functional calculations [54], the authors of Ref. [53] note that agreement with theory could only be obtained by introducing a 77 meV shift into the band calculations. According to Ref. [54], the three bands observed at the Fermi surface are primarily of d_{xz} , d_{yz} , and d_{xy} type. The two bands centered about (π, π) are of the hole type, and the band about (0, 0) is of the electron type. The Van Hove singularity lies 17 meV below $\varepsilon_{\rm F}$.

Previous APRES experiments revealed $k = (\pi, 0)$ saddle points and Van Hove singularities in many cuprates as can be seen in Table 1. The table shows that the *n*-type NCCO system



Figure 5. Flat bands near point $(\pi, 0)$ for Sr₂RuO₄ from ARPES data (from Ref. [53]). Note that in Ref. [53] the notation for Brillouin zone points is inverted from ours: here $\bar{X} = (\pi, \pi)$, $\bar{M} = (\pi, 0)$.

 Table 1. Superconducting transition temperature, temperature dependence of electrical resistance in the normal phase, and the position of the van Hove singularity as measured from the Fermi energy. (After Ref. [53])

Compound	$T_{\rm c}, {\rm K}$	$\rho_{ab}(T)$	$E_{\rm VH}$, meV	Reference
YBa ₂ Cu ₃ O _{7-y}	92	linear	< 10	[55]
YBa2Cu4O8	82	linear	19	[55]
Bi2(Sr0.93Pr0.03)2CuO6	10	linear	< 30	[56]
Bi2Sr2CaCu2O8+y	83	linear	< 30	[25]
Nd _{1.85} Ce _{0.15} CuO ₄	25	quadratic	350	[57]
Sr ₂ RuO ₄	0,93	linear [58]	17	[53]

is unique both in showing the $\rho(T) \propto T^2$ behavior [58] and in having its Van Hove singularity far from $\varepsilon_{\rm F}$. In Sr₂RuO₄ this singularity is as close to the Fermi energy as it is in the cuprates. The proximity of $T_{\rm c}$ to the Van Hove singularity has often been considered as the explanation of the high $T_{\rm c}$ in cuprates (see [59, 60] and review articles [3, 6, 12]). The low values of $T_{\rm c}$ in Bi-2201 and Sr₂RuO₄ cast some doubt on this view.

3. Basic multielectron models and the definition of Fermi quasiparticles in strongly correlated electron systems

Attempts at adapting band calculations to strongly correlated systems include (i) correcting the potential in the region of two-particle states [61] and (ii) the inclusion of self-action corrections to the potential [62]. Since the Kohn-Sham theorem is exact, one would expect, in principle, that quasiparticles in strongly correlated systems could also be treated using the density functional formalism — provided, of course, that the functional is local. The application of the density functional scheme to SEC systems deserves special discussion and need not be pursued here because we limit our consideration to model theories. Since the first part of this section, on the Hubbard, three-band p-d, and t-J models, inevitably overlaps with many previous reviews on the subject [4–13], the models will be reviewed only briefly, with particular emphasis on their applicability to the CuO₂ plane.

3.1 Single-band Hubbard model with repulsion

The Hamiltonian for a system of electrons in this model is of the form [63]

$$H = \sum_{i,\sigma} \left((\varepsilon - \mu) n_{i\sigma} + \frac{U}{2} n_{i,\sigma} n_{i,-\sigma} \right) + \sum_{i,j,\sigma} (t_{ij} a_{i\sigma}^+ a_{j\sigma} + \text{H. c.}),$$
(4)

where $n_{i\sigma} = a_{i\sigma}^+ a_{i\sigma}$, $a_{i\sigma}$ is the annihilation operator for an electron on site *i* with spin $\sigma = \pm 1/2$, ε is the single-electron energy in the crystal field, μ is the chemical potential, *U* the Hubbard repulsion, and t_{ij} the hopping integral between sites *i*, *j*. Consider the local basis of this model

$$|0\rangle, \quad |\sigma\rangle = a_{i\sigma}^+|0\rangle, \quad |2\rangle = a_{i+}^+ a_{i-}^+|0\rangle \tag{5}$$

with energies $\varepsilon_0 = 0$, $\varepsilon_{\sigma} = \varepsilon - \mu \equiv \varepsilon_1$, $\varepsilon_2 = 2\varepsilon_1 + U$. For the CuO_2 plane in the hole representation, $|0\rangle$ corresponds to the configuration $\operatorname{Cu}^+(d^{10})$, $|\sigma\rangle$ to $\operatorname{Cu}^{2+}(d^9)$, and $|2\rangle$ to $\operatorname{Cu}^{3+}(d^8)$. In undoped La₂CuO₄, copper is in the state Cu^{2+} , i.e., the ground state of the system has one-hole terms filled. Doping with holes has the effect of increasing the number of holes per cell, $n_{\rm h} = 1 + x$, making the configuration Cu³⁺ partially filled. However, x-ray spectroscopy has not shown Cu³⁺ to be present in a sufficient amount [64]. Holes added to the system in the doping process primarily fill oxygen orbitals, not considered in the Hubbard model. This is not to say this model is not applicable to oxides. The point is that more realistic models reduce to the Hubbard model for certain ranges of their parameters. Besides, the study of the properties of quasiparticles in the Hubbard model is interesting from the methodological point of view.

3.2 Three-band p-d model

This model extends the Hubbard model to the case of the CuO_2 layer [65, 66]:

$$H = \sum_{f,\sigma} \left((\varepsilon_{d} - \mu) n_{f\sigma} + \frac{U_{d}}{2} n_{f\sigma} n_{f,-\sigma} \right) + \sum_{i,\sigma} \left((\varepsilon_{p} - \mu) n_{i\sigma} + \frac{U_{p}}{2} n_{i\sigma} n_{i,-\sigma} \right) + \sum_{\langle i,f \rangle \sigma} t_{pd} (p_{i\sigma}^{+} d_{f\sigma} + \text{H. c.}) + \sum_{\langle i,f \rangle \sigma} t_{pp} (p_{i\sigma}^{+} p_{j\sigma} + \text{H. c.}) + V_{pd} \sum_{\langle i,f \rangle \sigma} n_{i\sigma} n_{f\sigma}.$$
(6)

Here f and i are copper and oxygen sites, respectively; ε_d and ε_p are the energies of a $d_{x^2-y^2}$ hole at copper and of a p_x , p_y holes at oxygen; U_d , U_p are the Coulomb parameters; t_{pd} is

the hopping integral between the nearest copper and oxygen sites; t_{pp} is the oxygen-oxygen hopping integral; and V_{pd} is the copper-oxygen interatomic Coulomb interaction. An important parameter of the problem is the energy of excitation for a charge transfer, $\Delta = \varepsilon_p - \varepsilon_d$. The p-d model has the undisputable merit of taking into account the chemical composition of the copper oxides. The model Eqn (6) enables a description of a large number of high-energyexcitation spectral techniques, such as x-ray absorption and x-ray photoelectron spectroscopy. On the other hand, models (4) and (6) are very similar in their low-energy behavior. The reason for this is indicated in Ref. [67], where it was demonstrated for the CuO₄ cluster that the 'hole at copper, hole at oxygen' complex has S = 0, and that a similar triplet state lies 2 to 4 eV higher in energy. Since the dopingproduced holes fall into the Zhang-Rice singlet, the singlecell local basis of (6) is identical to the Hubbard basis if the vacuum state is taken to be the copper (oxygen) $d^{10}p^6$ configuration and if, furthermore, the one-hole $|\sigma\rangle$ and twohole $|2\rangle$ states are brought into correspondence with the $(d^{10}p^5 \text{ and } d^9p^6 \text{ mixing})$ molecular orbitals and Zhang-Rice singlet, respectively. There is a considerable amount of literature analyzing the reduction of the three-band p-dmodel successively to the single-band Hubbard model and further to the t-J model (see Refs [68-73] and references in review articles [7-9]).

3.3 t - J model

The t-J model was originally derived from the Hubbard model in the limit $t/U \ll 1$. A canonical transformation eliminating two-particle configurations gives rise to the Hamiltonian [74, 75]

$$H_{t-J^*} = -t \sum_{\langle i,j\rangle\sigma} (c^+_{i\sigma} c_{j\sigma} + c^+_{j\sigma} c_{i\sigma}) + \frac{t^2}{U} \sum_{j,\delta,\delta'} (c^+_{j+\delta\uparrow} c^+_{j\downarrow} c_{j\downarrow} c_{j+\delta'\uparrow} + c^+_{j\uparrow} c^+_{j+\delta\downarrow} c_{j+\delta'\downarrow} c_{j'\uparrow} + c^+_{j+\delta\uparrow} c^+_{j\downarrow} c_{j+\delta'\downarrow} c_{j\uparrow} + c^+_{j\uparrow} c^+_{j+\delta\downarrow} c_{j\downarrow} c_{j+\delta'\uparrow}),$$
(7)

where $j + \delta$ and $j + \delta'$ are the nearest neighbors to site *j*. In the special case $\delta = \delta'$, neglecting the three-center terms in (7), we obtain the t-J Hamiltonian with $J = 4t^2/U$:

$$H_{t-J} = -t \sum_{\langle i,j \rangle \sigma} (c^+_{i\sigma} c_{j\sigma} + \text{H.c.}) + \sum_{\langle i,j \rangle} J \left(S_i \cdot S_j - \frac{n_i n_j}{4} \right).$$
(8)

The operators here act in bounded Hilbert space with twoparticle states excluded, $c_{i\sigma} \rightarrow c_{i\sigma}(1 - n_{i,-\sigma})$. The three-center terms contribute only in the presence of holes and can be rewritten in the form

$$H_{J}^{(3)} = -\frac{t^2}{U} \sum_{j,\sigma} \sum_{\delta \neq \delta'} (c_{j+\delta,\sigma}^+ n_{j,-\sigma} c_{j+\delta',\sigma} - c_{j+\delta,\sigma}^+ c_{j,-\sigma}^+ c_{j+\delta',-\sigma}).$$

$$\tag{9}$$

The first term in (9) accounts for intrasublattice hopping, which does not affect the antiferromagnetic order, whereas the second describes spin-reversal second-nearest-neighbor hopping. The inclusion of such hops yields the t-t'-J model [72]. An energy comparison for the Hubbard and t-J no-hole ground states and also for the t-J, $t-J^*$ and Hubbard one-hole ground states was carried out in Ref. [76] by exactly diagonalizing a one-dimensional 10-atom chain and a two-

dimensional 10-atom lattice. It was found that for U/t = 20all the models agree to within about 1%. However, for U = 8ta discrepancy of up to 20% is noted in two dimensions, necessitating corrections of higher order in t/U in the effective Hamiltonian. Thus, strictly speaking the t-J model derives from the Hubbard model in the limit $J \ll t$. However, because of its nontrivial properties, the t-J model is often used at arbitrary t to J ratios. This may be justified by referring to Ref. [77], in which it is shown that adding the Coulomb matrix element V_{ij} allows a later transition to the t-J model, for which the inequality $t \ll J$ is not necessary. The reason is that at large enough values of V_{ij} the system may develop instability with respect to charge density waves, and it is close to such an instability where it may become a physical realization of the t-J model with $J \sim t$ [77].

