

Separation of the spin-charge correlations in the two-band Hubbard model of high- T_c superconductivity

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The scrutiny of the complete mean field Green function solution [1] of the effective two-dimensional two-band Hubbard model of the high- T_c superconductivity in cuprates [2] unveils three important features of this model. (i) While the conjecture of the spin-charge separation in cuprates, repeatedly stressed by P.W. Anderson, is at variance with the existence of the Fermi surface in these compounds, the main findings of the present investigation point towards its actual occurrence and to an alternative explanation. (ii) The two-band Hubbard model recovers the superconducting state as a result of the minimization of the kinetic energy of the system, in agreement with ARPES data. (iii) The anomalous pairing correlations may be consistently reformulated in terms of localized Cooper pairs both for the hole-doped and the electron-doped cuprates.

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1. Introduction

The present paper is devoted to the discussion of the spin-charge separation relevance of some recently reported results [1] on an effective two-band Hubbard model of the high- T_c superconductivity in cuprates [2].

The spin-charge separation is known to be a dimensionality induced effect on the behaviour of the systems of interacting fermions. In three-dimensional systems, the occurrence of the interaction does not result in fundamental change of the single particle behaviour. Central to the Fermi-liquid theory describing this case is the preservation of the Fermi surface concept emerging from the Fermi exclusion principle for non-interacting fermions. The low-energy particle and hole excitations retain the key single particle features.

At the contrary, in the one-dimensional and quasi-one-dimensional systems of interacting fermions the Fermi surface concept does not survive. Only collective many-body excitations are present within this new state of the matter, called a Luttinger liquid. The collective modes of a Luttinger liquid separate into spin ("spinon") and charge ("holon") sectors that propagate with different collective-mode velocities. In the limit of very strong interactions, an even more puzzling behaviour, the spin-incoherent Luttinger liquid occurs [3].

The lamellar structure of the high- T_c cuprates has pointed to a quasi-two-dimensional behaviour, within which the CuO_2 planes play the essential role. While there are no general reasons to assume the failure of the Fermi surface concept in the two-dimensional case, in an early paper on high- T_c , arguing that the cuprates are essentially Mott-Hubbard insulators, Anderson [4] conjectured the

occurrence of the spin-charge separation as a basic feature of these systems. Later on, the scrutiny of the accumulated evidence offered him further heuristic arguments concerning the role of the spin-charge separation in the understanding of the various phases of the high- T_c cuprates [5]. During the two decades elapsed since its first formulation by Anderson, the spin-charge separation scenario has become the source of various "spinon-holon", "fractionalization", etc., theoretical models of the high- T_c superconductivity in cuprates.

The motivation for the derivation of the effective two-band Hubbard model [2] was quite different. We may trace its origins in another Anderson's idea in his paper [4], namely that the essential physics of the cuprates would be captured by a one-band Hubbard model.

Technically, however, the two-band Hubbard model emerged as a simplification of the more comprehensive p - d model [6], using a reduction procedure based on cell-cluster perturbation theory [7,8], consistent with the basic features evidenced by the study of the high- T_c cuprates (see, e.g., [9] for a review): (i) the occurrence of the Fermi surface in cuprates is a firmly established experimental fact; (ii) the cuprates are, in fact, charge-transfer insulators [11], which are characterized by a strong antiferromagnetic interaction inside the CuO_2 planes, while showing different band splittings in comparison with the Mott-Hubbard insulators; (iii) the nearest to the Fermi level stay the upper Hubbard band (single particle copper $d_{x^2-y^2}$ states) and the Zhang-Rice singlet (doubly occupied states in the direct space, generated [12] by a specific hierarchy of the ion-ion interactions); (iv) the cuprates exhibit hopping conduction, with an extremely low density of the free charge carriers.

Therefore, Plakida et al. [2] concluded that the simplification of the p - d model should retain precisely the abovementioned two band contributions to an effective Hamiltonian formulated in terms of Hubbard operators.

Using the equation of motion method for thermodynamic Green functions (GF) [13], the effective two-band Hubbard model was shown [14] to generate both the exchange and the spin fluctuation mechanisms currently assumed to result in superconducting pairing in cuprates and to be able [15] to produce electronic spectra of the normal state in agreement with ARPES data.

In [1] we derived the complete GF solution of the effective two-band Hubbard model within the generalized mean field approximation (GMFA), based on the rigorous implementation of consequences following both from the system symmetries (the invariance to translations and to spin reversal) and from the Hubbard operator algebra. This investigation has evidenced the existence of invariance properties of several statistical averages, as well as the exact vanishing of other ones. These results will be shown in this paper to shed new light on the spin-charge separation conjectured by P.W. Anderson.

