MODIFIED TWO-BAND TWO-DIMENSIONAL HUBBARD MODEL FOR THE DESCRIPTION OF THE HIGH CRITICAL TEMPERATURE SUPERCONDUCTING PHASE TRANSITION IN CUPRATES

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Abstract

A progress report on the development of numerical and rigorous solutions of the effective two-band two-dimensional Hubbard model of the high-temperature superconductivity in cuprates [N.M. Plakida et al., PRB 51, 16599 (1995)], within the equation of motion technique of the thermodynamic Green function approach, is given. Four important consequences of the rigorous mean-field solution are worth mentioning: (1) Occurrence, both in the normal and superconducting states, of the spin-charge separation, conjectured by P.W. Anderson on intuitive grounds. (2) Origin of the static *d*-wave pairing in the hopping singlet conduction. (3) Complete suppression of the *s*-type superconducting pairing by the crystal symmetry in square two-dimensional lattices and occurrence of a residual *s*-type term in rectangular lattices, in agreement with the experiment. (4) The energy band hybridization in the superconducting state points to an overall displacement of the energy spectrum toward lower energies, as pointed by very precise optical measurements.

1. Introduction

The present paper is a progress report on the development of a solution of the effective two-band two-dimensional Hubbard model of the high-temperature superconductivity in cuprates proposed by Plakida et al. [1], with special emphasis on the physics side rather than on technical mathematical details. The approach to the solution of the model in [1] was based on the equation of motion technique of the thermodynamic Green function (GF) [2], and a mean field (MF) GF solution was derived.

A generalization of the GF approach starting with a four-component Nambu operator [3] allows in principle the derivation of a solution for the superconducting phase as well. Such an undertaking, involving an approximate solution of the Dyson equation of the 4×4 GF matrix, evidenced [4] the capability of the model to generate both the exchange and the spin-fluctuation mechanisms of the superconductivity in cuprates. The exchange pairing, which is dominant and arises in the MF approximation was shown in [4] to originate in interband transitions among the Hubbard subbands and to be equivalent to the exchange pairing term involved in the simpler t-J model. A spin fluctuation pairing of the *d*-wave type, originating in interband transitions, was also found to arise beyond the MF approximation, as a purely many-body correlation term.

A solution of the Dyson equation of the normal state GF was reported in [5]. The essential role of the correlations, coming from electron scattering on the spin fluctuations induced by the kinematic interaction in the hole-doping case, was evidenced in the evaluation of the doping and temperature dependence of electron dispersions, spectral functions, the Fermi surface, and the

coupling constant λ. The agreement of the model predictions with the experimental data was found to be significantly improved provided the energy parameters entering the Hamiltonian are taken for adjustable phenomenological quantities.

The derivation of approximate numerical solutions of the effective two-band Hubbard model is usefully complemented by studies aimed at deriving rigorously properties of the GF matrix and of various correlation functions which follow from the system symmetries (crystalline ordering, spin reversal invariance) and the complicated algebra of the Hubbard operator set entering the model Hamiltonian [6-10].

The roots of the two-band Hubbard model stem from the experiment, which guided the derivation of the Hamiltonian of the model [1] from the broader *p-d* model [11, 12]. The discussion starts with a summary in Sec. 2, of the set of experimental data lying at the basis of the model. The easier derivation of consistent mathematical results also asks for a number of additional input items which are summarized in Sec. 3. The manifest Hermitian form of the Hamiltonian is written down in Sec. 4. Essentials of the MF solution of the GF matrix are given in Sec. 5. Physical consequences of the derived results are discussed in Sec. 6 and 7.

2. Experimental background of the model

Five kinds of experimental data are of interest:

1. *The crystal structure characterization*. All cuprates were found to be layered ternary perovskite structures, with an overwhelming contribution to the superconducting pairing coming from the CuO_2 planes (hence, the two-dimensional effective model, with the lattice constant parameters taken from experiment).

2. *The existence of the Fermi surface*, probed first by 2D-ACAR positron spectroscopy [13-15] and then by ARPES and optical methods [16] (hence, the energy bands lying at or near the Fermi level are to be retained in the model).

