# GENERALIZED MEAN FIELD ENERGY SPECTRUM OF THE MODIFIED TWO-BAND HUBBARD MODEL IN CUPRATES

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The effective two-band two-dimensional Hubbard model of the high-$T_c$ superconductivity in cuprates, as recently modified to include appropriately the zero doping limit [Gh. Adam, S.Adam, Rom. Journ. Phys., **54,** no. 9–10, 797–814 (2009)], is rigorously solved within the generalized mean field approximation of the equation of motion of the Green function matrix. The energy spectra, derived both for the normal state and the superconducting state, are finite over the whole available range of the doping, irrespective of the kind of doping (with holes or with electrons) of the cuprate system. The hopping-induced hybridization of the *normal state energy levels* is found *to preserve the centre of gravity* of the unhybridized levels. However, the hopping-induced hybridization of the *superconducting state energy levels* at a given momentum **q** inside the Brillouin zone *displaces the centre of gravity* of the hybridized normal levels. This is consistent with the overall displacement of the energy spectrum of the superconducting state as found from very precise optical measurements.

## 1. INTRODUCTION

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] provides a description of it based on four basic principles:

(1) *Deciding role of the experiment* in the definition of the fundamental features of the cuprates.

(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.

In [2] the $4 \times 4$ Green function matrix defined for a suitable Nambu operator has been proposed, the equation of motion of which provides the approach to the solution of the superconducting state. Progress along this line was reported in [3], where it was first proved that the exchange superconducting mechanism found within the *t-J* model arises in the mean field approximation of the Green function solution, while an approximate solution of the Dyson equation adds the spin-fluctuation mechanism as a second source to the superconducting pairing.

The rigorous solution [4] of the generalized mean-field Green function of the standard Hamiltonian of the effective two-band Hubbard model was derived using the symmetry group properties which leave invariant the physical system (spin reversal, lattice translations, and discrete crystallographic point group transforms). This has allowed the recovery, within the model predictions [5, 6], of the P.W. Anderson's conjecture ([7] and references therein), concerning the spin-charge splitting in cuprates, which is of fundamental importance for the understanding of the phase diagrams in these compounds.

Further investigation [8] 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.

The present paper reports the derivation of the mean field energy spectrum of the modified two-band effective Hubbard model Hamiltonian proposed in [8]. The most important result is the finding that, in the superconducting state, the hopping-induced hybridization leads to the displacement of the centre of gravity of the hybridized normal levels at every momentum **q** inside the Brillouin zone, such that the whole spectrum is displaced toward the lower energies, in agreement with very precise optical data [9].

The sections 2 and 3 summarize the experimental data, respectively the general abstractions, concepts, and facts underlying the model. The modified model Hamiltonian is written down in section 4 and a sketch of the Green function approach is given in section 5. The generalized mean field (GMFA) energy spectrum is derived in section 6, followed by conclusions in section 7.

## 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.

1. *The 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.

As a consequence, an effective two-dimensional (2D) model for the $CuO_2$ plane is requested. The lattice constants of the 2D model, which are taken from the experiment, define the specificity of a particular compound.

2. *The existence of the Fermi surface* was undoubtedly evidenced, first by 2D-ACAR positron spectroscopy [10]–[12] and then by ARPES and optical methods [13]. Therefore, 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* was evidenced, with $U > \Delta > W$ describing the relationship between the energy band parameters, where $W$ denotes the individual bandwidth, $\Delta$ denotes the interband energy gap given essentially by the *p-d* splitting within the $CuO_2$ plane, and $U$ is the Coulomb repulsion among the electrons.

This property has three direct consequences. First, the hybridization results in the Zhang-Rice singlet subband. Second, the simplest 2D model is to be a two-band model, incorporating the Zhang-Rice singlet and the upper Hubbard subband. Third, 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.

First, this property points to the occurrence of a low density hopping conduction consisting of both fermion and boson (singlet) carriers. Second, it asks for the Hubbard operator description [14] of the system states.

5. *The occurrence of cuprate families* characterized by specific stoichiometric reference structures, doped with either holes or electrons.

This property shows that the doping parameter $\delta$ is essential in the theoretical description of the cuprates. Therefore, $(\delta, T)$ phase diagrams arise which have to be accounted for within the theoretical model.

