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Mean Field Green Function Solution of the Two-Band Hubbard Model in Cuprates

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The paper discusses the generalized mean field solution of the Green function matrix of the effective two-band two-dimensional Hubbard model of the high-T_c superconductivity in cuprates, as recently modified to include appropriate boundary conditions at zero doping. Two main results are found. (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.

Key words and phrases: high-T_c superconductivity, cuprates, two-band Hubbard model, Green function, mean field approximation.

1. Basic principles of the theoretical description of cuprates

The high critical temperature superconductivity in cuprates is still a puzzle of the today solid state physics, in spite of the unprecedented wave of interest and number of publications. The two-band two-dimensional Hubbard model [1–3] provides a description of it based on four basic principles:

(1) *Deciding role of the experiment.*
The derivation of reliable experimental data on various cuprate properties asks for manufacturing high quality samples, performing high-precision measurements by adequate experimental methods. The next section summarizes the wealth of data provided by experiment.
(2) *Hierarchical ordering* of the interactions inferred from data.
(3) *Derivation of the simplest model Hamiltonian* following from the Weiss principle, i.e., hierarchical implementation of the various interactions into the model.
(4) *Mathematical solution* by right quantum statistical methods which secure rigorous implementation of the existing physical symmetries and observe the principles of mathematical consistency and simplicity.

2. Experimental input to the theoretical model

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.

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2.2. *Existence of the Fermi surface* was undoubtedly evidenced, first by 2D-ACAR positron spectroscopy at the beginning of the nineties [4–6] and then by ARPES and optical methods [7].

Consequence: The energy bands lying at or nearest to 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 [8] 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. Input: abstractions, concepts, facts

Besides the straightforward inferences following from the experiment, a number of additional input items need consideration.

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 [9].

3.3. *Fact*: The hopping induced energy correction effects are *finite* over the whole range of the doping parameter δ [10], hence appropriate boundary conditions are to be imposed in the limit of vanishing doping.

4. Model Hamiltonian

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

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

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

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

$$h_{h,i} = \frac{\mathcal{K}_{11}}{2} \sum_{\sigma} \left(\tau_{1,i}^{\sigma 0,0\sigma} - \tau_{1,i}^{0\sigma,\sigma 0} \right) + \frac{\mathcal{K}_{22}}{2} \sum_{\sigma} \left(\tau_{1,i}^{2\sigma,\sigma 2} - \tau_{1,i}^{\sigma 2,2\sigma} \right) + \\ + \frac{\mathcal{K}_{21}}{2} \sum_{\sigma} 2\sigma \Big[\left(\tau_{1,i}^{2\bar{\sigma},0\sigma} - \tau_{1,i}^{0\sigma,2\bar{\sigma}} \right) + \left(\tau_{1,i}^{\sigma 0,\bar{\sigma} 2} - \tau_{1,i}^{\bar{\sigma} 2,\sigma 0} \right) \Big] .$$

The Hubbard 1-forms define the hopping conduction neighbourhood of i-th lattice site,

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

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

In (1), ρ implements boundary conditions at vanishing doping. This Hamiltonian serves to the definition of the quasi-particle spectrum and superconducting properties.

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 $(\mathbf{r}, t)$ representation [11]. 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 $(\mathbf{r}, \omega)$ representation, which is obtained from the $(\mathbf{r}, t)$-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 use of spectral theorems.

Performing one more Fourier transform from the space variable $\mathbf{r}$ to the momentum variable $\mathbf{q}$ we get the momentum-energy $(\mathbf{q}, \omega)$-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 [2, 3] $\hat{X}_{i\sigma} = (X_i^{\sigma 2} \ X_i^{0\bar{\sigma}} \ X_i^{2\bar{\sigma}} \ X_i^{\sigma 0})^{\top}$ and its adjoint operator $\hat{X}_{j\sigma}^{\dagger} = (X_j^{2\sigma} \ X_j^{\bar{\sigma}0} \ X_j^{\bar{\sigma}2} \ X_j^{0\sigma})$ (the superscript $\top$ denotes the transposition).