3. *The charge-transfer insulator nature of the cuprates* with the relationship between the energy band parameters, $U > \Delta > W$, where U is the Coulomb repulsion among the electrons, Δ denotes the interband energy gap given essentially by the *p-d* splitting within the CuO_2 plane, and W denotes the individual bandwidth. (Three direct consequences follow: the hybridization of the

p-d crystal field levels results in the Zhang-Rice singlet subband; the simplest 2D model is to be a two-band model, incorporating the Zhang-Rice singlet and the upper Hubbard subband; finally, since $\Delta \sim 2W$, the model is to be developed and solved in the strong correlation limit, hence it will exhibit the highest mathematical complexity.)

4. *The occurrence of tightly bound electrons in the metallic state*. (Two consequences: occurrence of a low density hopping conduction with both fermion and boson (singlet) carriers; the system states ask for the Hubbard operator description [17]).

5. *The occurrence of cuprate families*, each being characterized by a specific stoichiometric reference structure and a specific kind of doping with either holes or electrons. (Therefore, the doping parameter δ is essential in the theoretical description of the cuprates. (δ, T) phase diagrams arise which have to be accounted for within the theoretical model.)

3. Additional input items

Three additional input items, which do not follow from the experimental data, are

necessary for consistent or easier derivation of the theoretical results.

1. *The abstraction* of the physical CuO_2 plane with doped electron states by a *doped effective spin lattice*: is done by a one-to-one mapping from the copper sites inside the CuO_2 plane onto the spin states of an effective spin lattice. At each lattice site *i* of the effective spin lattice, there are four possible spin states: $|0\rangle$ (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 and a_y respectively, 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 direct consequence of the doping. The hopping conductivity consists both of single spin hopping (fermionic conductivity) and singlet hopping (bosonic conductivity).

2. The hopping induced energy correction effects are *finite* over the entire range of the doping parameter δ [9]. As a consequence, the energy spectrum inside a cuprate family is to go continuously into the energy band levels of the stoichiometric reference structure characterizing the limit of the vanishing doping.

3. *The global description of the hopping conduction around a spin lattice site* is done by means of the Hubbard 1-forms [6].

4. Model Hamiltonian

The originally derived model Hamiltonian of the 2D Hubbard model [l] was rewritten in terms of Hubbard 1-forms [6] and then put in locally manifest Hermitian form [9, 10]

$$H = H_0 + \rho H_h = \sum_i (h_{0,i} + \rho h_{h,i}), \quad h_{0,i}^{\dagger} = h_{0,i}, \quad h_{h,i}^{\dagger} = h_{h,i}, \tag{1}$$

with the single particle and hopping contributions at the spin lattice site *i* given, respectively, by

$$h_{0,i} = E_1 \sum_{\sigma} X_i^{\sigma\sigma} + E_2 X_i^{22}, \tag{2}$$

$$h_{h,i} = \frac{\mathrm{K}_{11}}{2} \sum_{\sigma} (\tau_{1,i}^{\sigma 0,0\sigma} - \tau_{1,i}^{0\sigma,\sigma 0}) + \frac{\mathrm{K}_{22}}{2} \sum_{\sigma} (\tau_{1,i}^{2\sigma,\sigma 2} - \tau_{1,i}^{\sigma 2,2\sigma}) +$$

$$+ \frac{\mathrm{K}_{21}}{2} \sum_{\sigma} 2\sigma [(\tau_{1,i}^{2\bar{\sigma},0\sigma} - \tau_{1,i}^{0\sigma,2\bar{\sigma}}) + (\tau_{1,i}^{\sigma 0,\bar{\sigma} 2} - \tau_{1,i}^{\bar{\sigma} 2,\sigma 0})]. \tag{3}$$

The Hubbard 1-forms define the hopping conduction neighbourhood of the lattice site *i*:

$$\tau_{1,i}^{\alpha\beta,\gamma\eta} = \sum_{m \neq i} \nu_{im} X_i^{\alpha\beta} X_m^{\gamma\eta}, \quad (\tau_{1,i}^{\alpha\beta,\gamma\eta})^{\dagger} = -\tau_{1,i}^{\beta\alpha,\eta\gamma} \tag{4}$$

The Hubbard operators for the initial and final spin states $|\alpha\rangle$ and $|\beta\rangle$, respectively, at the spin lattice site *i*, are defined as $X_i^{\alpha\beta} = |i\alpha\rangle \langle i\beta|$.