## 3. ABSTRACTIONS, CONCEPTS, FACTS

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

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 consists both of single spin hopping (fermionic conductivity) and singlet hopping (bosonic conductivity).

2. *Concept:* The global description of the hopping conduction around a spin lattice site can be done by means of the Hubbard 1-forms [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 $X_i^{\alpha\beta} = |i\alpha\rangle \langle i\beta|$.

A Hubbard 1-form defines the hopping conduction neighbourhood of the lattice site $i$,

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

The actual labels ($\alpha\beta$, $\gamma\eta$) are defined by the available in-band or inter-band hopping transitions within the effective spin lattice.

Projection techniques based on cell-cluster perturbation theory [15]-[17] showed that the relative intensity of the hopping process relating the sites $i$ and $m$ of the spin lattice is determined by the non-vanishing Wannier coefficient $v_{im}$ following from the overlap of the wave functions of the $d$-copper and $p$-oxygen states. The coefficients $v_{im}$ show (non-exponential) decrease with the distance $r_{im} = |\mathbf{r}_m - \mathbf{r}_i|$ in between the sites $i$ and $m$. Significantly different from zero are the Wannier coefficients within the first three coordination spheres around a given reference site $i$. An instance of typical values for a square lattice is [1,18]: for the nearest neighbouring (nn) $m$-sites (the first coordination sphere), $v_{im} \sim v_1 = 0.14$; for the next nearest neighbouring (nnn) $m$-sites (the second coordination sphere), $v_{im} \sim v_2 = -0.13v_1$, while for the $m$-sites located at the third coordination sphere, $v_{im} \sim v_3 = 0.16v_1$.

3. *Fact*: The hopping induced energy correction effects are *finite* over the whole range of the doping parameter $\delta$ [8], hence the energy spectrum is to go continuously into the energy band structure characterizing the stoichiometric reference structure obtained in the limit of the vanishing doping.

## 4. MODEL HAMILTONIAN

The model Hamiltonian of the 2D Hubbard model serves to the definition of the quasi-particle spectrum and superconducting properties. The originally derived expression [1], called in what follows the standard Hamiltonian of the model, was

rewritten in terms of Hubbard 1-forms [4] and then put in locally manifest Hermitian form [8]

$$H = H_0 + \rho H_h = \sum_i \left( h_{0,i} + \rho h_{h,i} \right), \quad h_{0,i}^\dagger = h_{0,i}, \quad h_{h,i}^\dagger = h_{h,i}. \tag{2}$$

Here, $\rho$ implements boundary conditions at vanishing doping. The summation label $i$ runs over the sites of an infinite two-dimensional spin lattice with the lattice constants $a_x$ and $a_y$ respectively defined by the crystal structure of the cuprate.

The expressions of the single particle, $h_{0,i}$, and hopping, $h_{h,i}$, terms at the lattice site $i$ involve sums over the spin projection σ, the values of which are $\sigma = \pm 1/2$, $\bar{\sigma} = -\sigma$.

The single particle term at site $i$ is given by

$$h_{0,i} = E_1 \sum_\sigma X_i^{\sigma\sigma} + E_2 X_i^{22}, \tag{3}$$

Here, $E_1 = \tilde{\varepsilon}_d - \mu$ denotes the hole subband energy for the renormalized energy $\tilde{\varepsilon}_d$ of a $d$-hole and the chemical potential $\mu$. The energy parameter of the singlet subband is $E_2 = 2E_1 + \Delta$, where $\Delta \approx \Delta_{pd} = \varepsilon_p - \varepsilon_d \simeq 2eV$ is an effective Coulomb energy $U_{eff}$ corresponding to the difference between the two energy levels of the model.