The spin-charge correlation functions associated to normal hopping processes are found to vanish identically, while the GMFA pairing shows a unique correlation function relating the singlet destruction/creation processes with the surrounding charge density. This charge-charge pairing mechanism is shown to be equivalent to the occurrence of doping related correlations of Cooper pairs which are localized inside the hopping radius around the singlet destruction/creation event. Therefore, a kinetic energy minimization process is responsible for the occurrence of the superconducting phase inside the model, in agreement with ARPES data [9,10].

The paper is organized as follows. The Hamiltonian of the model is described in Sec. II. The main results of the GMFA-GF solution of the model are collected in Sec. III. The occurrence of doping related localized Cooper pairs is discussed in Sec. IV. The concluding section V summarizes the main results and points to open questions.

2. Model hamiltonian

The individual constituents of the model are quasi-particles (holes) that are quasi-localized at the sites i of an infinite two-dimensional array, the lattice constants of which, a_x and a_y , are defined by those of the underlying CuO₂ plane of the crystal lattice. In [2], a square array ($a_x=a_y=a=1$) was assumed. For the 123 compounds, the array is a rectangle which is very slightly different from a square ($|a_x-a_y|/\max(a_x,a_y) \leq 1$).

Significant simplification of the algebraic calculations asked by the derivation of the GMFA-GF solution was obtained [1] through the definition of the Hubbard 1-forms of labels ($\alpha\beta, \gamma\eta$),

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

The Hubbard 1-form (1) carries, at the site i , the overall effect of the hopping processes described by the pair of Hubbard operators ($X_i^{\alpha\beta}, X_m^{\gamma\eta}$) at the lattice sites (i, m) related by non-vanishing hopping parameters ν_{im} . Since the numerical coefficients ν_{im} stem from the overlap of the wave functions of the holes placed at the i -th and m -th lattice sites respectively, their values decrease (non-exponentially) with the distance $|\mathbf{r}_m - \mathbf{r}_i|$ between the two lattice sites. Here we take them for phenomenological parameters, carrying non-vanishing characteristic values within the first three coordination spheres of the lattice node i . From [2] and [5], the following typical values may be inferred: for the nearest neighbouring m -sites (the first coordination sphere), $\nu_{im} \sim \nu_1 = 0.14$; for the next nearest neighbouring m -sites (the second coordination sphere), $\nu_{im} \sim \nu_2 = -0.13\nu_1$, while for the m -sites located at the third coordination sphere, $\nu_{im} \sim \nu_3 = 0.16\nu_1$.

Using (1), the Hamiltonian of the effective two-band Hubbard model [2] was rewritten in the form [1]

$$H = E_1 \sum_{i,\sigma} X_i^{\sigma\sigma} + E_2 \sum_i X_i^{22} + K_{11} \sum_{i,\sigma} \tau_{1,i}^{\sigma 0,0\sigma} + K_{22} \sum_{i,\sigma} \tau_{1,i}^{2\sigma,\sigma 2} + K_{21} \sum_{i,\sigma} 2\sigma(\tau_{1,i}^{2\sigma,0\sigma} + \tau_{1,i}^{\sigma 0,\sigma 2}) \quad (2)$$

where the spin projection values in the sums over σ are $\sigma = \pm 1/2$, $\bar{\sigma} = -\sigma = -\sigma$.

The Hubbard operators (HOs) $X_i^{\alpha\beta} = |\alpha\rangle\langle\beta|$ are defined for the four states of the model at each lattice site i : $|0\rangle$ (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 inside the singlet subband).

The HOs may be either fermionic or bosonic. There are processes (e.g., hole creation/annihilation, interband transitions) which are described by fermionic HOs. Processes like singlet creation/annihilation, or the characterization of the charge and spin densities are described in terms of bosonic HOs. As a consequence, the HO algebra is very complicated. Two fermionic HOs anticommute, $\{X_i^{\alpha\beta}, X_j^{\gamma\eta}\} = \delta_{ij}(\delta_{\beta\gamma} X_i^{\alpha\eta} + \delta_{\eta\alpha} X_i^{\alpha\beta})$, while any other pair of HOs satisfies the commutation relations, $\{X_i^{\alpha\beta}, X_j^{\gamma\eta}\} = \delta_{ij}(\delta_{\beta\gamma} X_i^{\alpha\eta} - \delta_{\eta\alpha} X_i^{\alpha\beta})$. At every lattice site i , the multiplication rule $X_i^{\alpha\beta} X_i^{\gamma\eta} = \delta_{\beta\gamma} X_i^{\alpha\eta}$ and the completeness relation $X_i^{00} + X_i^{\sigma\sigma} + X_i^{\bar{\sigma}\bar{\sigma}} + X_i^{22} = 1$ hold. The latter secures rigorous fulfilment of the constraint of no double occupancy of any quantum state $|\alpha\rangle$.