In (1), ρ implements boundary conditions at vanishing doping.

5. Rigorous mean field solution of Green function matrix

The retarded and advanced Green function (GF) matrices are defined in terms of Nambu operators in the space-time ($\vec{r}$, t)-representation [2]. Using the equations of motion of the involved Heisenberg operators, differential equations of motion are derived. In this representation, splittings of the higher order correlation functions are also done.

In the dual space-energy ($\vec{r}, \omega$)-representation obtained from the ($\vec{r}$, t)-representation by appropriate Fourier transforms, the differential equations of motion are transformed in algebraic equations of motion. Analytic extensions in the complex energy plane result in a unique GF in the complex plane. Calculations of statistical averages are done in this representation by the use of spectral theorems.

Performing one more Fourier transform from the space variable $\vec{r}$ to the momentum variable $\vec{q}$, we get the momentum-energy ($\vec{q}, \omega$)-representation. Within this representation, we get: compact functional GF expressions, equations for the energy spectra, statistical average calculations from spectral theorems, spectral distributions inside the Brillouin zone.

The Green function matrices of the model define space-time correlations for the four-component Nambu column operator [3, 4] $\hat{X}_{i\sigma} = (X_i^{\sigma 2} X_i^{0\bar{\sigma}} X_i^{2\bar{\sigma}} X_i^{\sigma 0})^{\mathrm{T}}$ (where the superscript T denotes the transposition) and its adjoint operator $\hat{X}_{j\sigma}^{\dagger} = (X_j^{2\sigma} X_j^{\bar{\sigma}0} X_j^{\bar{\sigma}2} X_j^{0\sigma})$.

To get a standard eigenvalue problem for the spectrum, the ($\vec{q}, \omega$)-representation of the generalized mean field approximation (GMFA) GF solution is written in terms of the *energy matrix* [9]

$$\tilde{G}_{\sigma}^{0}(\vec{q},\omega) = \tilde{\chi}^{\frac{1}{2}}[I\omega - \tilde{\mathcal{E}}_{\sigma}(\vec{q})]^{-1}\tilde{\chi}^{\frac{1}{2}}\ , \tag{5}$$

$$\tilde{\mathcal{E}}_{\sigma}(\vec{q}) = \tilde{\chi}^{-\frac{1}{2}}\tilde{A}_{\sigma}(\vec{q})\tilde{\chi}^{-\frac{1}{2}};\ \ \tilde{\chi} = \left\langle \{\hat{X}_{i\sigma}, \hat{X}_{i\sigma}^{\dagger}\} \right\rangle \tag{6}$$

$$\tilde{A}_{\sigma}(\vec{q}) = \sum_{\vec{r}_{ij}} e^{i\vec{q}\cdot\vec{r}_{ij}} \tilde{A}_{ij\sigma};\quad \vec{r}_{ij} = \vec{r}_j - \vec{r}_i\ ;\quad \tilde{A}_{ij\sigma} = \left\langle \{[\widehat{X}_{i\sigma}, H], \widehat{X}_{j\sigma}^{\dagger}\} \right\rangle\ .$$

The $\tilde{\chi}$ matrix is diagonal:

$$\tilde{\chi} = \begin{pmatrix} \hat{\chi} & \hat{0} \\ \hat{0} & \hat{\chi} \end{pmatrix},\quad \hat{\chi} = \begin{pmatrix} \chi_2 & 0 \\ 0 & \chi_1 \end{pmatrix},\quad \hat{0} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}. \tag{7}$$

