Progress in the Mean-field Green Function Solution of the Two-band Hubbard Model in Cuprates

Gh. Adam, S. Adam
e-mail: adamg@jinr.ru, Laboratory of Information Technologies, JINR, Dubna
DFT IFIN-HH, Magurele – Bucharest, 077125, Romania

1. The rigorous solution [1] of the generalized mean-field Green function of the standard Hamiltonian of the two-dimensional two-band Hubbard model in cuprates [2, 3] has allowed the proof, within this model [4, 5], of the spin-charge splitting conjectured by Anderson ([6] and references therein) to be of fundamental importance for the understanding of the complicated phase diagrams in these compounds.

Further investigations [7] evidenced the fact that the effects of the hopping on the energy spectrum should be finite at any doping rate both in hole-doped and electron-doped cuprates. The straightforward consequence was the renormalization of the hopping part of the Hamiltonian with a factor able to remove the spectrum infinities in the limit of zero doping.

Under the phenomenological assumption

$$H = H_0 + \chi_1\chi_2 H_h \qquad (1)$$

where H_0 and H_h denote the standard one-site and hopping contributions to the Hamiltonian respectively, and χ_1 and χ_2 denote the electron- and hole-doping rates respectively, the mean-field spectrum was calculated and some distinctive subtle effects evidenced by phase sensitive experiments [8] and optical spectra measurements [9] have been proved to follow [10] from the modified Hamiltonian (1).

2. In the formulation of the starting hypotheses of the model, the experiment plays the deciding role. There are five kinds of experimental data which are essential for the derivation of a consistent theoretical model.

2.1. *Crystal structure characterization* points to the occurrence of layered ternary perovskite structures, with an overwhelming contribution to the superconducting pairing coming from the CuO_2 planes.

Consequence: An effective two-dimensional (2D) model for the CuO_2 plane is requested.

2.2. *Existence of the Fermi surface* was undoubtedly evidenced, first by 2D-ACAR positron spectroscopy at the beginning of the nineties and then by ARPES and optical methods.

Consequence: The energy bands lying at or near the Fermi level are to be retained in the model.

2.3. *The charge-transfer insulator nature of the cuprates* occurs with the following relationship between the energy band parameters, $U > \Delta > W$.

Consequence 1: The hybridization results in the Zhang-Rice singlet subband.

Consequence 2: The Zhang-Rice singlet and the upper Hubbard subbands enter the simplest model.

Consequence 3: Since $\Delta \sim 2W$, the model is to be developed and solved in the strong correlation limit.

2.4. *Tightly bound electrons* in the metallic state.

Consequence 1: Occurrence of low density hopping conduction consisting of both fermion and boson (singlet) carriers.

Consequence 2: This asks for the Hubbard operator description of the system states.

2.5. *Occurrence of cuprate families* which are characterized by specific stoichiometric reference structures, doped with either holes or electrons.

Consequence 1: The doping parameter δ is essential in the theoretical description of the cuprates.

Consequence 2: The (δ, T) phase diagrams arise which have to be accounted for.

3. Other essential contributions to the right formulation of the model and derivation of the solution come from a number of abstractions, concepts, and facts.

3.1. *Abstraction* of the physical CuO_2 plane with doped electron states by a *doped effective spin lattice*. This is done by a one-to-one mapping from the copper sites inside the CuO_2 plane to the spins of the effective spin lattice. There are four possible spin states at each lattice site i in the effective spin lattice: $|0\rangle$ (vacuum), $|\sigma\rangle = |\uparrow\rangle$ and $|\bar{\sigma}\rangle = |\downarrow\rangle$ (single particle spin states inside the hole subband), and $|2\rangle = |\uparrow\downarrow\rangle$ (singlet state in the singlet subband).

The spin lattice constants equal a_x, a_y, the CuO_2 lattice constants.

The effective spin lattice is characterized by antiferromagnetic spin ordering at zero doping.

The doping of the electron states inside the CuO_2 plane is equivalent to the *creation of defects* inside the spin lattice, by spin vacancies and/or singlet states.

The occurrence of a hopping conductivity inside the spin lattice is a consequence of the doping. The hopping conductivity may consist either of single spin hopping (fermionic conductivity) or singlet hopping (bosonic conductivity).

3.2. *Concept*: The global description of the hopping conduction around a spin lattice site can be done by means of the Hubbard 1-forms [1].

3.3. *Fact*: The hopping induced energy correction effects are *finite* over the whole range of the doping parameter δ [7], hence appropriate boundary conditions are to be imposed in the limit of vanishing doping.

4. The energy spectrum of the Hamiltonian (1) was derived within the equation of motion technique for thermodynamic Green functions as first proposed by Plakida [11].