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

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. Inband ($\mathcal{K}_{11}, \mathcal{K}_{22}$) and interband ($\mathcal{K}_{21}=\mathcal{K}_{12}$) processes are present.

The physically relevant information contained in the Hamiltonian (2) is extracted by the equation of motion method for thermodynamic Green functions. The results of the mean field approximation of this procedure are summarized in the next section.

3. Mean field approximation

We define [16] the four component σ -Nambu operator,

$$\hat{X}_{i\sigma} = (X_i^{\sigma 2} X_i^{0\sigma} X_i^{2\bar{\sigma}} X_i^{\sigma 0})^T \quad (3)$$

where the superscript T denotes the transposition. Then $\hat{X}_{i\sigma}^\dagger = (X_i^{\sigma 2} X_i^{0\bar{\sigma}} X_i^{2\bar{\sigma}} X_i^{\sigma 0})$ denotes the adjoint operator of $\hat{X}_{i\sigma}$. The set of all the sixteen correlation functions of the pairs of Hubbard operators emerging from $\hat{X}_{i\sigma}(t)$ and $\hat{X}_{j\sigma}^\dagger(t')$ can be written in terms of the retarded and advanced 4×4 GF matrices (in Zubarev notation [13])

$$\begin{aligned} \tilde{G}_{ij\sigma}^r(t-t') &= -i\theta(t-t') \langle \{ \hat{X}_{i\sigma}(t), \hat{X}_{j\sigma}^\dagger(t') \} \rangle, \\ \tilde{G}_{ij\sigma}^a(t-t') &= i\theta(t'-t) \langle \{ \hat{X}_{i\sigma}(t), \hat{X}_{j\sigma}^\dagger(t') \} \rangle, \end{aligned} \quad (4)$$

where $\langle \dots \rangle$ denotes the statistical average over the Gibbs grand canonical ensemble.

The GMFA-GF solution resulting from (4) can be written in compact form in the (\mathbf{q}, ω) -representation,

$$\tilde{G}_\sigma^0(\mathbf{q}, \omega) = \tilde{\chi} [\tilde{\chi} \omega - \tilde{A}_\sigma(\mathbf{q})]^{-1} \tilde{\chi} \quad (5)$$

$$\tilde{\chi} = \langle \{ \hat{X}_{i\sigma}, \hat{X}_{i\sigma}^\dagger \} \rangle, \quad (6)$$

$$\tilde{A}_\sigma(\mathbf{q}) = \sum_{r_j} e^{i_q r_j} \tilde{A}_{j\sigma}, r_j = r_j - r_i \quad (7)$$

$$\tilde{A}_{j\sigma} = \langle \{ \hat{Z}_{i\sigma}, \hat{X}_{j\sigma}^\dagger \} \rangle, \hat{Z}_{i\sigma} = [\hat{X}_{i\sigma}, H] \quad (8)$$

Here, ω denotes, in the complex energy plane, the value $\omega+i\varepsilon$ for retarded GF, and $\omega-i\varepsilon$ for advanced GF, $\varepsilon=0^+$.

For the alternative $\bar{\sigma}$ -Nambu operator,

$$\hat{X}_{i\sigma} = (X_i^{\bar{\sigma} 2} X_i^{0\sigma} X_i^{2\sigma} X_i^{\bar{\sigma} 0})^T \quad (9)$$

GMFA-GF results are obtained [1] in terms of the $\bar{\sigma}$ -frequency matrix $\tilde{A}_{ij\sigma} = \langle \{ [\hat{X}_{i\bar{\sigma}}, H], \hat{X}_{j\bar{\sigma}}^\dagger \} \rangle$

The elements of the frequency matrices $\tilde{A}_{ij\sigma}$ and $\tilde{A}_{ij\bar{\sigma}}$ have been found to share a same algebraic structure,

$$\langle \{ Z_i^{\lambda\mu}, X_i^{\nu\varphi} \} \rangle = \delta_{ij} \langle C_i^{\lambda\mu, \nu\varphi} \rangle + (1 - \delta_{ij}) V_{ij} \langle T_{ij}^{\lambda\mu, \nu\varphi} \rangle, \quad (10)$$

where the expressions of the specific one-site terms $C_i^{\lambda\mu, \nu\varphi}$ and two-site terms $T_{ij}^{\lambda\mu, \nu\varphi}$ have been rigorously simplified by making use of the translation invariance of the lattice and the Hubbard operator algebra.