3.4 Multiband p-d model

The actual orbital structure of copper is important not only for the analysis of valence band spectra far away from the Fermi surface, but also for symmetry analysis of the states near to it. The nonzero population of the d_{z^2} orbitals was found in experiments [78, 79] on the polarization dependence of x-ray absorption in Cu L_3 , which showed a correlation between T_c and the d_{z^2} orbital population. As for the t_{2g} orbitals, these are deep in the valence band (about 4 eV from the top [5]). Thus, the minimum a realistic model of the CuO₂ layer must contain is two d orbitals, $d_{x^2-y^2}$ and d_{z^2} , and p_x and p_y orbitals at each oxygen ion. In calculations involving apical oxygen, an oxygen p_z orbital is added. A model of this type suggested for the copper oxides [80] has a Hamiltonian of the form

$$H = H_{d} + H_{p} + H_{pd} + H_{pp} , \qquad (10)$$

$$H_{d} = \sum_{r} H_{d}(r) ,$$

$$H_{d}(r) = \sum_{\lambda\sigma} \left[(\varepsilon_{d\lambda} - \mu) d^{+}_{r\lambda\sigma} d_{r\lambda\sigma} + \frac{1}{2} U_{d} n^{\sigma}_{r\lambda} n^{-\sigma}_{r\lambda} \right]$$

$$+ \sum_{\sigma\sigma'} (V_{d} n^{\sigma}_{r1} n^{\sigma'}_{r2} - J_{d} d^{+}_{r1\sigma} d_{r1\sigma'} d^{+}_{r2\sigma'} d_{r2\sigma}) ,$$

$$H_{p} = \sum_{i} H_{p}(i), \ H_{p}(i) = \sum_{\alpha\sigma} \left[(\varepsilon_{p\alpha} - \mu) p^{+}_{i\alpha\sigma} p_{i\alpha\sigma} + \frac{1}{2} U_{p} n^{\sigma}_{i\alpha} n^{-\sigma}_{i\alpha} \right]$$

$$+ (V_{p} n^{\sigma}_{i1} n^{\sigma'}_{i2} - J_{p} p^{+}_{i1\sigma'} p_{i1\sigma'} p^{+}_{i2\sigma'} p_{i2\sigma}) ,$$

$$\begin{split} H_{\rm pd} &= \sum_{\langle i,r\rangle} H_{\rm pd}(i,r) \,, \\ H_{\rm pd}(i,r) &= \sum_{\alpha\lambda\sigma\sigma'} (T_{\lambda\alpha}p^+_{i\alpha\sigma} + d_{r\lambda\sigma} + {\rm H.\,c.} + V_{\lambda\alpha}n^{\sigma}_{r\lambda}n^{\sigma'}_{i\alpha} \\ &- J_{\alpha\lambda}d^+_{r\lambda\sigma}d_{r\lambda\sigma'}p^+_{i\alpha\sigma'}p_{i\alpha\sigma}) \,, \\ H_{\rm pp} &= \sum_{\langle i,j \rangle} \sum_{\alpha\beta\sigma} (t_{\alpha\beta}p^+_{i\alpha\sigma}p_{j\beta\sigma} + {\rm H.\,c.}). \end{split}$$

Within the multiband p-d model, the applicability of its three-band variety can be analyzed. Clearly, in the limit $\Delta_d = \varepsilon(d_{z^2}) - \varepsilon(d_{x^2-y^2}) \rightarrow \infty$ the multiband model becomes the three-band model. At the same time, for copper oxides $\Delta_d \sim 1$ eV, so that changing from large values of Δ_d to $\Delta_d \sim 1$ eV enables the influence of the orbital structure of

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copper to be studied. The simplest such calculation was carried out by exact diagonalization for the CuO₄ cluster [81].

The eigenstates of the cluster are indexed by the number of holes it contains, n = 0, 1, 2, ... For n = 0 we have the vacuum state $d^{10}p^6$. For n = 1, the eigenstates are the usual one-hole molecular orbitals of b_{1g} and a_{1g} symmetry, $d_{x^2-y^2}$ and d_{z^2} hybridizing with the p orbitals of the former and latter symmetry, respectively. For n = 2 we have the mixed configurations p⁵d¹⁰p⁵, p⁶d⁹p⁵, p⁶d⁸p⁶, p⁴d¹⁰p⁶, giving rise to a set of spin singlets and triplets in various orbital states. The energy difference between the two lowest terms, the singlet ${}^{1}A_{1g}$ and triplet ${}^{3}B_{1g}$, is shown in Fig. 6 for three different sets of model parameters. It is seen that for large Δ_d $(\Delta_d \ge 10 \text{ eV})$ the triplet lies $\Delta \varepsilon_S \approx 2 \text{ eV}$ above the singlet (in agreement with Ref. [67]), which allows it to be neglected in a low-energy description. As the parameter \varDelta_d decreases, however, so does the singlet-triplet splitting, and in the region $\Delta_d \sim 1 \text{ eV}$ we have $\Delta \epsilon_S \approx 0.5 \text{ eV}$ for typical values of the model parameters. A similar conclusion was reached for the cluster CuO₆ by means of the self-consistent field method including the configuration interaction [82] and also using perturbation theory [83], both studies exhibiting the crossover of the singlet ${}^{1}A_{1g}$ and triplet ${}^{3}B_{1g}$ with the variation in c/a. Analysis showed [84] that the principal effect of the two-hole B_1 states on the effective single-band t-t'-J Hamiltonian is to renormalize the second nearest-neighbor hopping parameter t'. This renormalization may be quite large and may even change the sign of t'. The variation of the quantity t'from compound to compound shows a correlation with the optimal doping temperature $T_{\rm c}^{\rm max}$. The crossover of the Zhang-Rice singlet and B1 term invalidates the single-band model.

Thus, the applicability of the three-band p-d, single-band Hubbard, and t-J models is limited, in terms of the energies involved, by the condition $E \ll \Delta \varepsilon_S$ and may be very limited for $\Delta \varepsilon_S \leqslant 0.5$ eV.



Figure 6. Energy difference of the lowest terms of two holes (a singlet and a triplet) versus the crystal field parameter $\Delta_d = \varepsilon (d_{z^2}) - \varepsilon (d_{x^2-y^2})$, for three sets of model parameters (in eV): *I*, $U_d = 12$, $U_p = 8$, $\Delta = 3$, $t_{pd} = 1.5$, the remaining parameters are zero; *2*, $V_d = 4.5$, the remaining parameters are the same as in 1; *3*, $U_d = 12$, $U_p = 8$, $\Delta = 2$, $t_{pd} = 1.5$, $t_{pp} = 0.2$, $V_d = 4.5$, $V_p = 3$, $V_{pd} = 0.6$, $J_d = J_p = 0.5$, $J_{pd} = 0.2$. (After Ref. [81]).

3.5 Quasiparticles in strongly correlated electron systems

The direct use of the concept of the electron as a quasiparticle in line with the Landau theory of the Fermi liquid [85] is hardly possible in the theory of SECs because in the half-filled Hubbard model, strong correlations rearrange the ground state to the point where even the Fermi surface itself disappears. However, combining the ideas of Landau and those of Hubbard, it proves possible to introduce the concept of a Fermi quasiparticle for systems with SEC as well. Consider first local states, involving no hopping between unit cells. Figure 7 shows the local bases of the (a) Hubbard and (b) multiband p-d models; in the latter case, only selected excited states, namely n = 1 and n = 2, are shown. Following Landau, we define the energy of a quasiparticle as the change in the energy of an *N*-electron system on adding one electron, that is,

$$\Omega_{pq} = E_q(N+1) - E_p(N), \qquad (11)$$

where $E_p(N)$ is the *p*th term for the *N*-electron system. Unlike Fermi-liquid theory, rather than applying definition (11) to the whole of the crystal, we shall limit it to that particular cell where the quasiparticle is produced. We will consider separately the particle's hopping behavior and its dispersion. For the Hubbard model, only two such particles may be considered:

$$\Omega_{-} = \varepsilon_1 - \varepsilon_0 = \varepsilon_1, \quad \Omega_{+} = \varepsilon_2 - \varepsilon_1 = \varepsilon_1 + U,$$
(12)

for the lower and upper Hubbard bands, respectively. In the multiband case, adding one electron increases the number of possible interlevel transitions. Mathematically, the localized quasiparticles so introduced are naturally described in terms of the Hubbard operators

$$\chi^{pq} = |p\rangle\langle q|\,,\tag{13}$$

constructed on a complete set of local multielectron states. Note that while the X operator is traditionally defined to involve a single-site state only, the states we employ here are those of a cell, i.e., multielectron molecular orbitals rather than atomic orbitals. In view of the projection properties of X operators, any local operator can be expressed as a linear combination of them. In particular, this applies to the oneelectron annihilation operator for cell *i* with band index λ :

$$a_{i\lambda\sigma} = \sum_{pq} |p\rangle \langle p|a_{i\lambda\sigma}|q\rangle \langle q| = \sum_{pq} \gamma_{\lambda\sigma}(p,q) X_i^{pq} \,. \tag{14}$$

Relation (14) illustrates the difference between the singleelectron and multielectron descriptions of Fermi quasiparti-



Figure 7. Local bases of the single-band Hubbard (a) and multiband p-d (b) models. For simplicity, only some of the excited terms in the one-hole and two-hole sectors of Hilbert space is shown for the multiband model. The arrows indicate quasiparticle annihilation processes.

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cles. Whereas the single-electron operator decreases the number of electrons by one for all sectors of Hilbert space simultaneously, X^{pq} describes the 'partial' annihilation of an electron for the initial state q with N + 1 electrons and the final state p with N electrons, the matrix element $\gamma_{\lambda\sigma}(p,q)$ giving the probability amplitude for such a transition. Once the exact diagonalization of the Hamiltonian is done, the amplitudes immediately follow. Since SEC poses restrictions on the Hilbert space regions for states with high correlation energy, it is clear that a discussion in terms of X operators is more natural because these restrictions simply remove the corresponding processes from the right-hand side of (14), whereas the single-electron operator $a_{i\lambda\sigma}$ cannot do this. Thus, splitting the electron annihilation process into partial components for each pair of possible initial and final states is the first important factor in the definition of quasiparticles. Another is the question of the spectral weight of a quasiparticle. Indeed, one can select a $|q\rangle \rightarrow |p\rangle$ transition process which changes the number of electrons by unity, has an energy of the form (11) and a non-zero matrix element $\gamma(p,q)$ in Eqn (14), but whose spectral weight is zero if this is a transition from one empty (unfilled) state to another empty state. In order to obtain the spectral weight, one needs to calculate the corresponding Green's function. This is conveniently done using the notation of Ref. [86], where each pair of 'initial and final states' (p,q) is associated with a vector $\boldsymbol{\alpha} = \boldsymbol{\alpha}(p,q)$. The Green's function within the cell is calculated exactly, giving

$$D_{i,j(0)}^{\alpha,\beta}(\omega) = \left\langle \langle X_i^{\boldsymbol{a}} | X_j^{\boldsymbol{\beta}} \rangle \right\rangle_{\omega}^{(0)} = \delta_{ij} \delta_{\alpha\beta} \frac{F(\boldsymbol{a})}{\omega - \Omega_{\boldsymbol{a}} + \mathrm{i}\delta} , \qquad (15)$$

where $F(\boldsymbol{\alpha})$ is the filling factor, $F(\boldsymbol{\alpha}) = \langle X^{p,p} \rangle + \langle X^{q,q} \rangle$ for Fermi quasiparticles, and $\Omega_{\boldsymbol{\alpha}} = \Omega_{pq} = E_q - E_p$. The singleelectron Green's function is

$$G_{ij,\sigma}(\omega) = \left\langle \left\langle a_{i\lambda_{1}\sigma} | a_{j\lambda_{2}\sigma}^{+} \right\rangle \right\rangle_{\omega} = \sum_{\alpha\beta} \gamma_{\lambda_{1}\sigma}(\alpha) \gamma_{\lambda_{2}\sigma}^{*}(\beta) D_{ij}^{\alpha\beta}(\omega) \,.$$
(16)

Accordingly, the local single-electron Green's function is

$$G_{ij,\sigma}^{(0)\lambda_1\lambda_2}(\omega) = \delta_{ij} \sum_{\alpha} \gamma_{\lambda_1\sigma}(\alpha) \gamma^*_{\lambda_2\sigma}(\alpha) \frac{F(\alpha)}{\omega - \Omega_{\alpha} + \mathrm{i}\delta} , \qquad (17)$$

showing that the spectral weight is determined by the product of the transition probability $|\gamma_{\lambda}(\alpha)|^2$ with the filling factor $F(\alpha)$. Taking the transition amplitudes and occupation numbers to be zero enables one to choose from a large number of transitions obeying (11), a much less number of quasiparticles with nonzero spectral weight. The occupation numbers of the terms are determined by the self-consistency equation for the chemical potential,

$$\sum_{n,p} n \langle X^{p,p} \rangle = n_{\rm h} \,, \tag{18}$$

where n = 0, 1, 2, ... is the number of holes, p indexes all the states in the corresponding sector of Hilbert space, and n_h is the number of holes per cell. The filling factor is thus concentration dependent, and the doping process gives rise to quasiparticles whose spectral weight is proportional to the doping level. Part of them fall within the gap forming in-gap states with deep impurity levels [87]. For the single-band

Hubbard model with no doping we find that at T = 0, for both quasiparticles in the paramagnetic phase $F(\Omega_+) = F(\Omega_-) = 1/2$, so that the number of states in each Hubbard zone is, including spin, 1 rather than 2 as for a freeelectron band. This change is often referred to as a change in statistics: strong correlations turn electrons into spinless fermions. As seen from our definition, the statistics do indeed change, but the two-fold spin generation is conserved in the paramagnetic phase, and an external magnetic field acts to split a Hubbard band. The number of states in a given Hubbard band ranges from zero to unity depending on the filling factor. For an infinite lattice, intercell interactions and hops may be included by applying perturbation theory in the X representation. The most frequently used approaches are various splitting schemes for higher-order Green's functions or, alternatively, the diagram technique for X operators [86, 88, 89]. Because of the complexity of commutation relations for X operators, however, this diagram technique is more complicated than that for fermions and bosons, and so have not come into general use. In recent years there has been much interest in slave-boson and slave-fermion techniques, with exact commutation accounted for by imposing additional constraints on the allowable Hilbert space. In practice, however, the exact local constraints are usually taken into account on the average, thus introducing uncontrollable errors. Although approximate Hubbard model analyses are numerous [79, 13, 89], their discussion is beyond the scope of the present review.

