Theory of high-T_c superconductors within a realistic Anderson lattice model

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(Received 11 July 1988)

A realistic Anderson lattice Hamiltonian for $La_{2-x}Sr_xCuO_4$ is derived from an extensive tight-binding parametrization of *ab initio* band structure. A solution of the Hamiltonian by the $1/N$ expansion technique gives remarkably good agreement with the data on thermodynamic, transport, and critical properties, e.g., the location of the holes on the oxygen and saturation of T_c at 15% doping are reproduced.

One likely origin for the superconductivity in a strongly correlated electron band is an indirect one via the Hubbard U (see below). For a half-filled Hubbard band, such a system is believed to be a strongly fluctuating quantum Heisenberg antiferromagnet.[1] The limit of the introduction of a *small* number of holes into such a half-filled band has been largely treated within the resonating-valence-bond[2] (RVB) approach. Here we concentrate primarily on the opposite limit of large number of holes; a limit which we find is better treated within an itinerant picture (as is consistent with recent measurements of the Fermi surface[3]), and by generalization of the Hubbard model to the Anderson lattice Hamiltonian[4] (ALH). We present a detailed description of $La_{2-x}Sr_xCuO_4$ using the ALH both in the normal and superconducting states.

(1) We carry out an accurate parametrization of the band structure[5] of $La_{2-x}Sr_xCuO_4$ to generate the ALH. (2) We solve the ALH, using a $1/N$ expansion, in the normal and superconducting states. (3) In mean field (leading N), we find a Fermi fluid above T_c with a mass enhancement of $m^*/m \sim 5$ and a superconducting *long-range*-order (LRO) parameter below T_c. (4) We find a narrow but observable critical region. (5) We find a correct behavior for the trend of thermodynamic and transport properties both above and below T_c, as a function of the hole concentration x_h, with one adjustable parameter.

To describe the La_2CuO_4 band structure, we need to include for the itinerant states the p orbitals of the oxygens; the s, p, and t_{2g} orbitals of the Cu; and the d states of La. These then hybridize with the local $d_{x^2-y^2}$ and d_{z^2} orbitals on the Cu. Our ALH is then

$$\mathcal{H}=\sum_{\mathbf{k},\alpha,\sigma}\varepsilon_{\mathbf{k}\alpha}c^{\dagger}_{\mathbf{k}\alpha\sigma}c_{\mathbf{k}\alpha\sigma}+E_1\sum_{i,\beta,\sigma}D^{\dagger}_{i\beta\sigma}D_{i\beta\sigma}+\sum_{\mathbf{k},\alpha,i,\beta,\sigma}(V_{\mathbf{k}\alpha\beta}D^{\dagger}_{i\beta\sigma}c_{\mathbf{k}\alpha\sigma}e^{i\mathbf{k}\cdot\mathbf{r}_i}+\text{H.c.})+\frac{U}{2}\sum_{i,(\beta,\sigma)\neq(\beta',\sigma')}N_{di\beta\sigma}N_{di\beta'\sigma'}-\mu\hat{\mathbf{N}}\,, \tag{1}$$

where $\varepsilon_{\mathbf{k}\alpha}$ are the unhybridized itinerant bands, E_1 is the energy of the $d_{x^2-y^2}$ and d_{z^2} orbitals on the Cu sites (denoted by $\beta=0,1$, respectively), and $V_{\mathbf{k}\alpha\beta}$ are the hybridizing matrix elements between them. $c^{\dagger}_{\mathbf{k}\alpha\sigma}$ and $D^{\dagger}_{i\beta\sigma}$ are the creation operators in the itinerant and localized manifolds α and β, respectively, and σ is the spin index. We prefer to invert the band structure and work with holes filled up to a chemical potential μ. The fourth term in Eq. (1) is the Hubbard repulsion U with $N_{di\beta\sigma}=D^{\dagger}_{i\beta\sigma}D_{i\beta\sigma}$. An identification may be made between the local-density-approximation (LDA) band structure and the Hartree solution to (1). A tight-binding parametrization of the band structure[5] then generates the values of $\varepsilon_{\mathbf{k}\alpha}$ and $V_{\mathbf{k}\alpha\beta}$. E_1 determined in this way, however, incorporates an unknown Hartree shift, so we take it as an adjustable parameter.