The energy matrix can be written in the *block structure* form:

$$\tilde{\mathcal{E}}_{\sigma}(\vec{q}) = \begin{pmatrix} \hat{E}_{\sigma}(\vec{q}) & \hat{\Phi}_{\sigma}(\vec{q}) \\ (\hat{\Phi}_{\sigma}(\vec{q}))^{\mathrm{T}} & -(\hat{E}_{\bar{\sigma}}(\vec{q}))^{\mathrm{T}} \end{pmatrix}. \tag{8}$$

The normal and anomalous 2×2 energy matrices are obtained as follows

$$\hat{E}_{\sigma}(\vec{q}) = \begin{pmatrix} \omega_2 & 2\sigma\omega_{21} \\ 2\sigma\omega_{21} & \omega_1 \end{pmatrix},\quad \hat{\Phi}_{\sigma}(\vec{q}) = \begin{pmatrix} -2\sigma T_2 & T_{21} \\ -T_{21} & 2\sigma T_1 \end{pmatrix} \tag{9}$$

$$\omega_2 \equiv \omega_2(\vec{q}) = (E_1 + \Delta) + [a_{22} + d_{22}(\vec{q})]\cdot\rho_{22} \tag{10a}$$

$$\omega_1 \equiv \omega_1(\vec{q}) = E_1 + [a_{22} + d_{11}(\vec{q})]\cdot\rho_{11} \tag{10b}$$

$$\omega_{21} \equiv \omega_{21}(\vec{q}) = [a_{21} + d_{21}(\vec{q})]\cdot\rho_{21} \tag{10c}$$

$$T_2 \equiv T_2(\vec{q}) = [K_{22}b_1 + (1-\delta)\xi_1 b_2(\vec{q}) + \delta\xi_1 b_3(\vec{q})]\cdot\rho_{22} \tag{11a}$$

$$T_1 \equiv T_1(\vec{q}) = [K_{11}b_1 + (1-\delta)\xi_1 b_2(\vec{q}) + \delta\xi_1 b_3(\vec{q})]\cdot\rho_{11} \tag{11b}$$

$$T_{21} \equiv T_{21}(\vec{q}) = [K_{21}b_1 + (1-\delta)\xi_2 b_2(\vec{q}) + \delta\xi_2 b_3(\vec{q})]\cdot\rho_{21} \tag{11c}$$

$$\rho_{mn} = \rho/\sqrt{\chi_n\chi_m}\ , \quad \{mn\} \in \{22,11,21\}$$

where expressions for the r.h.s. terms were reported in [10].

6. Physical consequences of spin reversal invariance

(i) The average occupation numbers are independent on the spin projection σ and the site label *i*, $\langle n_{i\sigma}\rangle = \langle n_{i\bar{\sigma}}\rangle = \chi_2$, $\langle n^h_{i\sigma}\rangle = \langle n^h_{i\bar{\sigma}}\rangle = \chi_1 = 1-\chi_2$. At zero doping level in hole doped cuprates $\chi_1 = 1$, $\chi_2 = 0$, point to the fact that the hole subband is full, while the singlet subband is empty. Under a hole doping rate δ, $\chi_2 = \delta$, $\chi_1 = 1 - \delta$, and the chemical potential is shifted towards a new equilibrium value.

(ii) The one-site singlet destruction or creation processes result in identically vanishing statistical averages, $\langle X_i^{02}\rangle = \langle X_i^{20}\rangle = 0$, whence the diagonal form of the $\tilde{\chi}$ matrix (7).

(iii) The *normal one-site* matrix elements stemming from hopping result in renormalization corrections to the energy parameters E_1 and E_2 of (1).

The normal *intraband* hopping matrix element are independent on the spin projection σ and result in identical corrections a_{22} to E_1 and E_2.

The normal *interband* hopping matrix elements change sign under the spin reversal $\sigma \to \bar{\sigma}$. However, they result into *spin-projection-independent hybridization effects* of the hole and singlet subband energy levels.