4. Exact numerical results

Since there are no exact solutions available for Hubbard type models in two dimensions, all exact results are obtained from numerical finite-cluster calculations, either by exactly diagonalizing the model Hamiltonian or by the quantum Monte Carlo (QMC) method. Because there has been a review of such results [7], here we mainly concentrate on the most recent work done in the period 1994–1996. It seems appropriate, however, to begin with a discussion of the exactly solvable one-dimensional Hubbard model.

4.1 Spectral density in the one-dimensional Hubbard model

Owing to the availability of an exact solution in the form of the Bethe ansatz [90], the relevant properties have been studied in considerable detail in the low-temperature region. It has been established, in particular, that SEC effects give rise to Luttinger-liquid properties [91-93]. The characteristic feature of a one-dimensional Luttinger liquid is that the electron distribution function $n_k = \langle a_k^+ a_k \rangle$ has no discontinuity at the Fermi level, namely, $n_k - n_{k_F} \sim$ $sgn(k - k_F)|k - k_F|^{\alpha}$, where α is a nonuniversal, interaction dependent constant. In the limit $U = +\infty$, for the Hubbard model $\alpha = 1/8$ [94]. The spectral density near the Fermi energy has the form $A(\omega) \propto |\omega - \varepsilon_{\rm F}|^{\alpha}$ instead of the delta function obtained for quasiparticles in the theory of Fermi liquids. It is because of the spectral density vanishing at the Fermi level in the one-dimensional Hubbard model that the description of an electron or a hole in SEC systems as a quasiparticle with charge e and spin 1/2 has been abandoned [95]. At the same time, a peak in the $A(k, \omega)$ characteristic of Fermi-liquid quasiparticles was obtained by the QMC method [96]. In a recent paper [97] the spectral density was calculated in the limit $U = \infty$ for arbitrary filling, based on

the exact many-particle wave function obtained [98] using the Bethe ansatz in this limit. The authors of Ref. [97] note the enhanced role of many-particle effects in $A(k, \omega)$ as the wave vector moves from k = 0 and $k = \pi$. Manifestations of this are the decreased weight of the Van Hove singularities, the appearance of power-law singularities of the type $A_{-}(\omega) \propto |\omega - \varepsilon_{\rm F}|^{-3/8}$ (for n < 1), and non-quasi-particle tails. The spectral density of single-particle states for the lower Hubbard band is illustrated in Fig. 8, which shows blurred Van Hove singularities at the band edges and a power-law singularity at the center (for n = 1/2). The inclusion of three-particle electron-hole excitations in addition to single-particle excitations accounts for more than 99.99% of the total spectral weight. In the same paper [97], the applicability of the Luttinger-liquid concept is analyzed. The value $\alpha = 1/8$ occurs for $|\omega - \varepsilon_{\rm F}| < t^2/U$, and outside this interval $\alpha = -3/8$. For $U \to \infty$, the Luttingerliquid region contracts to zero; for larger (but finite) U, there must be a peak in $A(\omega)$ for $\omega \sim t^2/U$ as a result of the divergence at $\alpha = -3/8$; this is precisely the peak that was obtained by the QMC method in Ref. [96].



Figure 8. Density of states for the lower Hubbard band as obtained from the exact solution in one dimension for $U = \infty$ [97] for a 1/4-filled band.

4.2 Two-dimensional Hubbard model and the t-J model

For an undoped Mott-Hubbard insulator, QMC is the most convenient choice because, due to the electron - hole symmetry, this approach avoids the well-known negative charge problem [99]. As shown by a series of calculations using the QMC method (for 4×4 , 8×8 , and 12×12 clusters [100– 102]) and the exact diagonalization technique (see review article [7]), the ground state has antiferromagnetic order in agreement with perturbation theory in t/U. This is not at all as trivial a fact as it may seem: suffice it to recall a host of alternative scenarios, such as RVB or flux phases (i.e., those with a nonzero flux of vector potential across an elemental contour). These phases also do not acquire stability in the t-Jmodel [103, 104], nor when next-nearest-neighbor spin-spin interactions are considered [105]. The dynamics of a hole in an antiferromagnetically ordered background has been studied by exactly diagonalizing the Hubbard [106, 107] and t-J [108] models, the main conclusion being that the band becomes narrower as a result of correlation, and instead of a band of width W = 8t, a narrow quasiparticle band of width $W \sim J \sim t^2/U$ arises. The dispersion for one hole moving in a background of a fluctuating antiferromagnetic state was obtained by exactly diagonalizing the t-J model for 16- and 18-atom clusters [76] and is shown in Fig. 9. Here the solid line is described by

$$\omega(k) = J [0.5(\cos k_x + \cos k_y)^2 - 1], \qquad (19)$$

and accounts for the main contribution, given by intrasublattice hopping. While the fact that the top of the valence band (bottom of the hole band) lies at $(\pi/2, \pi/2)$ agrees with the ARPES data on Sr₂CuO₂Cl₂, another cluster-calculation result of Refs [7, 76], that the electron energies at points $(\pi/2, \pi/2)$ and $(0, \pi)$, $(\pi, 0)$ are close to degeneracy, does not. One further important result is that the insulating gap is filled upon doping and that, simultaneously, the spectral weight increases at the band edges [108-112]. The change in the electron structure at the undoped insulator-hole metal transition was studied using the Hubbard-OMC approach in Ref. [113], in which the spectral density $A(k, \omega)$ is obtained by the 'maximum entropy' method [114]. Figure 10 shows the spectral density and band structure of quasiparticles for a two-dimensional Hubbard model in the undoped case. The calculations were performed on an 8×8 cluster at U = 8t and U = 12t and two temperatures, $\beta t = 3$ (T = 0.33t) and $\beta t = 10$ (T = 0.1t). For T = 0.1t, the magnetic correlation length ζ exceeds the cluster size, allowing a comparison with T = 0 results. For T = 0.33t, ζ is less than the lattice size and therefore short-order effects occur.



Figure 9. Dispersion for a single hole in the background of the quantum ferromagnetic state, from the exact diagonalization of the t-J Hamiltonian for a cluster of 16 atoms (open and closed circles) and a cluster of 18 atoms (open and closed squares are for J/t = 0.2 and 0.4, respectively). (After Ref. [76]).

The antiferromagnetic phase of a Mott insulator has two narrow bands below and two bands above ε_F , as is seen in Fig. 10. Dispersion at the top of the valence band is the same as in previous studies and shows a maximum at the point $(\pi/2, \pi/2)$ and a very nearly degenerate state with $k = (\pi, 0)$ at X. A nontrivial point to note here is the behavior of the spectral density, whose maxima are sometimes below and sometimes above ε_F , depending on the wave vector. It is not



Figure 10. Spectral density (a) and dispersion (b) for quasiparticles in the two-dimensional Hubbard model with U = 8t, $\beta t = 10$ for the undoped case n = 1. (After Ref. [113]).

entirely clear why the authors of Ref. [113] divided the bands into coherent ones with $|\omega - \mu| \approx 3t$ and incoherent ones with $|\omega - \mu| \approx 6t$, because the peak widths are of the same order for both types. A similar calculation [115] for an 8×8 lattice at U/t = 10, T = t/4 for the undoped case also displayed four peaks, two below and two above $\varepsilon_{\rm F}$, but, unlike [113], the redistribution of peak intensities for different k was found to conserve the peaks themselves — except for $k = (\pi, 0)$ (Fig. 11). This difference is probably due to a different analytical continuation procedure employed for calculating the spectral density from the Monte-Carlo-calculated Green's function. The high-energy PES satellites obtained in Ref. [115] from Hubbard-QMC calculations, agree not only qualitatively but also quantitatively with PES spectra from the exact diagonalization of the two-dimensional t-J model for 16- and 18-atom clusters.

Calculations for the doped case demonstrate the inadequacy of the rigid-band picture. Qualitatively, the results of Ref. [113] are very similar to the ARPES results in that the Fermi level is near point $k = (\pi/2, \pi/2)$ in the direction ΓM and that there is a flat band in the vicinity of X. One can also see shadow-band satellites near points $\Gamma(\omega - \mu \approx 5t)$ and $M(\omega - \mu \approx 7t)$. The similarity between the dispersion relations and bandwidths in the metallic and insulating phases enabled the authors of Ref. [115] to conclude that low-energy bands in the metallic state are influenced by the same manyparticle correlation effects as bands in an insulator, namely, that the width of a band is determined by magnetic



Figure 11. QMC-computed spectral density $A(k, \omega)$ for the two-band Hubbard model for an 8×8 lattice with U/t = 10, T = t/4 for the undoped case. The wave vector is in units of $\pi/4$. (After Ref. [115]).

correlations. The difference is that in an insulator these correlations are determined by long-range antiferromagnetic order, whereas in a metal, by short-range antiferromagnetic order.

The change in hole dispersion for a significant (above 10%) hole concentration was studied by exactly diagonalizing the t-J model for a 18-atom cluster [108]. The top of the band is shifted to the point (π, π) , and the Fermi momentum is near $(\pi/2, \pi/2)$ in the direction [1, 1] and $(\pi, 0)$ in the [1, 0] direction (Fig. 12). The solid line is the ordinary tight-binding dispersion relation

$$\omega(k) = -2t_{\rm eff}(\cos k_x + \cos k_y) \tag{20}$$

with $t_{\text{eff}} = 0.24$ for J/t = 0.4 and $t_{\text{eff}} = 0.15$ for J/t = 0.2. Note here the change in the nature of dispersion: for a large number of holes, the antiferromagnetic correlations are weaker, the system has metallic properties, and the dispersion (20) is basically due to nearest-neighbor hopping. A similar conclusion was reached in Ref. [116], although the band width obtained there is again of the order of J, not 8t. The Fermi surface is shown in Fig. 12c, where the states with n(k) > 1/2 were considered to be filled, and those with n(k) < 1/2, empty. For J < t the Fermi surface shape was found to be independent of J, analogous to the Hubbard model with $U \ge t$ [108]. One further nontrivial result is that the Fermi surface of strongly correlated holes is identical to that of free electrons. This explains why the Fermi surfaces calculated for doped metallic copper oxides are consistent with experimental data [117]. The question of why strongly correlated and free electrons have the same Fermi surfaces deserves special discussion, as also does the question of whether it may be considered proved that the concept of a Fermi liquid (or of a marginal Fermi liquid [95, 118]) is applicable to SEC systems. Although according to Ref. [108] the answer to the second question appears to be 'yes', in order to be perfectly sure it is still necessary to demonstrate that the width of a spectral density peak vanishes as ω^2 at $\omega \to 0$ (or as $\omega \ln \omega$ for a marginal Fermi liquid), which cannot be done for an infinite cluster. The first question is answered in part in Ref. [19], which presents a general analysis of quasiparticles in



Figure 12. Hole dispersion in the t-J model for a doping concentration > 10 %, from the exact diagonalization of a 18-atom cluster for (a) J/t = 0.4 and (b) J/t = 0.2. The length of a horizontal bar indicates the intensity of the spectral function for a given energy. (c) The Fermi surface in the t-J model for J/t = 0.4. Closed (open) circles denote filled (empty) states. The Fermi surface for noninteracting electrons at the same doping level is shown dashed (From Ref. [108]).