The calculation evidenced the occurrence of two kinds of particle number operators: related to the singlet subband,

$$n_{i\sigma} = X_i^{\sigma\bar{\sigma}} + X_i^{22}, n_{i\bar{\sigma}} = X_i^{\sigma\sigma} + X_i^{22} \quad (11)$$

and related to the hole subband,

$$n_{i\sigma}^h = X_i^{\sigma\sigma} + X_i^{00}, n_{i\bar{\sigma}}^h = X_i^{\bar{\sigma}\bar{\sigma}} + X_i^{00} \quad (12)$$

The completeness relation implies

$$n_{i\sigma} + n_{i\sigma}^h = n_{i\bar{\sigma}} + n_{i\bar{\sigma}}^h = 1 \quad (13)$$

The total particle number operators at site i are

$$N_i = n_{i\sigma} + n_{i\bar{\sigma}}, N_i^h = n_{i\sigma}^h + n_{i\bar{\sigma}}^h \quad (14)$$

Due to the spin reversal invariance of the physical system, the statistical averages calculated from σ -Nambu and $\bar{\sigma}$ -Nambu operators respectively, have resulted in the following kinds of relationships:

(i) The average occupation numbers are independent on the spin projection σ and on the site label i ,

$$\begin{aligned} \langle n_{i\sigma} \rangle &= \langle n_{i\bar{\sigma}} \rangle = \chi_2 \\ \langle n_{i\sigma}^h \rangle &= \langle n_{i\bar{\sigma}}^h \rangle = \chi_1 = 1 - \chi_2 \end{aligned}$$

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 (half-filling). 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, $\langle X_i^{02} \rangle = \langle X_i^{20} \rangle = 0$. As a consequence, the $\tilde{\chi}$ matrix (6) is *diagonal*, with non-vanishing matrix elements given by χ_1 and χ_2 , Eq. (15).

(iii) The *normal one-site* matrix elements originating in hopping processes result in renormalization corrections to the energy parameters E_1 and E_2 of (2).

The normal *intraband* hopping matrix element corrections are independent on the spin projection σ and result in identical contributions E_1 and E_2 .

The normal *interband* hopping matrix elements change sign under the spin reversal $\sigma \rightarrow \bar{\sigma}$.

The emerging interband contributions to the frequency matrices $\tilde{A}_{ij\sigma}$ and $\tilde{A}_{ij\bar{\sigma}}$ show the same σ -dependence. However, they result into *spin-projection-independent hybridization effects* of the hole and singlet subband energy levels.

(iv) The *anomalous one-site* matrix elements which stem from the hopping processes satisfy the identity $\langle C_i^{\sigma 2,0\sigma} + C_i^{0\bar{\sigma},\bar{\sigma} 2} \rangle = 0$, wherefrom two conclusions follow. First, the anomalous one-site *interband* hopping contributions to the frequency matrix vanish identically, irrespective of the relationship between the lattice constants a_x and a_y . Second, the anomalous one-site *inband* hopping contributions coming from the hole and singlet subbands respectively are equal to each other. Within a square array, both of them vanish identically, while within a slightly deformed square array they bring quite small contributions to the frequency matrix.

Therefore, the static one-site pairing is *absent* from the Hubbard model (2), such that the GMFA superconducting pairing *cannot arise via the minimization of the potential energy of the system*.

(v) Both the normal and anomalous two-site terms $\langle T_{ij}^{\lambda\mu,\nu\varphi} \rangle$ (10) stem from hopping processes. For any pair of lattice sites (i,j) , they involve *identically vanishing spin-charge correlations*,

$$\langle N_i S_j^z \rangle = \langle N_i^h S_j^z \rangle = 0, \quad S_j^z = (X_j^{\sigma\sigma} - X_j^{\bar{\sigma}\bar{\sigma}}) \quad (16)$$

These identities point to the *spin-charge separation* of the two-site normal correlation functions, which consist [1] exclusively of charge-charge, spin-spin and singlet-hopping terms.

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

$$X_{ij}^{pair} = \nu_{ij} \langle X_i^{02} N_j \rangle = -\nu_{ij} \langle N_j^h X_i^{02} \rangle \quad (17)$$

Since the singlet carries charge and no spin, (17) may be assumed to point to the occurrence of a static *charge-charge* correlation mechanism of superconductivity within the model (2).