The hopping term at site $i$ is given in terms of Hubbard 1-forms (1),

$$h_{h,i} = \frac{\mathcal{K}_{11}}{2} \sum_\sigma \left( \tau_{1,i}^{\sigma 0,0\sigma} - \tau_{1,i}^{0\sigma,\sigma 0} \right) + \frac{\mathcal{K}_{22}}{2} \sum_\sigma \left( \tau_{1,i}^{2\sigma,\sigma 2} - \tau_{1,i}^{\sigma 2,2\sigma} \right) +$$
$$+ \frac{\mathcal{K}_{21}}{2} \sum_\sigma 2\sigma \left[ \left( \tau_{1,i}^{2\bar{\sigma},0\sigma} - \tau_{1,i}^{0\sigma,2\bar{\sigma}} \right) + \left( \tau_{1,i}^{\sigma 0,\bar{\sigma} 2} - \tau_{1,i}^{\bar{\sigma} 2,\sigma 0} \right) \right]. \tag{4}$$

The hopping energy parameters $\mathcal{K}_{ab} = 2t_{pd}K_{ab}$ ($a, b = 1, 2$) depend on $t_{pd}$, the hopping $p$-$d$ integral, and on energy band dependent form factors $K_{ab}$. The label 1 points to the hole subband, while 2 to the singlet subband.

### 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 [19]. 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 **r** to the momentum variable **q** we get the momentum-energy (**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 GF matrices of the model, $\tilde{G}_{ij\sigma}\left(t-t'\right)$, define space-time correlations for the four-component Nambu column operator $\hat{X}_{i\sigma}=\left(X_i^{\sigma 2}\,X_i^{0\bar{\sigma}}\,X_i^{2\bar{\sigma}}\,X_i^{\sigma 0}\right)^{\top}$ [2, 3] (where the superscript $\top$ denotes the transposition) and its adjoint operator $\hat{X}_{j\sigma}^{\dagger}=\left(X_j^{2\sigma}\,X_j^{\bar{\sigma}0}\,X_j^{\bar{\sigma}2}\,X_j^{0\sigma}\right)$.

To get a standard eigenvalue problem for the spectrum, the GF solution obtained in the generalized mean field approximation (GMFA) is written in the (**q**,$\omega$)-representation in terms of the *energy matrix* [8],

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

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

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

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

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

where $\chi_2=\left\langle n_{i\sigma}\right\rangle=\left\langle n_{i\bar{\sigma}}\right\rangle$ and $\chi_1=\left\langle n_{i\sigma}^h\right\rangle=\left\langle n_{i\bar{\sigma}}^h\right\rangle=1-\chi_2$ 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,

$$\tilde{\mathcal{E}}_\sigma\left(\mathbf{q}\right)=\begin{pmatrix}\hat{E}_\sigma\left(\mathbf{q}\right)&\hat{\Phi}_\sigma\left(\mathbf{q}\right)\\\left(\hat{\Phi}_\sigma\left(\mathbf{q}\right)\right)^{\dagger}&-\left(\hat{E}_{\bar{\sigma}}\left(\mathbf{q}\right)\right)^{\top}\end{pmatrix}.\tag{8}$$

In what follows we denote

$$\rho_{mn} = \rho / \sqrt{\chi_m \chi_n} \quad \{mn\} \in \{22, 11, 21\}. \tag{9}$$

The normal $2 \times 2$ energy matrix is given by

$$\hat{E}_\sigma(\mathbf{q}) = \begin{pmatrix} \omega_2 & 2\sigma\omega_{21} \\ 2\sigma\omega_{21}^* & \omega_1 \end{pmatrix} \tag{10}$$

Here $\omega_2$ denotes the hopping renormalized energy of the singlet subband, $\omega_1$ denotes the hopping renormalized energy of the hole subband, while $\omega_{21}$ is the hybridization energy. They are $\mathbf{q}$-dependent quantities,

$$\omega_2 \equiv \omega_2(\mathbf{q}) = (E_1 + \Delta) + [a_{22} + d_{22}(\mathbf{q})] \cdot \rho_{22} \tag{11}$$

$$\omega_1 \equiv \omega_1(\mathbf{q}) = E_1 + [a_{22} + d_{11}(\mathbf{q})] \cdot \rho_{11} \tag{12}$$

$$\omega_{21} \equiv \omega_{21}(\mathbf{q}) = [a_{21} + d_{21}(\mathbf{q})] \cdot \rho_{21} \tag{13}$$

