Studies in the Two-Band Hubbard Model of High-T_c Superconductivity

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Abstract

The complete mean field Green function solution of the effective two-dimensional two-band Hubbard model of the high-T_c superconductivity in cuprates [N.M. Plakida et al., Phys. Rev. B, **51**, 16599 (1995)] has been obtained. It 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 and optical data. (iii) The anomalous pairing correlations may be consistently reformulated in terms of localized Cooper pairs both for hole-doped and electron-doped cuprates.

1. Introduction

The two-band Hubbard model of high-T_c superconductivity [1] emerged as a simplification of the more comprehensive p-d model [2], using a reduction procedure based on cell-cluster perturbation theory [3], consistent with the basic features evidenced by the study of the high-T_c cuprates (see, e.g., [4] 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 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 singlet subband (doubly occupied states in the direct space, generated 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.

Using the equation of motion method for thermodynamic Green functions (GF) [5], the effective two-band Hubbard model was shown [6] to generate both the exchange and the spin fluctuation mechanisms currently assumed to result in superconducting pairing in cuprates and to be able [7] to produce electronic spectra of the normal state in agreement with ARPES data.

Here we summarize the results of two recent studies of the generalized mean field approximation (GMFA) solution of the Green function of the effective two-band Hubbard model [8, 9]. Based on the rigorous implementation of consequences following both from the system symmetries (the invariance to translations, point symmetry, and spin reversal) and from the Hubbard operator algebra, the existence of invariance properties of several statistical averages, as well as the exact vanishing of other ones, have been found [8]. These results have been shown [9] to shed new light on the spin-charge separation conjectured by P.W. Anderson [10].

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 [4] and optical [11] data.

2. Model Hamiltonian

Significant simplification of the algebraic calculations asked by the derivation of the GMFA-GF solution was obtained [8] through the definition of the Hubbard 1-forms of labels $(\alpha\beta,\gamma\eta)$,

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

This expression 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}.

Using (1), the Hamiltonian of the effective two-band Hubbard model [1] was rewritten in the form [8]

$$\begin{aligned} H &= E_1\sum_{i,\sigma}X_i^{\sigma\sigma}+E_2\sum_i X_i^{22}+\mathcal{K}_{11}\sum_{i,\sigma}\tau_{1,i}^{\sigma0,0\sigma}+\\ &+ \mathcal{K}_{22}\sum_{i,\sigma}\tau_{1,i}^{2\sigma,\sigma2}+\mathcal{K}_{21}\sum_{i,\sigma}2\sigma(\tau_{1,i}^{2\bar\sigma,0\sigma}+\tau_{1,i}^{\sigma0,\bar\sigma2}). \end{aligned} \tag{2}$$

The Hubbard operator (HO) algebra is very intricate, involving both anticommutation and commutation relations, as well as specific properties at a given lattice site i.

3. Mean field approximation

We define [12] the four component σ-Nambu operator,

$$\hat X_{i\sigma}=(X_i^{\sigma2}\ X_i^{0\bar\sigma}\ X_i^{2\bar\sigma}\ X_i^{\sigma0})^\top \tag{3}$$

where the superscript $\top$ denotes the transposition. Then $\hat X_{j\sigma}^\dagger=(X_j^{2\sigma}\ X_j^{\bar\sigma0}\ X_j^{\bar\sigma2}\ X_j^{0\sigma})$ denotes the adjoint operator of $\hat X_{j\sigma}$. 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 [5])

$$\begin{aligned} \tilde G^r_{ij\sigma}(t-t') &= -\mathrm{i}\theta(t-t')\langle\{\hat X_{i\sigma}(t),\hat X_{j\sigma}^\dagger(t')\}\rangle,\\ \tilde G^a_{ij\sigma}(t-t') &= \mathrm{i}\theta(t'-t)\langle\{\hat X_{i\sigma}(t),\hat X_{j\sigma}^\dagger(t')\}\rangle, \end{aligned} \tag{4}$$

where $\langle\cdots\rangle$ 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 $(\mathbf{q},\omega)$-representation,

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

$$\tilde\chi = \langle\{\hat X_{i\sigma},\hat X_{i\sigma}^\dagger\}\rangle, \tag{6}$$

$$\tilde{\mathcal{A}}_\sigma(\mathbf{q}) = \sum_{\mathbf{r}_{ij}}\mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}_{ij}}\tilde{\mathcal{A}}_{ij\sigma},\ \mathbf{r}_{ij}=\mathbf{r}_j-\mathbf{r}_i\ , \tag{7}$$

$$\tilde{\mathcal{A}}_{ij\sigma} = \langle\{\hat Z_{i\sigma},\hat X_{j\sigma}^\dagger\}\rangle,\ \hat Z_{i\sigma}=[\hat X_{i\sigma},H]. \tag{8}$$

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

The spin and lattice symmetry invariance properties have evidenced the occurrence of two kinds of particle number operators: related to singlet subband, $n_{i\sigma}=X_i^{\bar\sigma\bar\sigma}+X_i^{22}$; $n_{i\bar\sigma}=X_i^{\sigma\sigma}+X_i^{22}$, and to the hole subband, $n^h_{i\sigma}=X_i^{\sigma\sigma}+X_i^{00}$, $\quad n^h_{i\bar\sigma}=X_i^{\bar\sigma\bar\sigma}+X_i^{00}$.