In order to handle the large U, we write $D_{i\beta\sigma}$ in a "boson-spinon" representation[6] (convenient when U is large)

$$D_{i\beta\sigma}=b_i^{\dagger}d_{i\beta\sigma}+a_i\delta_{\beta 0}d^{\dagger}_{i\beta-\sigma}\,\mathrm{sgn}\sigma\,, \tag{2}$$

where $b_i^{\dagger}$ is a Bose field representing d^{10} Cu and $d^{\dagger}_{i\beta\sigma}$ is a fermion field representing d^9. Because the d_{z^2} states are almost completely filled, it is sufficient to include only the component of d^8 with two $d_{x^2-y^2}$ holes, represented by the Bose field a_i. The three fields on site i are connected by the constraint

$$\sum_{\beta,\sigma}d^{\dagger}_{i\beta\sigma}d_{i\beta\sigma}+b_i^{\dagger}b_i+a_i^{\dagger}a_i=\hat{\mathbf{Q}}_i=1\,, \tag{3}$$

which, since $[\hat{\mathbf{Q}}_i,\mathcal{H}]=0$, conserves probabilities over the boson and fermion subspaces on site i. Equation (1) can now be written in the bosonized form[4]

$$\mathcal{H}=\sum_{\mathbf{k},\alpha,\sigma}\varepsilon_{\mathbf{k}\alpha}c^{\dagger}_{\mathbf{k}\alpha\sigma}c_{\mathbf{k}\alpha\sigma}+E_2\sum_i a_i^{\dagger}a_i+E_1\sum_{i,\beta,\sigma}d^{\dagger}_{i\beta\sigma}d_{i\beta\sigma}$$
$$+\sum_{\mathbf{k},\alpha,i,\beta,\sigma}[V_{\mathbf{k}\alpha\beta}(b_i d^{\dagger}_{i\beta\sigma}+a_i^{\dagger}\delta_{\beta 0}d_{i\beta-\sigma}\mathrm{sgn}\sigma)c_{\mathbf{k}\alpha\sigma}e^{i\mathbf{k}\cdot\mathbf{r}_i}+\mathrm{H.c.}]-\mu\hat{\mathbf{N}}+\sum_i\lambda_i(\hat{\mathbf{Q}}_i-1)\,, \tag{4}$$

where

$$\hat{\mathbf{N}}=\sum_i\left[2a_i^{\dagger}a_i+\sum_{\beta,\sigma}d^{\dagger}_{i\beta\sigma}d_{i\beta\sigma}\right]+\sum_{\mathbf{k},\alpha,\sigma}c^{\dagger}_{\mathbf{k}\alpha\sigma}c_{\mathbf{k}\alpha\sigma}\,, \tag{5}$$

and $E_2=2E_1+U$. The last term in Eq. (4) adequately imposes the constraint of Eq. (3) at all temperatures of interest via the Lagrange multiplier λ_i.

Before we turn to an approximate solution of Eq. (4), we must establish a superconducting long-range-order parameter. This is not entirely trivial. Equation (4) is invariant under local gauge symmetry

$$e^{i\hat{\mathbf{Q}}_i\phi}\hat{\mathbf{A}}_i e^{-i\hat{\mathbf{Q}}_i\phi}=\hat{\mathbf{A}}_i e^{i\phi}\,, \tag{6}$$

where $\hat{\mathbf{A}}_i=a_i$, b_i, or $d_{i\beta\sigma}$; hence *b_i or a_i cannot have LRO individually.* Convenient choices of s-wave order parameter equivalently involve either the conventional form $\langle c^{\dagger}_{k\uparrow}c^{\dagger}_{k\downarrow}\rangle$ or the gauge-invariant combination $\langle b_i^{\dagger}a_i\rangle$.