The quantities $a_{mn}$ and $d_{mn}(\mathbf{q})$ denote respectively the one-site and two-site contributions to the matrix $\tilde{\mathcal{A}}_\sigma(\mathbf{q})$ coming from the *hopping Hamiltonian* (4):

$$a_{22} = \mathcal{K}_{11} \left\langle \tau_1^{0\bar\sigma, \bar\sigma 0} \right\rangle - \mathcal{K}_{22} \left\langle \tau_1^{\sigma 2, 2\sigma} \right\rangle, \tag{14}$$

$$a_{21} = \left(\mathcal{K}_{11} - \mathcal{K}_{22}\right) \cdot 2\sigma \left\langle \tau_1^{\sigma 2, \bar\sigma 0} \right\rangle + \mathcal{K}_{21} \left( \left\langle \tau_1^{0\bar\sigma, \bar\sigma 0} \right\rangle - \left\langle \tau_1^{\sigma 2, 2\sigma} \right\rangle \right), \tag{15}$$

$$d_{22}(\mathbf{q}) = \mathcal{K}_{22} \left[ \chi^S(\mathbf{q}) + \chi_2^2 \chi^0(\mathbf{q}) \right] - \mathcal{K}_{11} \chi^{s-h}(\mathbf{q}). \tag{16}$$

$$d_{11}(\mathbf{q}) = \mathcal{K}_{11} \left[ \chi^S(\mathbf{q}) + \chi_1^2 \chi^0(\mathbf{q}) \right] - \mathcal{K}_{22} \chi^{s-h}(\mathbf{q}). \tag{17}$$

$$d_{21}(\mathbf{q}) = \mathcal{K}_{21} \left[ \chi^S(\mathbf{q}) - \chi_1 \chi_2 \chi^0(\mathbf{q}) \right] - \mathcal{K}_{21} \chi^{s-h}(\mathbf{q}). \tag{18}$$

In (14) and (15) the statistical averages are taken over Hubbard 1-forms, Eq. (1). In (16)–(18) the quantities $\chi^S(\mathbf{q})$, $\chi^0(\mathbf{q})$, and $\chi^{s-h}(\mathbf{q})$ denote the discrete Fourier transforms of the corresponding direct space quantities,

$$\chi_{ij}^S = \left(1 - \delta_{ij}\right) v_{ij} \left\langle \mathbf{S_i S_j} \right\rangle \cdot \rho \tag{19}$$

$$\chi_{ij}^0 = \left(1 - \delta_{ij}\right) v_{ij} \cdot \rho \tag{20}$$

$$\chi_{ij}^{s-h} = \left(1 - \delta_{ij}\right) v_{ij} \left\langle X_i^{02} X_j^{20} \right\rangle \cdot \rho \tag{21}$$

**Proposition 1**. *The matrix element* $\langle X_i^{\sigma 2} X_j^{\bar\sigma 0} \rangle$ *is real.*

The proof makes use of the fact that hopping matrix element $\langle X_i^{02}\, X_j^{20} \rangle$ is real and uses for $\langle X_i^{02}\, X_j^{20} \rangle$ and $\langle X_i^{02}\, X_j^{20} \rangle^*$ the result of the order reduction procedure developed in [4].

**Corollary 1.** *The quantity $\omega_{21}(\mathbf{q})$, Eq. (13) is real, hence the normal $2 \times 2$ energy matrix $\hat{E}_\sigma\ (\mathbf{q})$, Eq.(10) is* symmetric.

**Remark 1.** *In the expressions (16)–(18) of the two-site hopping contribution to the normal energy matrix (10) use was made of the* spin-charge separation *of the two-site normal correlation functions which was explicitly written down in [5, 6].*

The anomalous $2 \times 2$ energy matrix is given by

$$\hat{\Phi}_\sigma\left(\mathbf{q}\right) = \begin{pmatrix} -2\sigma T_2 & T_{21} \\ -T_{21} & 2\sigma T_1 \end{pmatrix} \tag{22}$$

$$T_2 \equiv T_2(\mathbf{q}) = [\,\mathcal{K}_{22}b_1 + (1-\delta)\,\xi_1 b_2\,(\mathbf{q}) + \delta\xi_1 b_3(\mathbf{q})]\cdot\rho_{22} \tag{23}$$

$$T_1 \equiv T_1(\mathbf{q}) = [\,\mathcal{K}_{11}b_1 + (1-\delta)\,\xi_1 b_2\,(\mathbf{q}) + \delta\xi_1 b_3(\mathbf{q})]\cdot\rho_{11} \tag{24}$$

$$T_{21} \equiv T_{21}(\mathbf{q}) = [\,\mathcal{K}_{21}b_1 + (1-\delta)\,\xi_2 b_2\,(\mathbf{q}) + \delta\xi_2 b_3(\mathbf{q})]\cdot\rho_{21} \tag{25}$$

where expressions for the r.h.s. terms have been reported in [8].