SEC systems. In order to calculate the spectral density

$$\rho_k(\varepsilon) = \frac{1}{\pi} \operatorname{Im} G^{\mathsf{R}}(\varepsilon, k) \tag{21}$$

let us introduce the mass operator $\Sigma(\varepsilon, k)$: $G^{-1}(\varepsilon, k) = \zeta_k - \varepsilon - \Sigma(\varepsilon, k)$. By definition, $\Sigma(0, k) = 0$. Assuming that $\Sigma(\varepsilon, k)$ is not an 'overly singular function' [19], let us perform an expansion for small ε to obtain

$$\Sigma(\varepsilon, k) = \lambda_k \varepsilon + \mathrm{i} \gamma_k(\varepsilon) \,. \tag{22}$$

In the region where this expansion holds, $\gamma_k(\varepsilon) \ll \varepsilon$, we obtain

$$\rho_k(\varepsilon) = \frac{\gamma_k(\varepsilon)/\pi}{\left[\zeta_k - (1+\lambda_k)\varepsilon\right]^2 + \gamma_k^2(\varepsilon)} = Z_k \delta(\varepsilon - \tilde{\zeta}_k), \quad (23)$$

where $Z_k = (1 + \lambda_k)^{-1}$, $\tilde{\zeta}_k = \tilde{v}_k(k - k_F)$, $\tilde{v}_k = Z_k v$. Restricting ourselves to the low-energy region, as we should in the Landau theory [119], the Z factor can be completely eliminated by a proper renormalization. Integrating Eqn (23), we find

$$\int_{-\infty}^{\infty} \rho_k(\varepsilon) \, \mathrm{d}\varepsilon = Z_k < 1 \,, \tag{24}$$

which is in conflict with the condition for conservation of the total number of states

$$\int_{-\infty}^{\infty} \rho_k(\varepsilon) \, \mathrm{d}\varepsilon = 1 \,. \tag{25}$$

Showing that some of the states, namely those incoherent and far away from the Fermi surface, are not covered by Eqn (23). That non-quasiparticle incoherent states exist is clear from the exact diagonalization results for all the models discussed. It can be argued that due to SECs, some of the states [namely, $1 - Z_k$, the difference between (24) and (25)] are pushed from the Fermi level deep into the band. As seen from (23), the Fermi surface is determined by the same vector k_F as for free electrons, but with a reduced velocity \tilde{v}_F —hence the reduced band width. It is this fact which is noted in [10] in comparing ARPES data and band predictions.

4.3 Exact results for the p-d model

On changing from the single-band Hubbard model to a more realistic three-band p-d model, the following effects are obtained [120]: (1) the indirect exchange interaction (superexchange) J comes into play; (2) new quasiparticles are created; (3) the next-nearest-neighbor hopping integral t'appears, important for detailing the dispersion law; and (4) an asymmetry between electron and hole doping is observed. The possibilities for an insulating state of a system with SEC are illustrated in Fig. 13. Since for copper oxides we typically have $U_{\rm d} \sim 10$ eV, $\Delta \sim 2-3$ eV, they should be classified as charge-transfer insulators according to Ref. [121]. In an undoped state there is one hole for one CuO_2 cell, $n_h = 1$. Neglecting the p-d hybridization, this hole resides at copper, that is, the configuration of the cell is $Cu(d^9)O(p^6)$. Cu^{2+} ions with spin S = 1/2 form an antiferromagnetic lattice. The effect of hybridization is to mix the d⁹p⁶ and d¹⁰p⁵ states, thus decreasing the effective magnetic moment at copper. Along with zero quantum spin fluctuations, there is a quite noticeable covalent contribution [123], both of which combine to give the observable value $\mu_{eff} = 0.6\mu_{B}$. The p-d model has been able to give correct values for the insulating gap $E_{\rm g}$ and the indirect exchange integral J for a large number of insulating copper oxides, such as the T' phase of R₂CuO₄ (R = Pr, Nd, Sm, Eu, and Cd); the T phase of La₂CuO₄; T* phases of (La-Ca-Sr)₂CuO₄ and (La-Tb-Sr)₂CuO₄; (Ca-Sr)CuO₂, Bi₂Sr₂YCu₂O₈; and YBa₂Cu₃O₆ [124]. Good agreement with the experimental values of E_g and J can be obtained by fixing all the model parameters except the charge-



Figure 13. Possible band-structure diagrams for the three-band p-d model: (a) metal, (b) Mott-Hubbard insulator, (c) charge-transfer insulator, $U_d > \Delta$, (d) charge-transfer insulator with splitting of the Zhang-Rice-singlet and triplet states. B, AB, and NB denote bonding, antibonding, and nonbonding bands, respectively; UHB are LHB are the upper and lower Hubbard bands; ZRS is the Zhang-Rice singlet; T is the triplet; E_{CT} is the gap with charge transfer. (From Ref. [122]).

transfer energy. The parameter values chosen were $U_d = 8.5$ eV and $U_p = 4.1$ eV. In Ref. [124], the parameters for Sm₂CuO₄ were chosen to be $t_{pd} = 0.873$ eV and $t_{pp} = 0.366$ eV, and in going to other substances, t_{pd} and t_{pp} were taken to vary as $1/r^4$ and $1/r^3$, respectively. The change in the charge-transfer energy is mainly due to the change in the Madelung potential, reflecting the difference between the three-dimensional spatial lattices of the oxides listed above.

An exact diagonalization of the three-band p-d Hamiltonian has been performed for the largest-size cluster of all, Cu₄O₁₃ [107, 109, 110, 112, 125–130]. The multiband p-d model was treated by exactly diagonalizing Cu₂O₇ and Cu₂O₈ clusters [120, 131]. The finite-temperature spectral density for the three-band p-d model was obtained from QMC calculations of the imaginary-time Green's function [132-134]. The general conclusion to be drawn from the above studies is that the p-d and Hubbard electronic structures are similar if the Zhang-Rice band is identified with the lower Hubbard band. Doping redistributes the spectral weight, decreasing it at the edges of the gap and, as charge transfer proceeds, giving rise to new in-gap states which fill the gap as the carrier concentration increases. Unlike the Hubbard model, this effect is asymmetric with respect to electron and hole doping, the amount of asymmetry depending on the parameters of the model [135]. Similar predictions were also made with the multiband p-d model (10) by exactly diagonalizing the CuO₄ cluster [136]. Figure 14 shows the density of states for filled (PES) and empty (BIS) states for the CuO₂ plane for two hole concentrations [112]. It is seen that doping results in filling the gap, the in-gap states being related to the appearance of a hole at a ligand. The dispersion of the Zhang-Rice band [133] is in qualitative agreement with experiment (Fig. 15).

A recently developed trajectory QMC algorithm [137] allows a cluster of as many as $N_a = 108$ atoms to be treated.



Figure 14. The density of filled (PES) and unfilled (BIS) states in $La_{2-x}Sr_xCuO_4$ as obtained by exactly diagonalizing the three-band p-d model for the Cu₄O₁₃ cluster with (a) x = 0 and (b) x = 0.25. The model parameters were $U_d = 8.79t_{pd}$, $U_p = 4.24t_{pd}$, $t_{pp} = 0.41t_{pd}$, $\Delta = 3.37t_{pd}$, and $t_{pd} = 0.966$ eV. The Fermi energy is shown dashed. (After Ref. [112]).



Figure 15. The dispersion of the Zhang–Ride band obtained by the QMC method for a 4×4 CuO₂ lattice (filled squares), by the local-density-functional method (dashed line), and in the Hartree–Fock approximation (dotted line) for $U_d = 6$, $U_p = 0$, $t_{pp} = 0$, $\Delta = 4$, $t_{pd} = 1$, $\beta = 1/T = 10$, with hole concentration $\delta = 0.25$. Experimental points for Bi₂Sr₂CaCu₂O₈ are shown by filled circles (ARPES) and by empty rectangles (ARIPES). (From Ref. [134]).

It was found that the energy and the filling factor cease to depend on the cluster size starting from $N_a = 24$, and the amplitude of antiferromagnetic correlations, from $N_a = 54$ (for temperature T = 0.25t). Doping reduces the spin correlations function $S(\pi,\pi)$ dramatically (Fig. 16), and at large cluster sizes, the hole and electron doping become asymmetric in that holes suppress antiferromagnetism more strongly than electrons. This is a known experimental fact, which manifests itself in that the slope dT_N/dx in La_{2-x}Sr_xCuO₄ is greater than in $Nd_{2-x}Ce_xCuO_4$ [138]. The density of single-particle states for the undoped case was calculated using the same trajectory algorithm for the $Cu_{36}O_{72}$ cluster with $N_a = 108$ [139]. The results support the qualitative picture shown in Fig. 13 for an insulator with charge transfer. The main difference from Fig. 13d is that the bonding (B) band has merged with the lower Hubbard (LHB) band and that the correlated states have a much greater weight due to the influence of the nonbonding band (NB).

Physically, the mechanism of formation of in-gap states in multiband SEC models is easy to understand by considering exact multielectron bases of the type shown in Fig. 7b [87]. Without doping, the only filled term is the lowest one, n = 1, which corresponds to the bonding $d_{x^2-y^2} - p_{\sigma}$ molecular orbital of b_{1g} holes. Possible Fermitype quasiparticles are shown in Fig. 7b, where particle 1, to use the electron language, forms an empty conduction band, whereas 2, 4 and the two-hole terms lying above (not shown for simplicity) form a complex valence band. In hole doping, the ground term n = 2 and the single-particle term are filled with the respective probabilities x and 1 - x. As a result, the particle 3 in Fig. 7b has a spectral weight proportional to x, and its energy falls within the insulating gap. Similarly, for electron doping the term n = 0 is filled with probability x, and the quasiparticle 6 in Fig. 7b forms an in-gap state.

One further example of exact work is the symmetry analysis of electronic wave functions in the antiferromagnetic phase of the copper oxides [140, 141]. One important result of this analysis is that the orbitals d_{z^2} and $d_{x^2-y^2}$ do not mix at the point $(\pi/2, \pi/2)$.



Figure 16. Copper-sublattice spin correlation function calculated using the quantum Monte Carlo method from the three-band p-d model for $\Delta = \varepsilon_p - \varepsilon_d = 1$, $U_d = 6$, $\beta = 1/T = 4$, t = 1. (a) Dependence on the order number of the copper coordination shell at *I*, $N_a = 24$; *2*, $N_a = 30$; *3*, $N_a = 54$; *4*, $N_a = 78$; and *5*, $N_a = 108$. (b) Effect of doping on the $k = (\pi, \pi)$ Fourier component at *I*, $N_a = 12$; *2*, $N_a = 24$; *3*, $N_a = 48$; *5*, $N_a = 78$; and *6*, $N_a = 108$. (After Ref. [137]).

5. Fermi quasiparticles in an infinite lattice

The problems to be discussed in this section are basically the following: the properties of quasiparticles in undoped CuO₂ layers; the role of multiband effects; a comparison with **ARPES** data for various insulating and superconducting copper oxides; and Fermi surface changes resulting from doping.