4. Localized cooper pairs

Rigorous mathematical transformations which rule out exponentially small quantities while preserving all the relevant contributions to the anomalous two-site correlation functions [1], yield for hole-doped cuprates ($i \neq j$)

$$\chi_{ij}^{pair} \approx \frac{K_{21}}{\Delta} \nu_{ij} \sum_{\sigma} 2\bar{\sigma} \langle \tau_{1,i}^{\sigma 2, \bar{\sigma} 2} N_j \rangle \quad (18)$$

while for the electron-doped cuprates ($i \neq j$)

$$\chi_{ij}^{pair} \approx \frac{K_{21}}{\Delta} \nu_{ij} \sum_{\sigma} 2\sigma \langle N_j^h \tau_{1,i}^{0\bar{\sigma}, 0\sigma} \rangle \quad (19)$$

Taking into account the expression (1) of $\tau_{1,i}^{\alpha\beta,\gamma\eta}$, these equations result into two-site ($m=j \neq i$) and three-site ($m \neq j \neq i$) contributions to the superconducting pairing. If an approximate decoupling of the three-site terms is performed following the general rule [17] that the fermionic components $X_i^{\alpha\beta} X_m^{\gamma\eta}$ should be separated from the bosonic components (N_j^h / N_j^h), we get the following dependence of the static superconducting pairing on the doping rate δ in hole-doped cuprates,

$$\chi_{ij}^{pair} \approx \frac{K_{21}}{\Delta} 4\nu_{ij} 2\bar{\sigma} [\nu_{ij} (1-\delta) \langle X_i^{2\sigma} X_j^{\bar{\sigma} 2} \rangle + \delta \langle \tau_{1,i}^{\sigma 2, \bar{\sigma} 2} \rangle] \quad (20)$$

while in electron-doped cuprates:

$$\chi_{ij}^{pair} \approx \frac{K_{21}}{\Delta} 4\nu_{ij} 2\sigma [\nu_{ij} (1-\delta) \langle X_i^{0\bar{\sigma}} X_j^{0\sigma} \rangle + \delta \langle \tau_{1,i}^{0\bar{\sigma}, 0\sigma} \rangle] \quad (21)$$

These equations unveil a view on the static superconducting mechanism emerging from (2) which recovers the exchange mechanism of the *t-J* model in terms of localized Cooper pairs. These pairs involve neighbouring spin states found in that energy band which crosses the Fermi level. It is worth noting that, in the absence of the doping, the pairing comes from pure two-site correlations, which, however result in zero weight in the frequency matrix due to the fact that the involved energy states are empty. With the increase of the doping, the terms originating in three-site correlations, which are proportional to δ , become increasingly important due to the inclusion of the whole hopping environment (i, m) around the i site where the singlet destruction/creation occurs.

5. Conclusions

A scrutiny of the complete mean field Green function solution [1] of the effective two-dimensional two-band Hubbard model of the high- T_c superconductivity in cuprates [2] was performed.

Our intention was to understand whether the spin-charge separation, repeatedly advocated by Anderson [4,5] to occur in cuprates, may be recovered within the present model or not. While the spin-charge separation conjecture is, strictly speaking, at variance with the existence of the Fermi surface in cuprates, the main findings of this

investigation show that the model (2) supports its actual occurrence in these compounds.

The fundamental feature which results in the spin-charge separation is the particular hierarchy of the ion-ion interactions yielding the Zhang-Rice singlet. While the singlet may decay into a hole state by single particle hopping, or may be created by the inverse process, there are *direct* destruction/creation singlet hopping processes which provide a distinct spinless boson field contribution to the system behaviour.

As a consequence, the correlation of the singlet destruction/creation processes at a given lattice site i with the surrounding charge density, which provides the GMFA anomalous contribution to the Green functions, may be viewed as a charge-charge correlation induced static mechanism of the superconductivity within the present model.

Since, on the other side, the system symmetries and the HO algebra result in vanishing spin-charge normal correlation functions, we arrive at the conclusion that the predictions of the model (2) result, within GMFA at least, in the spin-charge separation advocated by Anderson.

Further mathematical transformations of the anomalous hopping correlation functions resulted, however, in a description of the pairing mechanism through the occurrence of the interacting Cooper pairs within the hopping related region to the i -th reference node where singlet destruction/creation occurred. The obtained formulation allows us to relate the superconducting pairing to the doping rate δ , equations (20) and (21).

It is also worth mentioning that the complete absence of the one-site anomalous pairing, together with the occurrence of hopping related two-site anomalous pairing correlations, point to the fact that the Hubbard model (2) recovers the superconducting state as a result of the minimization of the kinetic energy of the system, in agreement with the ARPES data [9,10].

An open question which deserves further attention concerns the investigation of the spin-charge separation conjecture for the full Dyson equation of the Green function matrix (4).

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