**Remark 2.** *In the expressions (23)–(25) of the two-site hopping contribution to the anomalous energy matrix (22) explicit use was made of the identity* $\left\langle X_i^{02} S_j^z \right\rangle = 0,\ \ S_j^z = \left( X_j^{\sigma\sigma} - X_j^{\bar\sigma\bar\sigma} \right)/2,$ *describing the* spin-charge separation *of the two-site anomalous correlation functions which follows from the spin reversal invariance of the two-dimensional spin lattice [4].*

## 6. GMFA ENERGY SPECTRUM

All the 16 matrix elements of the Green function (5) share *a same denominator*, $D \equiv D(\mathbf{q},\omega) = I\omega - \tilde{\mathcal{E}}_\sigma(\mathbf{q})$, with the following monic bi-quadratic dependence in $\omega$ [4],

$$D\,(\mathbf{q},\omega) = (\omega^2 - u\omega + \upsilon)(\omega^2 + u\omega + \upsilon), \tag{26}$$

where $u$ and $\upsilon$ are *spin-independent quantities* which will be detailed below. The *zeros of $D(\mathbf{q},\omega)$*, 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 $\omega^2 - u\omega + \upsilon = 0$ solved previously [1] in the mean field approximation.

### 6.1. ENERGY SPECTRUM OF THE NORMAL STATE

The spectral equation

$$\omega^2 - u_0\omega + \upsilon_0 = 0 \tag{27}$$

has the coeffcients given respectively by

$$u_0 = \omega_2 + \omega_1 \tag{28}$$

$$\upsilon_0 = \omega_2\omega_1 - \omega_{21}^2. \tag{29}$$

The solutions of the spectral equation (27) provide the hybridization effect induced by the hopping on the upper and lower subbands of the model:

$$\Omega_2^0 = \omega_2 + \beta_0 \tag{30}$$

$$\Omega_1^0 = \omega_1 - \beta_0 \tag{31}$$

The small parameter $\beta_0$ satisfies the equation

$$\beta_0^2 + D_0\beta_0 - \omega_{21}^2 = 0; \quad D_0 = \omega_2 - \omega_1 \approx \Delta, \tag{32}$$

where from the numerically well-conditioned for $\beta_0$ follows as

$$\beta_0 = \frac{D_0\eta_0/2}{1 + \sqrt{1 + \eta_0}}; \quad \eta_0 = \left[\frac{2\omega_{21}}{D_0}\right]^2. \tag{33}$$

**Remark 3.** *We have* $\Omega_2^0 + \Omega_1^0 = \omega_2 + \omega_1$, *hence the hopping induced hybridization of the normal state levels* preserves the centre of gravity *of the unhybridized levels.*

### 6.2. ENERGY SPECTRUM OF THE SUPERCONDUCTING STATE

From the factorization (26), it results that $\Omega_3 = -\Omega_2$ and $\Omega_4 = -\Omega_1$, with $\Omega_2$ and $\Omega_1$ obtained from the secular equation

$$\omega^2 - u\omega + \upsilon = 0. \tag{34}$$

Numerically well-conditioned forms of the coefficients $u$ and $\upsilon$ are

$$\upsilon^2 = \upsilon_0^2 + \varphi \;\Rightarrow\; \upsilon = \sqrt{\upsilon_0^2 + \varphi} \;\Rightarrow\; \delta\upsilon = \upsilon - \upsilon_0 = \varphi/(\upsilon + \upsilon_0).$$
$$u^2 = u_0^2 + 2\delta\upsilon + \psi \;\Rightarrow\; u = -\sqrt{u_0^2 + 2\delta\upsilon + \psi} \tag{35}$$
$$\Rightarrow\; \delta u = u - u_0 = (2\delta\upsilon + \psi)/(u + u_0).$$