To get a standard eigenvalue problem for the spectrum, the $(\mathbf{q}, \omega)$-representation of the generalized mean field approximation (GMFA) GF solution is written in terms of the *energy matrix* [10],

$$\widetilde{G}_{\sigma}^{0}(\mathbf{q}, \omega) = \widetilde{\chi}^{1/2} \Big[I\omega - \widetilde{\mathcal{E}}_{\sigma}(\mathbf{q}) \Big]^{-1} \widetilde{\chi}^{1/2} \ , \tag{2}$$

$$\widetilde{\mathcal{E}}_{\sigma}(\mathbf{q}) = \widetilde{\chi}^{-1/2} \widetilde{\mathcal{A}}_{\sigma}(\mathbf{q}) \widetilde{\chi}^{-1/2} \ ; \quad \widetilde{\chi} = \langle \{ \hat{X}_{i\sigma}, \hat{X}_{i\sigma}^{\dagger} \} \rangle ,$$

$$\widetilde{\mathcal{A}}_{\sigma}(\mathbf{q}) = \sum_{\mathbf{r}_{ij}} \mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}_{ij}} \widetilde{\mathcal{A}}_{ij\sigma} \ ; \quad \mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i \ ; \widetilde{\mathcal{A}}_{ij\sigma} = \langle \{ [\hat{X}_{i\sigma}, H], \hat{X}_{j\sigma}^{\dagger} \} \rangle \ .$$

The $\widetilde{\chi}$ matrix is diagonal,

$$\widetilde{\chi} = \begin{pmatrix} \hat{\chi} & \hat{0} \\ \hat{0} & \hat{\chi} \end{pmatrix}, \quad \hat{\chi} = \begin{pmatrix} \chi_2 & 0 \\ 0 & \chi_1 \end{pmatrix}, \quad \hat{0} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix},$$

where $\chi_2 = \langle n_{i\sigma} \rangle = \langle n_{i\bar{\sigma}} \rangle$ and $\chi_1 = \langle n^h_{i\sigma} \rangle = \langle n^h_{i\bar{\sigma}} \rangle = 1 - \chi_2$ denote spin and site independent averages of particle number operators. In terms of the doping rate δ, it results that in the hole-doped cuprates, $\chi_2 = \delta,\ \chi_1 = 1-\delta$, while in the electron-doped cuprates, $\chi_1 = \delta,\ \chi_2 = 1 - \delta$.

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

$$\widetilde{\mathcal{E}}_\sigma(\mathbf{q}) = \begin{pmatrix} \hat{E}_\sigma(\mathbf{q}) & \hat{\Phi}_\sigma(\mathbf{q}) \\ (\hat{\Phi}_\sigma(\mathbf{q}))^\dagger & -(\hat{E}_{\bar{\sigma}}(\mathbf{q}))^\top \end{pmatrix}. \tag{3}$$

With the choice [10] $\rho = \chi_1\chi_2$, the normal and anomalous 2×2 energy matrices are obtained as follows

$$\hat{E}_\sigma(\mathbf{q}) = \begin{pmatrix} \omega_2 & 2\sigma\omega_{21} \cdot \sqrt{\chi_1\chi_2} \\ 2\sigma\omega^*_{21} \cdot \sqrt{\chi_1\chi_2} & \omega_1 \end{pmatrix},$$

$$\hat{\Phi}_\sigma(\mathbf{q}) = \begin{pmatrix} -2\sigma T_2 \cdot \chi_1 & T_{21} \cdot \sqrt{\chi_1\chi_2} \\ -T_{21} \cdot \sqrt{\chi_1\chi_2} & 2\sigma T_1 \cdot \chi_2 \end{pmatrix},$$