5.1 Magnetic polarons in quantum antiferromagnets

In the absence of doping, SEC models of both the p-d Hubbard and t-J varieties, and those involving an SDWunstable metallic state [142] reduce to the two-dimensional S = 1/2 Heisenberg model [7–9]. In the tight-binding limit $U \ge t$, SDW equations yield a spin wave velocity identical to that in the Heisenberg model [143]. Formally, these two treatments of holes differ in that the former starts from a localized quasiparticle, which is dispersive due to intersite hopping, whereas in the latter the point of departure is a Hartree–Fock band with a Fermi surface having the 'nesting' property

$$\varepsilon(k+Q) = -\varepsilon(k) \,. \tag{26}$$

The Coulomb interaction, accounted for in the random phase approximation (RPA), causes a transition to an SDW state (antiferromagnetic if $Q = (\pi, \pi)$). Ab initio, spin-polarization Hartree-Fock calculations [144] for the antiferromagnets La₂CuO₄, La₂NiO₄, K₂NiF₄ and K₂CuF₄ describe an insulator with the gap (E_g) and superexchange integral (J)values consistent with experiment. However, the top of the valence band has a dispersion inconsistent both with the ARPES data and with exact numerical calculations, and is found to lie at the point $(\pi, 0)$ rather than $(\pi/2, \pi/2)$. The inclusion of the configuration interaction in the nine-band model results in shifts in the band energies and the top of the valence band lying at $(\pi/2, \pi/2)$ [144]. However, in all the approaches above, the holes have a similar physical meaning, namely, quasiparticles dressed in local spin fluctuations. We now turn to consider the basic concepts relevant to the subject and to discuss new results not covered in the previous reviews.

The string picture dates back to Ref. [74], in which the corresponding quasiparticle was dubbed a quasi-oscillator.

The meaning of this concept is that (quoting from Ref. [145]) "a charge carrier oscillates about the equilibrium position which slowly moves through the crystal. When moving away from the equilibrium position, the electron produces a chain of reversed spins - i.e., an antiphase antiferromagnetic ordering — along its path. On its return to an equilibrium position along the same path, the electron erases the antiphase ordering thus restoring the normal, antiferromagnet ordering." Unlike free electrons, a quasiparticle is described by a superposition of many-particle states. Variational [146-148] and closely related projection-operator [149-151] calculations rely on a finite-size set of basis operators in which, along with the original one-electron operators, various mechanisms for spin-reversal and intersite in-string hopping are included. The difference between a free particle and a quasiparticle is clearly demonstrated in the exact-diagonalization t-J calculation of the spectral density $A(k,\omega)$ in Ref. [152]. In this work, the polaron annihilation operator is taken in the form

$$c_{k,\uparrow} = \frac{1}{\sqrt{N}} \sum_{j} \sum_{\lambda=0}^{3} \exp(ik \cdot R_j) \alpha_{\lambda}(k) A_{j,\lambda}, \qquad (27)$$

$$A_{j,0} = c_{j,\uparrow}, \quad A_{j,l} = \sum_{h \in N(j)} S_j^- c_{h,\downarrow} , \qquad (28)$$

$$A_{j,2} = \sum_{h \in N(j)} \sum_{l \in N(h)} S_j^- S_h^+ c_{l,\uparrow} , \qquad (29)$$

$$A_{j,3} = \sum_{h \in N(j)} \sum_{l \in N(h)} \sum_{m \in N(l)} S_j^- S_h^+ S_l^- c_{m,\downarrow} \,.$$
(30)

Here N(j) denotes the set of the nearest neighbors to site R_j , and $\alpha_{\lambda}(k)$ are the variational parameters. For a free electron, the spectral density (Fig. 17) has a wide spectrum for practically all k. The large incoherent contribution to $A(k, \omega)$ indicates the inadequacy of the free electron description. For a quasiparticle, in contrast, we obtain narrow peaks in the much-less-dispersive spectral density, and the small contribution from incoherent non-quasi-particle states indicates that Eqn (27) is a good choice as far as the description of the magnetic polaron is concerned.



Figure 17. Spectral functions for a magnetic polaron (solid lines) and a free electron (dashed lines) in the absence of doping in the t-J-model framework, obtained by exactly diagonalizing a 4 × 4 cluster. (After Ref. [152]).

5.2 Multiband models

Multiband models are employed both for developing efficient single-band models [73, 84, 153] and for directly calculating the quasiparticle band structure [154–157]. The important point to bear in mind is that, apart from strong intra-atomic Coulomb correlations, covalent effects, i. e., interatomic p–d hybridization, are important in copper oxides. Whereas the former are easier to incorporate in the framework of a local approach, for the latter, in contrast, a change to *k* space is more convenient. In a search for an approach in which both the covalence and SEC effects would be accounted for, the method of local unitary transformations was proposed [158], in which the Hamiltonian of the model is mapped onto the space of weakly correlated p orbitals.

The alternative approach of Ref. [159] is an extension of the band-theory tight-binding method. Let us divide the lattice into nonintersecting clusters (unit cells) and rewrite the original Hamiltonian as a sum over the cells plus a sum over the intercell hops and interactions,

$$H = H_0 + H_1, \quad H_0 = \sum_i H_i, \quad H_1 = \sum_{i,j} H_{i,j},$$
 (31)

where *i* indexes cells rather than sites. When an exact diagonalization of H_i has been done, Hubbard operators can be constructed on the basis of the multielectron molecular orbitals. Using relations (14) and their spin-operator analogues, the intercell Hamiltonian can also be written in the X representation. As a result, the original Hamiltonian is written in the exact form

$$H_{0} = \sum_{in\gamma} (E_{n\gamma} - n\mu) X_{i}^{\gamma\gamma}, \quad H_{1} = \sum_{ij} \sum_{\gamma_{1}\gamma_{2}\gamma_{3}\gamma_{4}} A_{\gamma_{1}\gamma_{2}}^{\gamma_{5}\gamma_{4}} X_{i}^{\gamma_{1}\gamma_{2}} X_{j}^{\gamma_{4}\gamma_{3}}.$$
(32)

The single-band Hubbard Hamiltonian in the X representation is formally the same, the only difference being in the structure of the local basis E_{my} . For the Hubbard model this basis consists of four states (5), whereas in (10), for a cell in the form of a CuO₂ cluster, the number of states in the local basis is \sim 100. Thus, Hamiltonian (32) differs quantitatively, rather than qualitatively, from its single-band Hubbard counterpart in the X representation. Therefore, the methods developed for the Hubbard model may be used here as well, with the perturbation being the intercell hopping and interactions and the zeroth approximation accounting in an exact way for both the SEC and covalent effects within the cell. Note here that the matrix elements involved in the problem depend on the size of the cluster. Denoting the number of atoms in the cell by N, each eigenstate contains a factor $1/\sqrt{N}$. The matrix element $\langle \gamma_1 | a_{i\lambda\sigma} | \gamma_2 \rangle$ contains a factor 1/N. The hopping operator $c_i^+ c_j$ acquires a factor $1/N^2$, and the four-fermion Coulomb interaction operator, a factor $1/N^4$. The renormalization of the effective intercell hopping, $\tilde{T} = T_{pd}/N^2$, may generally be compensated by the increase in the number of scattering channels, so that representation (32) does not make it easier to obtain an exact solution, nor does it offer any advantages in the vicinity of the Mott-Hubbard transition, where the bandwidth W is of the order of the insulating gap E_{g} . Copper oxides, however, are far from the Mott – Hubbard transition [160] and usually obey the condition $W \ll E_g$, so that the band-narrowing effect is felt by each individual quasiparticle.

In order to calculate the band structure of the quasiparticles, various formulations of perturbation theory in intercell hopping can be employed. In the simplest, the 'Hubbard I' approximation, the dispersion relation is of the form [156]

$$\det\left\{\delta_{mn}\delta_{fg}\left(\omega-\Omega(\boldsymbol{a}_{m})\right)-F(\boldsymbol{a}_{m})\left[A_{fg}^{mm}(k)+B_{fg}^{mn}(k)\right]\right\}=0,$$
(33)

where the subscripts f and g refer to two antiferromagnetic sublattices, the indices m and n designate quasiparticles, and A and B are the p-d and p-p intercell hopping matrices. The cluster treatment has been applied to the three-band p-d[161-163] and five-band p-d [73, 84] models using the CuO₄ cluster as a cell. The problem of nonorthogonal molecular orbitals, stemming from there being a common oxygen ion to two neighboring CuO₄ clusters, was resolved by constructing Wannier functions centered at copper sites and defining the Hubbard operators on the basis of them. Despite the difference in the unit cell used, Refs [81, 84] arrive at the same conclusion about the influence of d_{7^2} orbitals, namely that the stabilization of the B_1 triplet due to the Hund configuration $|d_{x^2-v^2}d_{z^2}\rangle$ restricts the applicability of the single-band model of the CuO₂ layer. The effects arising from the proximity of the two-hole singlet and the triplet are treated in Ref. [81] which calculates the hole dispersion in the antiferromagnetic phase in the no-doping case (Fig. 18). Figure 18 also shows ARPES data for Sr₂CuO₂Cl₂ [14] as well as the t-J dispersion calculated in the self-consistent Born approximation (30). In the calculation of Ref. [27], quantitative agreement with experiment is obtained along ΓM , but not in the ΓX and XY directions. An attempt to improve the agreement by including a next-nearest-neighbor hop t' [164] succeeded for the XY line, somewhat worsened the agreement on the ΓM line, and gave nothing for ΓX . There is no experimental evidence to support the conclusion of the t-J model about the nearly degenerate energies at points $(\pi/2, \pi/2)$ and $(\pi, 0)$. In our view, it is the limited applicability of the t-J model itself, discussed above, that



Figure 18. Electron dispersion near the top of the valence band of an undoped antiferromagnetic CuO₂ layer in comparison with ARPES data [14]. Open rectangles, theory; circles with vertical bars, experimental data [14]. Solid and dashed curves are from the t-t'-J [164] and t-J [27] models, respectively. (After Ref. [81]).

explains all these discrepancies. In fact, for all points in the Brillouin zone there is good agreement with experiment in a narrow region $\Delta E \sim 0.1$ eV near the top of the valence band, and greater discrepancies deeper into the band. At the same time, a calculation with the d_{z^2} orbitals [81] shows the distinctly better agreement over the entire Brillouin zone. The fact that it is precisely at $(\pi/2, \pi/2)$ where the t-J model is good presumably relates to the fact that $d_{x^2-y^2}$ and d_{z^2} cannot mix for symmetry reasons. At the bottom of Fig. 18 one can also see a nondispersive level corresponding to hole excitation into the two-particle triplet state. The absence of dispersion and the incoherent nature of the excitations were also found in an extended t-J model with triplet holes [165].

The introduction into the t-t'-t''-J model of matrix elements for hopping to the second (t') and third (t'')coordination shells [166] removed the main disagreement between the t-t'-t''-J model and experiment, related to the nearly degenerate nature of the quasiparticle energies $E(\pi/2, \pi/2)$ and $E(\pi, 0)$. Intracell hopping (t' and t'') pushes the level $E(\pi, 0)$ into the valence band in agreement with the ARPES data. A comparison of the $A(k, \omega)$ obtained for undoped and doped ($x \approx 10\%$) clusters of 16, 18 and 20 atoms using the exact-diagonalization method shows that the main effect of doping is to shift $A(k, \omega)$ by $\approx 0.5t$ for the wave vectors $(k, 0), \pi/2 \leq k \leq \pi$, which is precisely the reason for the formation of a plane wave near $(\pi, 0)$. Recall that the magnitude of the hopping integrals t' and t'' depends on the detailed nature of the multiband models in their low-energy reduction to t-J [72, 73].

One further perturbation approach to treating clusters involves the diagram technique for X operators [86]. This method has proved useful in considering superconductivity in the p-d model [167, 168] and explaining the electron-hole asymmetry in the phase diagram of *n*- and *p*-type copper oxides [169].

5.3 Electronic structure of doped systems

At finite hole concentrations one faces the problem of the distortion of antiferromagnetic order by other holes, which has been treated both in the tight-binding approximation [170] and in the weak-binding limit ('spin-bag' model [143]).

In the SDW state, a doped hole reduces the sublattice magnetization locally on the scale of the coherence length

$$\zeta_{\rm SDW} = \frac{v_{\rm F}}{\pi \Delta_{\rm SDW}} \,, \tag{34}$$

where $v_{\rm F}$ is the velocity at the Fermi surface, and $\Delta_{\rm SDW}$, the order parameter of the SDW state.