Normal state. To solve Eq. (4) we extend the spin degeneracy σ from $2\rightarrow$ to large N. Such a procedure permits a systematic expansion[4,7,8] in powers of $1/N$ (the expectation is that the qualitative features of the results will remain unchanged when $N\rightarrow 2$). We expand the normal self-energy to leading order in $1/N$ [Fig. 1(a)] equivalent to a mean-field approximation[4,7] to b_i and λ_i, i.e., $b_i=\langle b\rangle$ and $\lambda_i=\lambda$. The violation of gauge symmetry involved here is only apparent (see, e.g., Ref. 4). In the normal state $\langle b\rangle$ and λ are calculated by minimizing the free energy with respect to $\langle b\rangle$ and λ to get

$$N\sum_{\mathbf{k},\beta,\alpha}V_{\mathbf{k}\beta\alpha}\langle d^{\dagger}_{0\beta\sigma}c_{\mathbf{k}\alpha\sigma}\rangle=-\lambda\langle b\rangle\,, \tag{7a}$$

$$n\sum_{\beta}\langle d^{\dagger}_{0\beta\sigma}d_{0\beta\sigma}\rangle=\left(\tfrac{1}{2}N-\langle b\rangle^2\right), \tag{7b}$$

and conservation of hole number gives the relation

$$\frac{N}{N_s}\sum_{\mathbf{k},\alpha}\langle c^{\dagger}_{\mathbf{k}\alpha\sigma}c_{\mathbf{k}\alpha\sigma}\rangle+N\sum_{\beta}\langle d^{\dagger}_{0\beta\sigma}d_{0\beta\sigma}\rangle=1+x_h\,. \tag{7c}$$

In (7c), x_h is the number of holes due to Sr doping, proportional to Sr concentration x up to $x=0.15$. The $\mathbf{k}$ sums in (7) are over the full three-dimensional (3D) Brillouin zone.

The expectation values in Eq. (7) are related to various single-particle Green's functions. All three are calculated numerically from Eq. (4) by solving the mean-field band structure and employing the tetrahedron algorithm. The self-consistent relations (7) are then solved numerically.

The resulting density of states (DOS) for La_2CuO_4 in Fig. 2 shows an uppermost partly filled band ~ 1 eV wide, consisting mostly of $d_{x^2-y^2}$, with a filled d_{z^2} band just below it, below which lies the upper edge of the itinerant band at 6.3 eV. Sr doping is dealt with just by adding the appropriate number of holes. Adding holes is seen to lower the d bands, resulting in a discontinuity at $x\sim 0.12$ where the Fermi level goes into the itinerant bands. In Fig. 3 we see that added holes indeed go onto the oxygens[9] as experimental data[10] confirms. The density of states at ε_F is seen to agree with the trend and absolute value determined from susceptibility[11] and specific-heat[12] measurements. The Hall resistivity in Fig. 3 is in fair agreement with a single point[13] determined on a film; its trend also agrees with ceramic data.[14] The picture that emerges of the normal phase then is of a strongly correlated Fermi liquid whose mass enhancement is $m^*/m\sim 5$.

Superconducting state. We have examined the superconducting phase by studying the generalized (normal and anomalous) self-energy using the well-known Nambu-Gorkov formalism. We have included the leading-order self-energies of each type; the graphs for the anomalous self-energy are shown in Figs. 1(b) and 1(c). They are of order $1/N$. The details of assigning the order to various graphs and some of the algebra involved in obtaining the equations for the superconducting phase is dis-

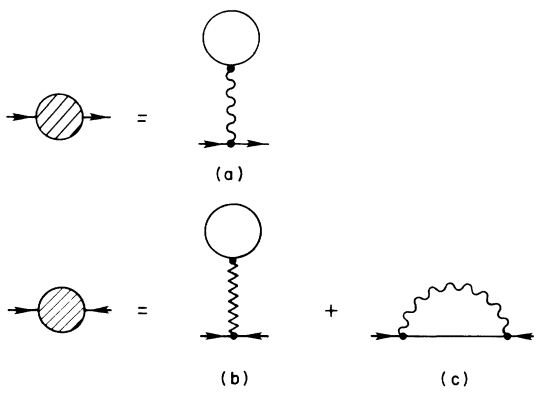

FIG. 1. Diagrams for the self-energy. (a) Leading-N [order (1)] contribution to the normal self-energy. (b),(c) Leading (order $1/N$) contributions to the anomalous self-energy. Wavy line is b boson, zig-zag line is a boson.