While the use of general symmetry properties (system invariance to the spin reversal, to the lattice translations and to the crystallographic point group transforms) has allowed [1] the derivation of a rigorous Green function solution, the formulation of the mean-field Green function solution in terms of the energy matrix [7] has allowed the derivation of the energy spectrum from a standard eigenvalue problem, having as consequences the proof of the need of the renormalization factor $\chi_1\chi_2$ in (1).

This resulted in rigorous derivation of the elements of the energy matrix and of the Green function matrix in the momentum-energy $(\mathbf{q},\omega)$-representation.

All the 16 matrix elements of the Green function share *a same denominator*, $\mathcal{D} \equiv \mathcal{D}(\mathbf{q},\omega) = I\omega - \widetilde{\mathcal{E}}_\sigma(\mathbf{q})$, with the following monic bi-quadratic dependence in ω:

$$\mathcal{D}(\mathbf{q},\omega) = (\omega^2 - u\omega + v)(\omega^2 + u\omega + v), \quad (2)$$

where u and v are *spin-independent quantities* detailed in [7]. The *zeros of* $\mathcal{D}(\mathbf{q},\omega)$, provide the *GMFA energy spectrum of the system*. In the *normal state*, the energy spectrum is given by the roots of the second order equation $\omega^2 - u\omega + v = 0$ solved previously [2] in the mean field approximation.

The explicite expressions are cumbersome and are referred to [7, 10]. Two important consequences are worth noting, however.

4.1. The anomalous contributions to the Green function and the energy matrix elements come exclusively from the hopping term H_h of (1).

– The *two-site* anomalous terms come from the singlet hopping conduction and involve the characteristic anomalous charge-charge correlations $\langle X_i^{02} N_j\rangle$ which can be shown rigorously to be mathematically equivalent to Cooper pair anomalous correlations.

– The *one-site* anomalous term which come from the hopping conduction and do contribute s-type pairing, *vanish identically* in tetragonal cuprate structures. However, in orthorhombic cuprate structures, such terms do bring a small anomalious s-type contribution to the pairing, in qualitative agreement with phase sensitive experiments [8].

4.2. There are two main results established from the study of the energy spectrum of the energy matrix.

(i) Hybridization of normal state energy levels *preserves the center of gravity* of the unhybridized levels.

(ii) Hybridization of superconducting state energy levels *displaces the center of gravity* of the unhybridized normal levels. The whole spectrum is displaced towards lower frequencies.

This feature of the cuprates predicted by the two-band Hubbard model is in agreement with the optical spectra measurements [9]. It points to a fundamentally different redistribution of the s[ectrum in the superconducting state, which is related to the occurrence of gapeless energy lines inside the two-dimensional Brillouin zone of the model.

References

[1] Gh. Adam, S. Adam: *Rigorous derivation of the mean field Green functions of the two-band Hubbard model of superconductivity*, J. Phys. A: Math. Theor., **40**, (2007) 11205–11219.

[2] N.M. Plakida, R. Hayn, J.-L. Richard: *Two-band singlet-hole model for the copper oxide plane*, Phys. Rev. B, **51**, (1995) 16599–16607.

[3] N.M. Plakida, L. Anton, S. Adam, Gh. Adam: *Exchange and spin-fluctuation mechanisms of superconductivity in cuprates*, Zh. Eksp. Teor. Fiz., **124**, (2003) 367–378; [Engl. transl., JETP **97**, (2003) 331–342].

[4] Gh. Adam, S. Adam: *Separation of the spin-charge correlations in the two-band Hubbard model of high-Tc superconductivity*, J. Opt. Adv. Mat., **10**, No. 7, (2008) 1666–1670.

[5] S. Adam, Gh. Adam: *Features of High-Tc Superconducting Phase Transitions in Cuprates*, Romanian Journ. Phys., **53**, No. 9–10 (2008) pp. 993–999.

[6] P.W. Anderson: *Sources of quantum protection in high-T_c superconductivity*, Science, **288**, (2000) 480–482.

[7] Gh. Adam, S. Adam: *Finiteness of the hopping induced energy corrections in cuprates*, Romanian Journ. Phys., **54**, No. 9-10 (2009).

[8] C.C. Tsuei and J.R. Kirtley, Phys. Rev. Lett., **85**, (2000) 182–185.

[9] H.J.A. Molegraaf, C. Presura, D. van der Marel, P.H. Kes, and M. Li, *Superconductivity-induced transfer of in-plane spectral weight in $Bi_2Sr_2CaCu_2O_{8+\delta}$*, Science, **295**, (2002) 2239–2241.

[10] Gh. Adam, S. Adam: *Mean field Green function solution of the two-band Hubbard model in cuprates*, Lecture at MMCP 2009, July 7–11, 2009, JINR-Dubna, to be published.

[11] N.M. Plakida: *Superconductivity in the two-band singlet-hole model for copper oxyde plane*, Physica C **282–287**, (1997) 1737–1738.