As little as 2% Sr-produced holes in La_{1.98}Sr_{0.02}CuO₄ or 14% Ce-produced electrons in Nd_{1.86}Ce_{0.14}CuO₄ suppress the three-dimensional antiferromagnetic order. As shown in Ref. [171], short-range order persists with a correlation length $\zeta \sim d_{\rm Cu-Cu}/\sqrt{x}$ ($d_{\rm Cu-Cu} = 3.8 \,\rm A$ being the copper spacing in the CuO_2 plane), indicating holes to be responsible for the reduction of short-range order in the CuO₂ plane. Incommensurate spin fluctuation in $La_{2-x}Sr_{x}CuO_{4}$, with the $\chi''(q,\omega)$ peak near $q = Q = (\pi,\pi)$ splitting in four due to $\pm \delta$ shifts along the x and y axes, were observed for x = 0.075 and x = 0.14 [172]. The most recent neutron scattering data on the family of $La_{2-x}Sr_xCuO_4$ single crystals with x = 0.04 - 0.18show that the splitting of the peak varies with the hole concentration (Fig. 19), the measure of incommensurability, δ , depending on the concentration in the same way as τ_c . The threshold x_c above which δ differs from zero coincides with the superconductivity threshold. The existence of incommensurate spin fluctuations in YBa2Cu3O6+x remains an open question [30], possibly due to the holes being distributed in a special way between the CuO₂ layers and CuO chains [174, 175]. It has been shown [176] that upon doping, holes fill the chain states up to $x = x_c$ and that at $x > x_c$ they rapidly overflow to the plane, suppressing antiferromagnetism at $x_{\rm c} \approx x_0 \approx 0.4.$

Even in the region of optimum doping, an electron moves in a background of strong antiferromagnetic-type spin fluctuations. In the t-J, Hubbard, or p-d descriptions of quasiparticles at finite hole concentrations, much reliance is placed on the slave-boson and slave-fermion concepts [7–9], which make it possible to obtain an efficient band model satisfactorily describing both the spectroscopic and kinetic properties of the normal phase [177]. Figure 20 shows the dispersion of the Zhang–Rice band for two Brillouin zone directions in YBa₂Cu₃O₇ and YBa₂Cu₃O₈ [179], as predicted by the three-band p-d model. Good quantitative agreement is seen with the ARPES data of Ref. [178]. The splitting of the two bands in the figure is due to hole tunneling between neighboring CuO₂ planes.

If there were no fluctuations and long-range order were present, an SDW state gap would appear in the carrier spectrum. Since we actually have short-range order, however, the SDW gap is washed out. This is how the concept of the spin pseudogap emerges. To describe it, a modification of the standard mass-operator expression was proposed, [33]

$$\Sigma(k, i\varepsilon_n) = U^2 T \sum_{q,\omega_n} \chi(q, i\omega_n) G_0(k - q, i\varepsilon_n - i\omega_n), \quad (35)$$

 $\chi(q, i\omega_n)$ being the spin susceptibility, by phenomenologically introducing an expression for χ with a diffuse maximum near the antiferromagnetic wave vector $Q = (\pm \pi, \pm \pi)$. The quasiparticle density of states calculated in this way shows a decrease near the Fermi surface, which may be attributed either to a partial rearrangement of the band structure or, alternatively, to the appearance of a pseudogap. On the other hand, the states pushed away from the Fermi surface produce density-of-states peaks at the edges of the gap, seen as satellites or shadow bands in the photoelectron spectra.



Figure 19. Inelastic neutron scattering data (E = 14.7 meV) on $\text{La}_{2-x}\text{Sr}_{x-1}$ CuO₄ single crystals, showing spin fluctuations incommensurate with the wave vectors $\pi/2(1 \pm \delta, 1)$ for various hole concentrations. The energy resolution $\delta E = 2 \text{ meV}$. (After Ref. [173]).

Because electrons move in fluctuating antiferromagnetic regions, the appearance of shadow bands actually relates to local Umklapp processes, since the states k and k + Q are equivalent in the reduced Brillouin zone. That this is indeed so is confirmed by microscopic calculations of $A(k, \omega)$ within the Hubbard model using the QMC approach [35] or perturbation theory [36] (the term microscopic meaning that no phenomenological expressions are used for susceptibility). For the diagonal $k_x = k_y = k$, an Umklapp process in the antiferromagnetic phase results in the $k_1 = (k, k)$ and $k_2 = (\pi - k, \pi - k)$ quasiparticles having the same energy. In Fig. 11, which shows the $A(k, \omega)$ calculated for the halffilled Hubbard model, this is seen for $k_1 = 0.25\pi(1, 1)$ and $k_2 = 0.25\pi$ (3, 3). However, the intensities, which are equal in the S = 1/2 Heisenberg antiferromagnet, redistribute themselves in the finite U/t Hubbard model. For $k_2 = 0.25\pi (3, 3)$, the integral of $A(k, \omega)$ over the filled portion of the spectrum, which determines the intensity of the photoelectron spectrum,



Figure 20. Electron dispersion below the Fermi level in comparison with ARPES data for Y - Ba - Cu - O [178]. (After Ref. [179]).

is 23% of the total spectral weight (for U/t = 8). On doping, the filled states for $k = k_2$ decrease in weight, giving ~ 10% for $\langle n \rangle = 0.87$ and 4% for $\langle n \rangle = 0.70$ [35]. As regards the spin correlation length, the same calculations yield $\zeta \approx 1.5a$ for $\langle n \rangle = 0.88$ and $\zeta < a$ for $\langle n \rangle = 0.77$. According to Ref. [35], at the optimum doping the intensity of shadow band satellites slightly exceeds the noise level and is therefore measurable, whereas in overdoped samples these satellites are too weak to observe.

Very interesting results concerning quasiparticle spectra in the two-dimensional Hubbard model have been obtained by self-consistent mass-operator calculations [36] using the FLEX (fluctuation exchange) approximation. This approximation [180, 181] goes back to the early idea [182] of a selfconsistent perturbation theory satisfying the Ward identity and thereby also the particle number, momentum, and energy conservation laws. The resulting equations for Σ and G are usually solved numerically on the imaginary axis, after which a complex problem of analytical continuation to the axis of real frequencies must be addressed. In Ref. [36], numerical calculations are made for $\Sigma(k, \omega + i\gamma)$ with ω real and $\gamma < \pi T$ small, which makes the analytic continuation for $\gamma \rightarrow 0$ an easy task. Results for various concentrations $x = 1 - \langle n \rangle$ are presented in Fig. 21, in which the pseudogap at x = 0.12 in the density of states appears as a forerunner of an antiferromagnetic SDW state. The spin correlation length is found to be $\zeta = 2.5a$, in good agreement with the neutron data. Thus, both the QMC and FLEX approaches confirm that satellites with $\zeta \approx 2a$ are indeed possible.



Figure 21. Spectral density for the Hubbard model and the density of states (inset) for various hole concentrations. The wave vector *k* is taken along the $(\pi, 0) - (\pi, \pi)$ line. The satellites corresponding to shadow bands are indicated by arrows. (After Ref. [36]).

Figure 22 shows the quasiparticle dispersion constructed in the FLEX approximation from the positions of spectral density maxima near $X = (\pi, 0)$. For x = 0.22, there is only one band, with a saddle point at X giving a Van Hove singularity. For x = 0.12, below the optimum value, the main (large-weight) band has almost the same dispersion and shows a flatter portion for $\omega = 25$ meV above the Fermi level. To the right of X, the dispersion in this band shows a dramatic increase, leading to a drop in the density of states. Open squares for x = 0.12 indicate shadow bands. It is interesting that the shadow bands calculated in Ref. [36] do not, in contrast to Ref. [33], correspond to the poles of the Green's function but rather result from the redistribution of intensity due to quasiparticle attenuation processes. Under



Figure 22. Electron dispersion near the point $(\pi, 0)$ for various hole concentrations *x* using the FLEX approximation within the single-band Hubbard model. Dashed line, x = 0.22; squares, x = 0.12, filled (open) squares referring to the main (shadow) bands, respectively. Solid line, calculation for the antiferromagnetic phase with short-range order for x = 0.12 and magnetization per cell $m_{\rm S} = 0.21$. (After Ref. [36]).

long-range order conditions, the coupling between the k and k + Q states would indeed be secured by Umklapp processes. With short-range order, we have dynamic coupling determined by the decay of the state k into the final state k + Q as a result of attenuation. Spin fluctuations are not the only ones acting to renormalize the Hartree-Fock quasiparticle spectrum. Earlier, in Ref. [183], it was shown that the exact mass operator of the Hubbard model consists of three terms accounting for fluctuations in spin density, electron density, and two-particle excitations. An expression of this type was employed in three-band-model FLEX calculations in Ref. [184], which gives virtually identical results to those from the QMC method and indicates the spin fluctuations contribute the most to the mass operator. The plane waves near point xresult in there being a Van Hove singularity in the density of states N(E). A similar type of singularity is known in oneelectron band theory, but its origin there lies in band effects, whereas in models with strong correlations the flat band results from the strong correlations themselves. While band effects are easily suppressed by impurities, the correlationrelated band narrowing and small-dispersion features are stable to impurities.

The maximum in the imaginary part of the spin susceptibility Im $\chi(q, \omega)$ in Ref. [184] corresponds to spin fluctuations with an incommensurate wave vector and energy ω_s . For doping x < 0.25, $\omega_s \approx 0.01 - 0.03t$ and depends linearly on x. For the imaginary part of the electron mass operator, there is a nontrivial result [184] that Im $\Sigma = \omega$ for $\omega > \omega_s$ and Im $\Sigma = \omega^2$ for $\omega < \omega_s$. Thus, Fermi liquid properties are exhibited only at the very lowest energies. A similar result was obtained earlier for mixed-valence systems using the periodic Anderson model and the X-operator diagram technique [185].

5.4 Concentration dependence of the Fermi surface and the violation of Luttinger's theorem

In the spirit of the rigid-band model, the Fermi surface at low hole concentrations is very naively described as consisting of hole pockets centered about the point \overline{M} , whose volumes are proportional to the hole concentration x. Although direct experimental evidence of small hole pockets is lacking, the kinetic, and in particular the Hall data indicate that the carrier (hole) concentration $n_h \propto x$ [4–10]. Theoretical calculations using the t-J [186] and two-dimensional Hubbard [187] models do support this picture, but only if the concentration is not too low, $x \ge 0.10$. The region $x \approx 0.05$, with the insulator-metal transition and incipient superconductivity, has been little explored. Quality samples with a sufficiently uniform dopant distribution are hard to fabricate, possibly because of the phase separation process in an antiferromagnetic semiconductor, in which carriers of finite concentration accumulate to form a conducting drop [188, 189]. However, even far away from the insulator-metal transition the concentration dependence of the Fermi surface is nontrivial and exhibits non-Fermi-liquid effects. This question has been studied [187] within the FLEX approximation of the Hubbard model. It was found that the relaxation rate $\Gamma_k = -\text{Im} \Sigma_k(\omega = 0)$, which shows Fermi-liquid behavior $\Gamma_k \propto T^2$ in highly doped systems with $x \ge 0.20$, increases with decreasing temperature in the shadow band in underdoped systems (x = 0.11) instead. For the main band, the limit of Γ_k at $T \rightarrow 0$ is unclear, because FLEX calculations are performed numerically and at finite temperatures. Since a small scale of ω_q^* energies ($\omega_q^* \approx 1-5 \text{ meV}$) exists, determined

by the accuracy of the calculations, one can only speak of the anomalous behavior of Γ_k at $T > \omega_q^*$, which results in the violation of Luttinger's theorem [190]. The volume of the Fermi surface is given by

$$n_{\text{Lutt}}(T) = \frac{2}{N} \sum_{k} \theta \left(\mu - \varepsilon_k - \text{Re} \,\Sigma_k(\omega = 0) \right), \tag{36}$$

and the particle concentration is given by

$$n(T) = \frac{2}{N} \sum_{k} n_{k} = -\frac{2}{N} \sum_{k} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{\pi} f(\omega) \operatorname{Im} G_{k}(\omega + \mathrm{i}0^{+}),$$
(37)

where $f(\omega)$ is the Fermi distribution function. Luttinger's theorem states that for T = 0

$$n(T) = n_{\text{Lutt}}(T) \,. \tag{38}$$

which when extended by lifting the assumption $\Gamma_k = 0$, becomes [187]

$$n \approx n_{\text{Lutt}} + \frac{2}{\pi N} \sum_{k} \arctan\left(\frac{\Gamma_k}{\varepsilon_k + \text{Re}\,\Sigma_k(0) - \mu}\right),$$
 (39)

which is exact in the limit $T \rightarrow 0$. Figure 23 shows the deviations from Luttinger's theorem, obtained by directly solving the FLEX equations (solid line) and by using Eqn (39) (dashed line). Note that Eqn (38) may fail due to the temperature broadening of the Fermi distribution — hence



Figure 23. Deviations from Luttinger's theorem for underdoped systems, obtained by directly solving the FLEX equations (solid line) and from Eqn (39) (dashed line); *n* is the number of particles, n_{Lutt} is the volume of the Fermi surface. Calculation within the Hubbard model with U = 4t, t = 0.25 eV, T = 63 K. Inset shows temperature-induced increases in the particle concentration \tilde{n} , due to the diffusion of the Fermi distribution function at finite temperatures. It is seen that these increases are an order of magnitude less than the deviations from Luttinger's theorem. (After Ref. [187]).

the approximate equality symbol in (39). The inset to Fig. 23 shows, however, that this effect is small, at least an order of magnitude less than the deviation from Luttinger's theorem which we are discussing.