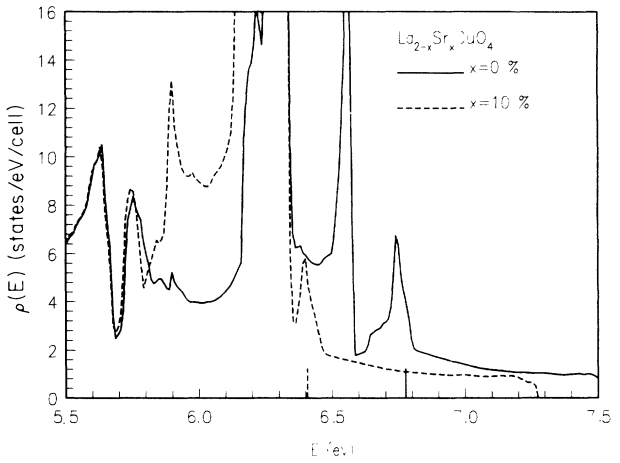

FIG. 2. DOS for La_2CuO_4 (solid curve) and $La_{1.9}Sr_{0.1}CuO_4$ (dashed curve) calculated in mean-field approximation with $E_1=9.42$ eV. Vertical lines indicate position of Fermi level.

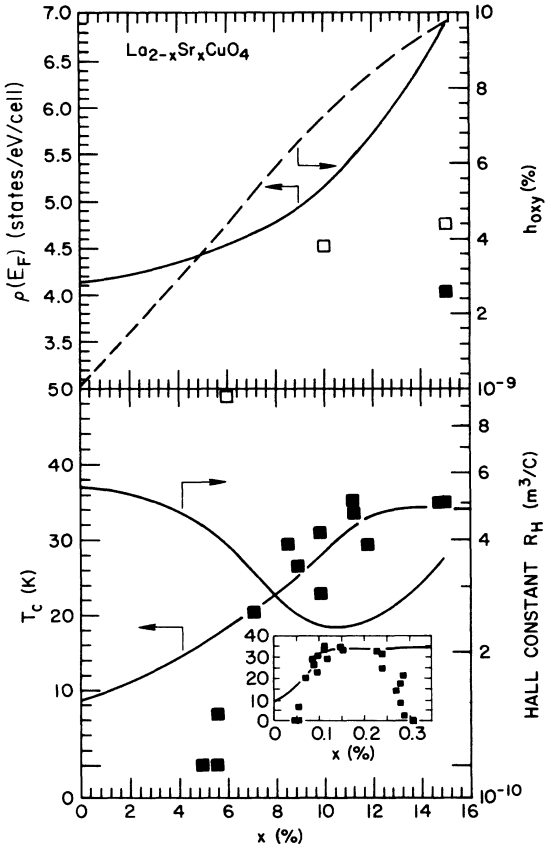

FIG. 3. Comparison between theory and experiment as a function of doping x. Top panel: DOS at ε_F (solid curve), experimental points are from susceptibility (open squares) and specific-heat jump (filled square); dashed curve, holes on planar oxygen p_x,p_y orbitals. Lower panel: solid curve and box, T_c at $U=6.5$ eV with $\tilde{u}=0.439$; filled squares are data. Dotted curve, R_H; open square, data point.

cussed at length in Ref. 15.

Notice, the gap equation derived here has no adjustable parameter such as μ^* of the Eliashberg theory for conventional superconductors. Here the corresponding pseudopotential term is explicitly evaluated.[15]

The solution below T_c is numerically difficult, but is simplied when we recognize that near the Fermi level, the normal-state band structure is nearly approximated by a single band $\varepsilon_{\mathbf{k}}$ hybridizing with an effective single d orbital via matrix elements $V_{\mathbf{k}}\sim V$. The gap equation may then be obtained analytically as

$$1=\left[\frac{2NV^2}{\tilde{E}_2}-\tilde{u}\right]\sum_{\mathbf{k}',n'}\frac{g^2_{\mathbf{k}'\mathbf{k}'}}{\omega_{n'}^2+E^2_{\mathbf{k}'}+\delta^2 g^2_{\mathbf{k}'\mathbf{k}'}}, \tag{8a}$$