(iv) The *anomalous one-site interband* hopping matrix elements vanish identically, whereas the *anomalous one-site intraband* ones satisfy the identity

$$\sum_\sigma 2\sigma\langle\tau_{1,i}^{0\bar{\sigma},0\sigma}\rangle = \sum_\sigma 2\sigma\langle\tau_{1,i}^{\sigma 2,\bar{\sigma}2}\rangle\,. \tag{12}$$

Within a square array, each average vanishes identically, while within a slightly deformed square array (like in YBCO cuprates) they are very small, but nonvanishing quantities [18].

(v) Both the normal and anomalous two-site terms stem from hopping processes. For any pair of lattice sites (*i*, *j*), they involve identically vanishing spin-charge correlations, $\langle N_i S_j^z\rangle = \langle N_i^h S_j^z\rangle = 0$, $\langle X_i^{02} S_j^z\rangle = 0$, $S_j^z = (X_j^{\sigma\sigma} - X_j^{\bar{\sigma}\bar{\sigma}})/2$. These identities point to the *spin-charge separation* [19] of the two-site correlation functions.

(vi) The *spin-independence* of the singlet-charge correlations following from $X_i^{02} n_{j\sigma} = X_i^{02} n_{j\bar{\sigma}}$, leads to a single characteristic two-site anomalous matrix element:

$$\chi_{ij}^{\text{pair}} = \upsilon_{ij}\langle N_j^h X_i^{02}\rangle \ \ (i \neq j)\,. \tag{13}$$

Since the singlet carries charge and no spin, (13) may be assumed to point to the occurrence of a static *charge-charge* correlation mechanism of superconductivity within model (1). The four-fermion anomalous and singlet hopping terms may be rigorously reduced to two-fermion expressions [6, 8].

7. GMFA energy spectrum

All the 16 matrix elements of the Green function (5) share *a same denominator*, $D \equiv D(\vec{q},\omega) = I\omega - \tilde{\mathcal{E}}_\sigma(\vec{q})$, with the following monic bi-quadratic dependence in ω:

$$D(\vec{q},\omega)=(\omega^2-u\omega+v)(\omega^2+u\omega+v)\,, \tag{14}$$

where u and v are *spin-independent quantities* detailed in [10]. The *zeros of* $D(\vec{q},\omega)$, provide the *GMFA energy spectrum of the system*.

7.1. Energy spectrum of the normal state. The spectral equation $(\omega^2-u_0\omega+v_0)=0$ has the coefficients given by $u_0=\omega_2+\omega_1$ and $v_0=\omega_2\omega_1-\omega_{21}^2$, respectively.

Its solutions are $\Omega_2^0=\omega_2+\beta_0$ for the upper subband and $\Omega_1^0=\omega_1-\beta_0$ for the lower subband respectively. The small parameter β_0 is given by

$$\beta_0=(D_0\eta_0/2)/(1+\sqrt{1+\eta_0})\,;\;\; \eta_0=(4\omega_{21}^2)/D_0^2;\;\; D_0=\omega_2-\omega_1.$$

7.2. Energy spectrum of the superconducting state. From factorization (14), it results that $\Omega_3=-\Omega_2$ and $\Omega_4=-\Omega_1$, with Ω_1 and Ω_2 obtained from the secular equation $(\omega^2-u\omega+v)=0$, where $v^2=v_0^2+\varphi \;\Rightarrow\; v=\sqrt{v_0^2+\varphi} \;\Rightarrow\; \delta v=v-v_0=\varphi/(v+v_0)$.

$u^2=u_0^2+2\delta v+\psi \;\Rightarrow\; u=\sqrt{u_0^2+2\delta v+\psi} \;\Rightarrow\; \delta u=u-u_0=(2\delta v+\psi)/(u+u_0)<0.$

The hybridization yields $\Omega_2=\Omega_2^0+\delta u/2+\beta_1$ and $\Omega_1=\Omega_1^0+\delta u/2-\beta_1$, where the small parameter β_1 is given by $\beta_1=(D_1\eta_1/2)/(1+\sqrt{1+\eta_1});\;\; \eta_1=(\psi-2\delta v)/D_1^2;\;\; D_1=\Omega_2^0-\Omega_1^0$.

In conclusion, there are two main results established from the study of the energy spectrum of energy matrix (8). (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, as pointed by very accurate optical measurements [20].

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