The reason why Luttinger's theory is violated is the nonzero value of Γ_k . While $\Gamma_k \neq 0$ is symmetric in states below and above the Fermi surface, the summation over k on the right-hand side of (39) causes some terms to compensate, giving $n = n_{\text{Lutt}}$. If, however, Γ_k is asymmetric, as is the case in the FLEX approximation (because the maximum value of Γ_k relates to shadow bands outside the main Fermi surface), n deviates from n_{Lutt} . Since a comparison shows that the solid and dashed lines agree well, the violation of Luttinger's theorem is due to the anomalous properties of Γ_k which, in turn, relate to the existence of the shadow bands. Indeed, the very concept of the shadow bands is due to the fact that the spectral density partially moves from beneath the Fermi surface to above it, so that the particles beneath become fewer, and it is no surprise that the theorem is violated. For x > 0.20, above the optimum doping values, it has been shown [187] that the attenuation $\Gamma_k \to 0$ for $T \to 0$, and Luttinger's theorem therefore holds. For this Fermi liquid region, both theoretical calculations and ARPES data indicate nesting of the Fermi surface in the (π, π) direction [10]. Although the nesting is most pronounced in Bi-2212, it is also seen in Bi-2201 and, possibly, also in YBaCuO and $La_{2-x}Sr_{x}CuO_{4}$. As is well known, this property makes the normal metallic state unstable toward SDW and CDW phases, leading to a partial rearrangement of the band structure. Superconductivity in such electron-hole pairing systems was treated in detail in Ref. [142], and with application to copper oxides, in Refs [191, 192]. The band theory of phase separation also employs the nesting concept [193].

6. Electronic properties of the normal phase

To avoid overlapping previous reviews [4-12], we will not discuss here the unusual temperature dependences exhibited by many normal phase properties, nor the marginal Fermiliquid concept or other approaches developed for explaining these dependences. In this section we restrict ourselves to two problems which are currently under active discussion, the spin pseudogap and charge ordering with the formation of one-dimensional domains (or stripe phases).

6.1 Spin pseudogap

The term spin gap stems from the observation that the temperature dependence of the inverse relaxation time $(T_1\overline{T})^{-1}$ in NMR experiments exhibits a maximum at T = 130-150 K, well above the T_c of YBa₂Cu₃O_{6+x} in the underdoping region [194, 195]. Later, inelastic neutron scattering studies [196] identified this gap as that for spin excitations with $q = Q = (\pi/a, \pi/a)$. Since what is actually observed is a decrease in the spectral weight $\chi''(Q, \omega)$ at low frequencies and an increase at high frequencies, the term 'pseudogap' was introduced. The pseudogap is also seen in NMR as a maximum in the temperature dependence of the spin – spin relaxation rate T^* . NMR evidence for the existence of a pseudogap at $T = T^*$ in various copper oxide superconductors is reviewed in Ref. [197]. The value of T^* decreases with increasing hole concentration, and for optimum doping, $T^* = T_c$ (Fig. 24). A pseudogap in the quasiparticle spectrum also shows up in infrared optical spectra, Raman spectro-

Figure 24. Variation of T_c and T^* with concentration. The squares denote various oxides: YBa₂Cu₃O_{6.6}(123O_{6.6}), YBa₂Cu₃O_{6.7}(123O_{6.7}), YBa₂Cu₄O₈(124O₈), and YBa₂Cu₃O_{6.95}(123O_{6.95}); n_s is the density of the superfluid component; m^* is the effective mass of the carriers. (After Ref. [198]).

8

 T^*

Normal metal phase

123O_{6.95}

Overdoping

12

 $n_{\rm s}/m^*$, 10⁷ cm⁻²

Superconducting phase

Optimum doping

123O_{6.6}

123O_{6.7}

Phase with a pseudogap

Underdoping

4

1240

scopy, and in the kinetic properties (see review [198]). Finally, in Figs 3 and 4, which show ARPES results for Bi-2212 oxides with varying hole concentration [15], one can directly see the opening of a gap at the Fermi surface along the $(\pi, 0) - (\pi, \pi)$ line as the hole concentration decreases. The macroscopic nature of the pseudogap is the subject of much discussion at present. In our view, the formation of local antiferromagnetic domains, which produce shadow bands and have been discussed in Sections 5.3 and 5.4, is quite enough to account for the pseudogap. There are other proposals, however, such as local quasiparticle pairing without inter-pair phase coherence [39] and the separation of the charge and spin degrees of freedom [45], among others. According to Ref. [199], the spin gap is due to the singlets formed from the spins of adjacent CuO₂ layers, the interaction between the spins being enhanced by strong in-plane spin fluctuations.

6.2 Quasi-one-dimensional charge ordering

When introduced into an antiferromagnetic insulator as a result of doping, holes form slowly fluctuating metallic stripes and move quasi-one-dimensionally along them. Between the stripes there are insulating regions, which induce a spin pseudogap due to a magnetic analogue of the proximity effect as shown in Ref. [200]. Experimentally, alternating conducting and nonconducting stripes were found in $Bi_2Sr_2CaCu_2O_{8+y}$ in extended x-ray absorption fine structure (EXAFS) and electron diffraction [201] measurements. Figure 25 shows the alternation of LTO (low-temperature orthorhombic) and LTT (low-temperature tetragonal) stripes



Figure 25. Schematic representation of the CuO₂ plane with conducting LTO and insulating LTT stripes. (After Ref. [201]).

with widths L = 2.65a and $W \approx 2a$, so that the total period of the structure is $\lambda_p = L + W = 4.65a$. The EXAFS technique showed an alternation of Cu–O bonds with apical oxygen below T_c , the length of the Cu–O bond being 2.53 A and 2.37 A for the LTO and LTT phases, respectively. In Ref. [201] the tetragonal phase is described as a one-dimensional, polaronic charge density wave (CDW), whereas the orthorhombic phase is associated with metallic conduction.

For a two-dimensional Fermi gas in the superlattice of quantum stripes of width L oriented along the x axis, the vector k_y is quantized due to the size effect, so that $k_y^{(n)} = n\pi/L$. For n = 2 we have $k_y^{(2)} = 0.38(2\pi/a)$, which is very close to the Fermi vector in the ΓM direction, $k_{\rm F} = 0.37(2\pi/a)$ [10]. Therefore the density-of-states peak due to the y-propagating standing wave of wavelength $\lambda \approx L$ falls in the vicinity of the Fermi surface which, according to estimates [201], increases T_c five-fold as compared with the uniform case. A system of stripe phases is a special case of the phase separation phenomenon. Insulating ordering may be produced both by charge and spin fluctuations. Presumably, the higher the hole concentration, the lower the relative contribution of spin fluctuations. For the optimally doped Bi-2212 system studied in Ref. [201], it is quite likely that charge ordering is responsible for the insulating properties of the nonconducting stripes.

The conclusion about the nonuniform distribution of charge in TmBa₂Cu₄O₈ was made based on NQR studies [202, 203]. In Ref. [202], two stripe types — straight stripes along [1, 1, 0] and zigzag stripes along [1, 0, 0] with a period of 2a — were proposed. Both separation possibilities lead to the formation of 'spin ladders' [204] with copper spins coupled by a strong antiferromagnetic exchange J. The ladders are separated by conducting stripes, with antiferromagnetic correlations weakened by the presence of carriers. For exchange between the ladders $\lambda \tau$, the spin excitation spectrum has a gap with a width from 0.5 τ at $\lambda = 0$ to zero at $\lambda = 0.25$ [204]. Thus, the ordering of separated electrons into a stripe phase may lead to a spin gap, although further

T, K

300

250

200

150

100

50

0

investigation is needed to clarify the temperature and concentration dependences of the gap-related effects in this mechanism.

7. Effects of the electronic system on the concentration dependences of T_N and T_c in underdoped copper oxides

In this section we will consider the suppressive effects of the electronic structure on the antiferromagnetism of a material doped with carriers or in which copper is substituted by other magnetic ions. Since, on *p*-type doping, a hole moves mainly over oxygen orbitals, an additional exchange $J_{Cu-O} \gg J_{Cu-Cu}$ arises, producing fluctuations in a Heisenberg antiferromagnet and rapidly suppressing three-dimensional longrange order. A static model with fluctuations was analysed in Ref. [205]. A t-J analysis of spin waves including the interaction of magnons with holes and with electron-hole pairs [206, 207] shows both the sublattice magnetization $M_{\rm i}$ and spin wave velocity v to increase nonlinearly with increasing hole concentration. The critical concentration x_c can be determined not only from the condition $M_i(x_c) = 0$, but also by requiring the vanishing of the magnon velocity [208]. As shown in Ref. [207], both approaches predict virtually the same value of x_c , and this value agrees quite well with the experimental $La_{2-x}Ba_xCuO_4$ data. By extending the calculations of Refs [206, 207] to finite temperatures, the concentration dependence of the Néel temperature was derived [209].

The asymmetry of the magnetic phase diagram for electron and hole doping originates from asymmetry in the electron structure [210], because whereas *p*-type systems display frustrations, in *n*-type systems we actually observe diamagnetic substitution. Neglecting covalence, i.e., assuming that in the absence of doping all copper ions are in the d⁹ state with spin S = 1/2, one additional electron produces the d¹⁰ configuration with S = 0, which is indeed equivalent to diamagnetic substitution — for example, in the La₂Cu_{1-y}Zn_yO₄ system. Experimentally, this equivalence was demonstrated by the similarity of the $T_N(y)$ dependences in La₂Cu_{1-y}Zn_yO₄ and Pr_{2-y}Ce_yCuO₄ [138].

Due to covalence, the ground state of the cell in the absence of doping is a superposition of a hole at copper and a hole at oxygen,

$$\left| GS(n_{\rm h}=1) \right\rangle = u \left| \, \mathrm{d}^9 \mathrm{p}^6 \right\rangle + v \left| \, \mathrm{d}^{10} \mathrm{p}^5 \right\rangle, \tag{40}$$

where *u* and *v* are the coefficients determined by the parameters of the p-d Hamiltonian, $u^2 = (1 + \Delta/v)/2$, $\Delta = \varepsilon_p - \varepsilon_d$, $v^2 = \Delta^2 + 8t_{pd}^2$. After adding an electron, the cell is in the state $|GS(n_h = 0)\rangle = |d^{10}p^6\rangle$, so that the diamagnetic substitution at a copper ion upon *n*-type doping occurs with probability $u^2 < 1$, not 1 as in the absence of covalent effects. As a result, the slope of the concentration curve is different in *n*-type systems and diamagnetically substituted systems [211]. Although this difference is small, because $u^2 \approx 0.8$ for realistic values of the relevant parameters, it agrees well with the data of Ref. [138].