where

$$\cot\theta_{\mathbf{k}}=(\varepsilon_d-\varepsilon_{\mathbf{k}})/2\langle b\rangle V,$$

$$E_{\mathbf{k}}=\varepsilon_d+\langle b\rangle V\tan\theta_{\mathbf{k}}, \tag{8b}$$

$$\tilde{u}=\frac{1}{N\rho_0\sin^2\theta_{\mathbf{k}_F}}\left[1-\frac{0.2}{N}\right], \tag{8c}$$

$$g_{\mathbf{k}',\mathbf{k}}=\sin\theta_{\mathbf{k}'}\cos\theta_{\mathbf{k}}, \tag{8d}$$

and the gap is

$$\Delta_{\mathbf{k}}=\delta g_{\mathbf{k}\mathbf{k}}, \tag{8e}$$

and where $\tilde{E}_2=E_2+\lambda$ and $\varepsilon_d=E_1+\lambda$. The sum over n' is the typical Matsubara sum for fermions.

Equation (8) is solved for T_c and the results are compared with data[14] in Fig. 3, taking $U=5.9$ eV, which is in the usually quoted range. Incidentally, without the $\tilde{u}$, T_c will be much too high and since the value of $\tilde{u}$ here is explicitly determined by considering the appropriate graphs; one may further conclude that the theory presented here delineates the delicate balance between competing mechanisms in the superconducting phase of these high-T_c materials.

Next, to explore the width of the critical region around T_c, it is crucial to account for the three-dimensional nature of the electronic dispersion. We model it by $\varepsilon_{\mathbf{k}}=\varepsilon_{\mathbf{k}_\parallel}+\hbar^2k_z^2/2m_z$ where $|k_z|$ is terminated at the zone boundary $G_z/2$. Since the parallel mass $m\equiv(1/2\pi)\int dl/|\nabla\varepsilon(k)|$ is *much* smaller than m_z [$m_z/m\sim 80$ (Ref. 16)] the three-dimensional Fermi surface is almost cylindrical. With these simplifications we make a Landau-Ginsburg expansion of Eq. (4) in powers of the superconducting order parameters. We find the critical region to be given by

$$\left|\frac{T-T_c}{T_c}\right|<C(\epsilon)\gamma^{-2}\left[\frac{T_c}{\varepsilon_F}\left(\frac{\varepsilon_d^2+(\langle b\rangle V)^2}{\varepsilon_d^2}\right)^{1/2}\right]^4, \tag{9}$$

where $\varepsilon_F=\varepsilon(k_F)$, $\gamma^{-1}=(3/2)^{1/2}m_z/m$, and $\epsilon=4-d$. $C(\epsilon)$ is a universal constant which to order ϵ (with $\epsilon=1$) ~ 400. Inside this region, the specific-heat exponent $\alpha\sim\frac{1}{10}\epsilon=\frac{1}{10}$. Inserting values for the constants in (9), we obtain a value of about 1 K for the width of the critical region. This is in agreement with recent data.[16,17]

We conclude with the following remarks concerning the principal features of our results. (1) By considering a realistic ALH for these high-T_c materials and solving it with the $(1/N)$ expansion techniques using slave bosons, one can explain a number of normal-state properties like susceptibility, Hall coefficient, and the location of the added holes in the system. (2) The magnitude of T_c, its variation, and eventual saturation with doping can also be explained with our model. (3) Quantum fluctuations in the phase of the boson field b do not change the conclusions *qualitatively*, despite destroying the LRO of $\langle b\rangle$, because in the normal phase one may show via a gauge transformation[7] that only $\langle|b|\rangle$ is essential to form the Fermi-liquid state. (4) It is nevertheless desirable to investigate higher order in $1/N$ corrections, e.g., to the χ/γ ratio and to T_c. (5) In the limit of $x_h\to 0$, the ALH can naturally produce the observed antiferromagnetic structure.[18] Here then spin fluctuations must predominate.[1] Therefore, as x_h gets smaller, we expect stronger suppression of T_c than that illustrated in Fig. 3. The overall picture, however, is that we have achieved a substantial degree of agreement with the data using one or, at most, two adjustable parameters.

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