The quantities $\varphi$ and $\psi$ are expressed in terms of the anomalous matrix elements (23)–(25) as follows:

$$\psi = |T_2|^2 + 2|T_{21}|^2 + |T_1|^2 \tag{36}$$

$$\varphi = \omega_1^2 \mid T_2 \mid^2 + 2\omega_1\omega_2 \mid T_{21} \mid^2 + \omega_2^2 \mid T_1 \mid^2 - 4\omega_{21}\left[\omega_1\Re\left(T_2^* T_{21}\right) + \omega_2\Re\left(T_1 T_{21}^*\right)\right] +$$
$$+ 2\omega_{21}^2\left[\Re\left(T_1 T_2^*\right) + \mid T_{21} \mid^2\right] + \mid T_1 T_2 - T_{21}^2 \mid^2 . \tag{37}$$

Since $u \to u_0$ as the doping rate $\delta \to 0$, the quantities $u$ and $u_0$ should have the same sign. This imposes the minus sign in the expression of $u$, Eq. (35).

The equation (34) has always real roots since its discriminant, which equates $\left(\omega_2 - \omega_1\right)^2 + 4\omega_{21}^2 - 2\delta\upsilon + \psi,$ is non-negative at any momentum $\mathbf{q}$ inside the Brillouin zone.

The solutions of the spectral equation (34) provide the hybridization effect induced by the hopping on the upper and lower subbands of the model in the superconducting state:

$$\Omega_2 = \Omega_2^0 + \delta u / 2 + \beta_1 \tag{38}$$

$$\Omega_1 = \Omega_1^0 + \delta u / 2 - \beta_1 . \tag{39}$$

The small parameter $\beta_1$ satisfies the equation

$$\beta_1^2 + D_1\beta_1 + \delta\upsilon / 2 - \psi / 4 = 0; \quad D_1 = \Omega_2^0 - \Omega_1^0 \approx \Delta . \tag{40}$$

where from the numerically well-conditioned for $\beta_1$ follows as

$$\beta_1 = \frac{D_1\eta_1 / 2}{1 + \sqrt{1 + \eta_1}}; \quad \eta_1 = \frac{\psi - 2\delta\upsilon}{D_1^2} . \tag{41}$$

**Remark 4.** *From the equations (38) and (39) it follows that the hybridization of the superconducting state energy levels* displaces the centre of gravity *of the hybridized normal levels. Since the above discussion shows that $\delta u < 0$ everywhere inside the Brillouin zone, this displacement points to an* overall shift of the superconducting state spectrum toward lower energies. *This result is consistent with very accurate optical spectra measurements [9].*

## 7. DISCUSSION AND CONCLUSIONS

The basic experimental data and concepts following from the investigation of the cuprates have been reviewed. The present investigation started with the renormalization of the hopping part of the two-band two-dimensional Hubbard model of the superconductivity in cuprates [1], as recently discussed in [8]. For the sake of generality, the phenomenological renormalizing factor entering the hopping part of the modified two-band Hubbard model Hamiltonian was left as a free parameter. It was simply required to result in finite energy spectra for all the

cuprate phases, in particular the antiferromagnetic phase exhibited by the stoichiometric reference structure at zero doping.

The energy spectrum following from the generalized mean field solution of the thermodynamic Green function matrix of the model was solved from the energy matrix (8). There are two main results established by this study.

(i) The hybridization of the normal state energy levels *preserves the centre of gravity* of the unhybridized levels.

(ii) The hybridization of the superconducting state energy levels *displaces the centre of gravity* of the hybridized normal levels. The whole spectrum is displaced towards lower frequencies in agreement with very sensitive optical spectra measurements [9].

These results add to the previously established ones within the effective two-band Hubbard model: the spin-charge separation of the normal and anomalous correlations conjectured by Anderson to be a fundamental feature of the cuprates [7], the intimate connection of the origin of the anomalous pairing with the singlet hopping conductivity in these compounds [5, 6], the kinetic nature of the anomalous pairing, with a small admixture of static anomalous pairing in orthorhombic compounds, as evidenced by very subtle phase sensitive experiments [20].

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