The suppression of antiferromagnetism and superconductivity due to the substitution of copper by various magnetic (Fe, Co, Ni) and non-magnetic (Zn, Al, Ga) ions has been studied in considerable detail. In Y-123, trivalent impurities generally substitute Cu1 sites in Cu–O chains, and divalent Zn and Ni substitute in-plane Cu2 sites [212]. The suppression effect of various impurities is conveniently compared using the La_{2-x}Sr_xCu_{1-y} M_y O₄ system (M = Fe, Co, Ni, Zn, Ga, Al) in which all impurities are located in the CuO₂ plane. Systems with Cu substituted by Ni are the most anomalous in behavior: the slope dT_N/dx for Ni is almost three times less than for Zn. For Zn, $dT_N/dx = -17$ K (at.%)⁻¹, and for Ni, $dT_N/dx = -5.5$ K (at.%)⁻¹ [213].

The $T_c(y)$ dependences for La_{1.85}Sr_{0.15}Cu_{1-y} M_yO_4 proved to be virtually the same for the nonmagnetic Zn, Al, Ga and magnetic Co impurities; the most rapid falloff of T_c was found for Fe and the slowest, for Ni [214]. Assuming a low-spin state for Co³⁺, it proved possible [214] to qualitatively explain the concentration dependences $T_c(y)$ and the magnetic properties of the impurities Co, Zn, Ga, Al, and Fe, but the situation with Ni is more difficult. From static susceptibility measurements, the magnetic moment at a nickel atom turned out to be even smaller than S = 1/2, instead of the S = 1 anticipated for Ni²⁺. A small magnetic moment and a slow falloff of $T_c(y)$ were also reported for YBa₂Cu_{3-y}Ni_yO₇ [215].

The multielectron analysis in Ref. [216] not only provided quantitative and qualitative agreement with the concentration dependences of T_c and T_N but also explained the anomalies that arise when Cu is substituted by Ni. Formally, the Ni²⁺ ion has the configuration d⁸, which is equivalent to hole doping as far as the number of holes per CuO₂ cell is concerned, and the ground state of the system should therefore be considered in the two-hole sector of Hilbert space. Due to the SEC effects, the contribution from the p⁶d⁸p⁶ configuration is suppressed, and the ground state (Zhang–Rice singlet) is described by a mixture of configurations

$$|GS(n_{\rm h}=2)\rangle = u_0 |{\rm p}^5 \,{\rm d}^{10} {\rm p}^5\rangle + v_0 |{\rm p}^5 \,{\rm d}^9 {\rm p}^6\rangle \,, \tag{41}$$

where $u_0^2 = (1 - \Delta_0/v)/2$, $\Delta_0 = \Delta - V_{pd}$, $v_0^2 = \Delta_0^2 + 8t_{pd}^2$. This result is obtained in the limit $U_d = \infty$, when the contribution from d⁸ is zero. For $U_d \approx 10$ eV, the contribution from d⁸ to the ground state is ~1%. Due to the Coulomb interaction between Cu and O, the charge transfer energy is renormalized, $\Delta_0 < \Delta$, increasing the role of covalence in the two-hole compared to the one-hole sector. As a result, we see from (41) that Ni²⁺ in the CuO₂ lattice is not in the state S = 1, but with probability u_0^2 has S = 0 in configuration d¹⁰ and with probability v_0^2 has S = 1/2 in d⁹. Taking $\Delta = 2$ eV, $t_{pd} = 1$ eV, and $V_{pd} = 0.6$ eV, the weights are found to be $u_0^2 = 0.28$ and $v_0^2 = 0.72$. The effective spin at nickel,

$$S_{\rm Ni} = v_0^2 \cdot 0.5 \,, \tag{42}$$

is 0.36 [215].

The concentration dependence of T_N for diamagnetic substitution has been calculated in two different ways. A QMC calculation using the two-dimensional low-anisotropy Heisenberg model showed that for an anisotropy-to-exchange ratio $K/J \sim 10^{-3}$, dT_N/dx is close to the experimental value. In the Hubbard model, diamagnetic substitution was modeled by spin wave scattering on a static magnetic impurity, with the magnon mass operator calculated in the random phase approximation [217]. As a result, $T_N(x)$ is given by

$$T_{\rm N}(x) = T_{\rm N}(0) \left(1 - \alpha x \ln \frac{1}{r}\right),\tag{43}$$

where $\alpha \sim 1$, $r = J_{||}/J_{\perp} \approx 6 \times 10^{-3}$ for La₂CuO₄. Since $T_{\rm N}(0) = J \ln(1/r)$,

$$\frac{\mathrm{d}T_{\mathrm{N}}}{\mathrm{d}x} = -\alpha \frac{T_{\mathrm{N}}^2(0)}{J} \,.$$

The inclusion of anisotropy produces a gap Δ_a in the spin wave spectrum and yields a renormalization $r \rightarrow [r^2 + (\Delta_a/2J_{\perp})^2]^{1/2}$. The value of Δ_a/J is of the same order (~ 10^{-3}) as r. The resulting slope dT_N/dx is also close to the experimental value for substituting Cu by Zn. As regards dT_N/dx for substitution by nickel, Eqn (41) shows that with probability v_0^2 the spin of the impurity, S = 1/2, is equal to that of the lattice, i.e., magnetic disorder is virtually absent (since the lattice does not change, it may be considered that, for $x \ll 1$, the parameters of the Hamiltonian are also the same, so that the exchange terms J_{Cu-Ni} and J_{Cu-Cu} are close in magnitude in this d⁹ state). With probability u_0^2 the substitution of Cu by Ni is equivalent to diamagnetic substitution, i.e., in $La_{2-x}Sr_xCu_{1-y}M_yO_4$ the fraction of diamagnetic centers, which is y for M = Zn, is $u_0^2 y$ in the case of Ni. This means that

$$\frac{dT_{\rm N}}{dy}({\rm Ni}) = u_0^2 \frac{dT_{\rm N}}{dy}({\rm Zn}) = -4.76 \text{ K} ({\rm at.\%})^{-1}, \qquad (44)$$

which is very close to the experimental value for Ni, $-5.5 \text{ K} (\text{at.}\%)^{-1}$. [213]. Thus, the mechanism of antiferromagnetism suppression for Zn and Ni substitutions is the same [216], the quantitative difference between the two stemming from the fact that their electronic structures are affected differently by substitution.

A clue to the understanding of the concentration dependence of T_c for Zn, Ga, Al and Co substitutes is provided by static susceptibility measurements [213, 214], which show that the effective magnetic moment of an impurity is close to that of Cu²⁺. A lattice with one site empty behaves, quite obviously, as a single paramagnetic center due to the sublattices not being compensated. A similar conclusion about a Zn-induced magnetic moment results from NMR data [215]. This implies that the T_c suppression following the substitution by formally nonmagnetic impurities is in fact due to the scattering of the Cooper pairs by magnetic moments that are induced by the impurity locally in an antiferromagnetic environment, i.e., we are actually dealing with the ordinary BCS magnetic suppression effect. With this understanding, and taking into account the quantitative difference in the concentration of diamagnetic centers on substitution by Zn and Ni, we also obtain an explanation of the anomalously weak suppression of $T_{\rm c}$ in the case when Cu is substituted by Ni. For the slope of $T_{c}(y)$, the following expression, analogous to (44), is obtained [216]:

$$\frac{\mathrm{d}T_{\mathrm{c}}}{\mathrm{d}y}(\mathrm{Ni}) = u_0^2 \frac{\mathrm{d}T_{\mathrm{c}}}{\mathrm{d}y}(\mathrm{Zn})\,. \tag{45}$$

The Ni-to-Zn $T_{\rm c}(y)$ is 0.38 for slope ratio 0.25 $La_{1.85}Sr_{0.15}Cu_{1-y}M_yO_4$ [213] and for YBa₂(Cu_{1-y} M_y)₃O_{7-x} [215], to be compared with the theoretical value of u_0^2 of 0.28. Thus, the notion that substituting Cu by Ni leads to the filling of the Zhang-Rice singlet and that the latter remains localized due to the small radius of the impurity state, provides a unified description of the concentration dependences of both $T_{\rm N}$ and $T_{\rm c}$.

It is also interesting to note that, on substituting copper by transition metals, the concentration dependences in underdoped systems differ from those in overdoped, as observed both for $La_{2-x}Sr_xCu_{1-y}M_xO_4$ (M = Zn, Ni) [218] and for $Bi_2Sr_2Ca_{1-x}Y_x(Cu_{1-y}M_y)_2O_{8+z}$ (M = Fe, Co, Ni, Zn) and $Bi_2Sr_{1.6}La_{0.4}Cu_{1-y}M_yO_{6+z}$ (M = Co, Zn) [219]. In overdoped systems the dependence of T_c on the hole (*p*) and impurity (*y*) concentration may be written in the form [218]

$$T_{\rm c}(p,y) = T_{\rm c}(p,0)g(y)$$
 (46)

where the function g(y) is independent of the hole concentration for all investigated substitutions of Cu by Fe, Co, No, and Zn in the B-2212, Y-123, and La-214 systems. Qualitative agreement with the Abrikosov–Gor'kov theory [220] can be achieved by assuming that the density of states N(0) at the Fermi level increases with hole concentration and that the scattering of quasiparticles by impurities is strong enough to be treated in the unitary limit.

Underdoped systems exhibit stronger T_c suppression than predicted by (46). According to Ref. [218], this is the region where localization effects are more important.

In *n*-type systems the differences in the suppression effect in replacing Cu by Zn, Fe, Co, and Ni agree quite well with theory [220]. Thus, for a nonmagnetic Zn impurity the suppression is very weak, whereas for magnetic Ni and Co, data from ceramic samples [221, 222] show the suppression to be already complete at a concentration ~1 %. Recent studies on single crystals of $Pr_{2-x}Ce_xCu_{1-y}M_yO_{4+z}$ with M = Ni, Co support the ceramic data and also show that $dT_c/dy = -20$ K (at.%)⁻¹ for both Ni and Co [223]. This is the highest T_c suppression rate among all the copper oxides for which the effect of substituting copper by transition metals has been studied to date.

8. Conclusions

Due to extensive experimental and theoretical work, much progress has been made in recent years in the understanding of the energy-band structure of the strongly correlated electron system of copper oxides. The spin-polaron antiferromagnetic-lattice description of holes in underdoped systems, which developed from mutually consistent numerical cluster calculations and various perturbation calculations for the CuO₂ lattice, is well supported by experimental studies, notably by the ARPES data. In the metallic phases one distinguishes two regions, underdoped and overdoped systems, the degree of doping being measured from the optimum doping level. Although overdoped systems obey Luttinger's theorem and have a large Fermi surface consistent with band calculations, SEC effects do still arise in that near point $X = (\pi, 0)$ the electron dispersion has a flat portion and that near $\varepsilon_{\rm F}$ the band is narrower than predicted by band theory. This metallic state is sometimes referred to as a strange metal because some experimental data, in particular the temperature dependence of the kinetic coefficients, indicate a non-Fermi-liquid behavior of the system. The concept of a marginal Fermi surface provides a good qualitative description of this strange behavior.

Even more strange, though, is the region of underdoped metallic compositions which, in addition to T_c , is also characterized by the spin pseudogap formation temperature T^* . The body of data summarized above demonstrates that the formation of the electronic structure in this composition

region involves strong local antiferromagnetic fluctuations, which control the pseudogap and the shadow bands, cause the mass operator to deviate from the Fermi-liquid behavior near the Fermi energy, and lead to the violation of Luttinger's theorem. At the phenomenological level, this system might be identified as an almost antiferromagnetic Fermi liquid, a concept which proved very successful in describing the deviation from the Korringa law of the spin-lattice relaxation rate in NMR spectra [224]. The hole concentration region near the insulator-metal transition remains least understood. Although, qualitatively, the concept of insulating and metallic phases coexisting with the percolationcontrolled insulator-metal transition is consistent with the phase separation phenomenon observed in a number of oxides, it remains unclear exactly when this separation is disordered and when ordered stripe phases appear. Since $La_{2-x}Sr_xCuO_4$ does not show any phase separation, the question arises as to precisely how and when the insulator metal transition occurs in a spatially uniform system.

Although the mechanisms of superconducting pairing have not been considered here, the dominant role of spin fluctuations in forming the electronic structure suggests that they are important in this respect as well. It is commonly believed that the exchange by spin fluctuations leads to d-type pairing [6-12], although the possibility of s-pairing due to exchange by antiferromagnetic fluctuations should also be noted [225].

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