The total particle number operators at site i are $N_i=n_{i\sigma}+n_{i\bar\sigma}$, $\quad N_i^h=n^h_{i\sigma}+n^h_{i\bar\sigma}$.

Furthermore, the following kinds of relationships have been obtained:

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

$$\langle n_{i\sigma}\rangle=\langle n_{i\bar\sigma}\rangle=\chi_2;\quad \langle n^h_{i\sigma}\rangle=\langle n^h_{i\bar\sigma}\rangle=\chi_1=1-\chi_2. \tag{9}$$

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. (9).

(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 *inband* 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 $\sigma \to \bar{\sigma}$. However, they result into *spin-projection-independent hybridization effects* of the hole and singlet subband energy levels.

(iv) The *anomalous one-site* matrix elements which stem both from the *interband* and *inband* hopping processes vanish identically. 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 contributions to $\tilde{\mathcal{A}}_{ij\sigma}$ stem from hopping processes. For any pair of lattice sites (i, j), they involve *identically vanishing spin-charge correlations*, $\langle N_i S_j^z \rangle = \langle N_i^h S_j^z \rangle = 0$, $S_j^z = (X_j^{\sigma\sigma} - X_j^{\bar{\sigma}\bar{\sigma}})/2$. These identities point to the *spin-charge separation* of the two-site normal correlation functions, which consist [8] exclusively of charge-charge, spin-spin and singlet-hopping terms.

(vi) The *spin-independence* of the singlet-charge correlations, $\langle X_i^{02} n_{j\sigma} \rangle = \langle X_i^{02} n_{j\bar{\sigma}} \rangle$, leads to a single two-site anomalous matrix element, $\chi_{ij}^{pair} = \nu_{ij} \langle X_i^{02} N_j \rangle = -\nu_{ij} \langle N_j^h X_i^{02} \rangle$. Since the singlet carries charge and no spin, this 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 two-site anomalous correlation functions [8], yield for hole-doped cuprates $(i \neq j)$

$$\chi_{ij}^{pair} \approx \frac{\mathcal{K}_{21}}{\Delta} \nu_{ij} \sum_{\sigma} 2\bar{\sigma} \langle \tau_{1,i}^{\sigma 2, \bar{\sigma} 2} N_j \rangle, \tag{10}$$

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

$$\chi_{ij}^{pair} \approx \frac{\mathcal{K}_{21}}{\Delta} \nu_{ij} \sum_{\sigma} 2\sigma \langle N_j^h \tau_{1,i}^{0\bar{\sigma}, 0\sigma} \rangle. \tag{11}$$

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 [13] that the fermionic components $X_i^{\alpha\beta} X_m^{\gamma\eta}$ should be separated from the bosonic components (N_j / N_j^h), we get the following dependence of the static superconducting pairing on the doping rate δ in hole-doped cuprates,

$$\chi_{ij}^{pair} \simeq \frac{\mathcal{K}_{21}}{\Delta} \cdot 4\nu_{ij} \cdot 2\bar{\sigma} [\nu_{ij} (1 - \delta) \langle X_i^{\sigma 2} X_j^{\bar{\sigma} 2} \rangle + \delta \langle \tau_{1,i}^{\sigma 2, \bar{\sigma} 2} \rangle], \tag{12}$$

while in electron-doped cuprates:

$$\chi_{ij}^{pair} \simeq \frac{\mathcal{K}_{21}}{\Delta} \cdot 4\nu_{ij} \cdot 2\sigma [\nu_{ij} (1 - \delta) \langle X_i^{0\bar{\sigma}} X_j^{0\sigma} \rangle + \delta \langle \tau_{1,i}^{0\bar{\sigma}, 0\sigma} \rangle]. \tag{13}$$

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.

References

[1] N.M. Plakida, R. Hayn, and J.-L. Richard, Phys. Rev. B, **51**, 16599 (1995).

[2] V.J. Emery, Phys. Rev. Lett. **58**, 2794 (1987); C.M. Varma, S. Schmitt-Rink, and E. Abrahams, Solid State Commun. **62**, 681 (1987).

[3] L.J. Feiner, J.H. Jefferson, and R. Raimondi, Phys. Rev. B **53**, 8751 (1996); V.Yu. Yushankhai, V.S. Oudovenko, and R. Hayn, Phys. Rev. B **55**, 15562 (1997).

[4] A. Damascelli, Z. Hussain, and Z.-X. Shen, Rev. Mod. Phys. **75**, 473 (2003).

[5] D.N. Zubarev, Sov. Phys. Usp. **3**, 320 (1960).

[6] N.M. Plakida, L. Anton, S. Adam, and Gh. Adam, ZhETF **124**, 367 (2003); English transl.: JETP **97**, 331 (2003).

[7] N.M. Plakida and V.S. Oudovenko, JETP **104**, 230 (2007).

[8] Gh. Adam and S. Adam, J.Phys.A: Math. Theor.**40**, 11205 (2007).

[9] Gh. Adam and S. Adam, J.Opt.Adv.Mat. (to be publ.)

[10] P.W. Anderson, Science, **235**, 1196 (1987); **288**, 480 (2000).

[11] J.E. Hirsch, Science, **295**, 2226 (2002).

[12] N.M. Plakida, Physica C **282–287**, 1737 (1997).

[13] A.N. Vasiliev, *Functional Methods in Quantum Field Theory and Statistical Physics*, (Gordon & Breach, Amsterdam, 1998).