$$\begin{gathered} \omega_2 \equiv \omega_2(\mathbf{q}) = (E_1 + \Delta) + [a_{22} + d_{22}(\mathbf{q})] \cdot \chi_1, \\ \omega_1 \equiv \omega_1(\mathbf{q}) = E_1 + [a_{22} + d_{11}(\mathbf{q})] \cdot \chi_2, \\ \omega_{21} \equiv \omega_{21}(\mathbf{q}) = [a_{21} + d_{21}(\mathbf{q})], \\ T_2 \equiv T_2(\mathbf{q}) = \mathcal{K}_{22} b_1 + (1-\delta)\xi_1 b_2(\mathbf{q}) + \delta\xi_1 b_3(\mathbf{q}), \\ T_1 \equiv T_1(\mathbf{q}) = \mathcal{K}_{11} b_1 + (1-\delta)\xi_1 b_2(\mathbf{q}) + \delta\xi_1 b_3(\mathbf{q}), \\ T_{21} \equiv T_{21}(\mathbf{q}) = \mathcal{K}_{21} b_1 + (1-\delta)\xi_2 b_2(\mathbf{q}) + \delta\xi_2 b_3(\mathbf{q}), \end{gathered}$$

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

6. GMFA energy spectrum

All the 16 matrix elements of the Green function (2) 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:

$$\mathcal{D}(\mathbf{q}, \omega) = (\omega^2 - u\omega + v)(\omega^2 + u\omega + v), \tag{4}$$

where u and v are *spin-independent quantities* detailed in [10]. 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 [1] in the mean field approximation.

There are two main results established from the study of the energy spectrum of the energy matrix (3).

(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.

6.1. Energy spectrum of the normal state

The spectral equation $\omega^2 - u_0\omega + v_0 = 0$ has the coefficients given respectively by $u_0 = \omega_2 + \omega_1$ and $v_0 = \omega_2\omega_1 - \chi_1\chi_2|\omega_{21}|^2$.

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 satisfies the equation $\beta_0^2 + D_0\beta_0 - \chi_1\chi_2|\omega_{21}|^2 = 0$; $D_0 = \omega_2 - \omega_1$, wherefrom

$$\beta_0 = \big(D_0\eta_0/2\big)/\big(1 + \sqrt{1+\eta_0}\big) \ ; \quad \eta_0 = \big(4\chi_1\chi_2|\omega_{21}|^2\big)/D_0^2 \ .$$

6.2. Energy spectrum of the superconducting state

From the factorization (4), it results that $\Omega_3 = -\Omega_2$ and $\Omega_4 = -\Omega_1$, with Ω_2 and Ω_1 obtained from the secular equation $\omega^2 - u\omega + v = 0$, where

$$v^2 = v_0^2 + \varphi \quad \Rightarrow \quad v = \sqrt{v_0^2 + \varphi} \quad \Rightarrow \quad \delta v = v - v_0 = \varphi/(v + v_0).$$

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

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 satisfies the equation $\beta_1^2 + D_1\beta_1 + \delta v/2 - \psi/4 = 0$; $D_1 = \Omega_2^0 - \Omega_1^0$, wherefrom

$$\beta_1 = \big(D_1\eta_1/2\big)/\big(1 + \sqrt{1+\eta_1}\big) \ ; \quad \eta_1 = \big(\psi - 2\delta v\big)/D_1^2.$$

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Функции Грина для решения двухзонной модели Хаббарда в приближении среднего поля в купратах

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В работе рассматривается использование техники уравнения движения функций Грина для решения эффективной двухзонной модели Хаббарда высокотемпературной сверхпроводимости в приближении среднего поля в купратах, которая недавно была модифицирована авторами для включения надлежащих граничных условий при нулевом легировании. Получены два новых результата. 1. Гибридизация нормальных уровней состояния энергии сохраняет центр тяжести негибридизированных уровней. 2. Гибридизация энергетических уровней состояния сверхпроводимости смещает центр тяжести негибридизированных уровней. Весь спектр смещается в сторону более низких частот.

Ключевые слова: высокотемпературная сверхпроводимость, купраты, двухзонная модель Хаббарда, функции Грина, приближение среднего поля.