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Green functions for strongly correlated electronic systems

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Abstract. By means of the path-integral formalism, a general procedure for the evaluation of the exact n-point Green functions at finite temperature is developed for the analysis of strongly correlated electron systems. The densities of states for two different types of electrons are written by using a non-standard perturbation expansion.

1. Introduction

Since the discovery of copper oxide superconductors, novel mechanisms have been proposed to account for the large value of the critical temperature and for the electronic properties of these compounds (see, for example, [1]). There is considerable controversy as to what gives the attractive interaction and indeed many possible ways by which the pairing force could be mediated have so far been suggested (see, for example, [2]). Even though a complete theoretical understanding of the properties of the new superconductors is still lacking, it is now generally agreed that the phenomenon arises from the existence of strong on-site electronic correlations in the highest occupied band, formed predominantly by the 3d $(x^2 - y^2)$ orbitals of the copper overlapping with the oxygen 2p (x or y) orbitals in the Cu–O planes. Motivated by these physical considerations, the Hubbard model has proved to be well suited to the study of high-T_c superconductors (HTS).

In this article we consider an extended version of the Hubbard model where $d_{i\sigma}$ and $p_{i\sigma}$ are operators which describe electrons with spin σ ($\equiv \uparrow, \downarrow$) at the ith site with energy ϵ_d and ϵ_p, respectively; t_{ij}^d (t_{ij}^p) is the hopping between the i and j for d (p) electrons, ($i \neq j$), neighbours and V_{ij} is a hopping matrix element, which connects different electrons placed at neighbouring sites i and j ($i \neq j$). We also introduce the on-site Coulomb repulsion U_p and U_d between the p and d electrons at the same site.

Therefore the model Hamiltonian is

$$H = \sum_{i,\sigma} \epsilon_d d_{i\sigma}^\dagger d_{i\sigma} + U_d \sum_i d_{i\uparrow}^\dagger d_{i\uparrow} d_{i\downarrow}^\dagger d_{i\downarrow} + \sum_{i,\sigma} \epsilon_p p_{i\sigma}^\dagger p_{i\sigma} + U_p \sum_i p_{i\uparrow}^\dagger p_{i\uparrow} p_{i\downarrow}^\dagger p_{i\downarrow}$$
$$+ V \sum_{i,\sigma} (d_{i\sigma}^\dagger p_{i\sigma} + p_{i\sigma}^\dagger d_{i\sigma}) + \sum_{ij\sigma} t_{ij}^d d_{i\sigma}^\dagger d_{j\sigma}$$
$$+ \sum_{ij\sigma} t_{ij}^p p_{i\sigma}^\dagger p_{j\sigma} + \sum_{ij\sigma} V_{ij} (d_{i\sigma}^\dagger p_{j\sigma} + p_{i\sigma}^\dagger d_{j\sigma})$$

where V represents a hybridization between p and d electrons at the same site.

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It is worth noting that in many cases a truncated version of this Hamiltonian has been used to analyse the HTS and often the limit of infinite U_d has been considered together with $U_p = 0$ [3–7].

Here we study the *total* Hamiltonian, that is we consider all the inter-site and intra-site terms which are included in H. In order to solve such a model we separate the Hamiltonian into an unperturbed component H_0 and an interaction one H_I; H_0 is the site-independent part and contains the effects of the on-site strong correlations and, in contrast, H_I contains the terms responsible for the correlations between different sites.

The unperturbed Hamiltonian can be diagonalized by use of a non-standard path-integral technique developed in [8]. From this diagonalization we can calculate the 'free' propagators and thus the full Green functions can be written by means of a suitable approximate Dyson equation [9].

We want to stress that in this approach all the calculations are performed at finite temperature and for finite values of the correlations energies U_p and U_d and the hybridization V. We believe that this technique, as it is able to take into account the effects of the on-site correlations in an exact way, may prove to be very useful in the study of HTS.

In this article we confine ourselves to the introduction of a generalized method for treating the Hamiltonian H, that is we calculate the 'free' and full propagators of the model and then we compute the spectral density of states for d and p electrons. The analysis of these densities of states for realistic situations will be the subject of a future article.

The article is organized as follows: in section 2 we solve H_0 exactly by using the path-integral formalism, so we are able to calculate the 'free' Green functions. From these results we may determine, in section 3, the full propagators by means of an approximate Dyson equation and then we can write down the spectral density of states for d and p electrons.

2. The model

Let us consider the following Hamiltonian

$$H = H_0 + H_I \tag{1}$$

where

$$H_0 = \sum_{i,\sigma} \epsilon_d d^\dagger_{i\sigma} d_{i\sigma} + U_p \sum_i d^\dagger_{i\uparrow} d_{i\uparrow} d^\dagger_{i\downarrow} d_{i\downarrow} + \sum_{i,\sigma} \epsilon_p p^\dagger_{i\sigma} p_{i\sigma} + U_p \sum_i p^\dagger_{i\uparrow} p_{i\uparrow} p^\dagger_{i\downarrow} p_{i\downarrow} + V \sum_{i,\sigma} (d^\dagger_{i\sigma} p_{i\sigma} + p^\dagger_{i\sigma} d_{i\sigma}) \tag{2}$$

and

$$H_I = \sum_{ij\sigma} t^d_{ij} d^\dagger_{i\sigma} d_{j\sigma} + \sum_{ij\sigma} t^p_{ij} p^\dagger_{i\sigma} p_{j\sigma} + \sum_{ij\sigma} V_{ij} (d^\dagger_{i\sigma} p_{j\sigma} + p^\dagger_{i\sigma} d_{j\sigma}). \tag{3}$$

First, we analyse H_0. Since different sites are decoupled in H_0, it is sufficient to consider the one-site case. The Fock space generated by H_0 has a finite dimension

and therefore the model can be solved completely in terms of 16 × 16 matrices by diagonalizing H_0 (16 being the dimensionality of the Fock space).

Indeed, noting that the total number of particles

$$N = d^\dagger d + p^\dagger p$$

and the total spin

$$S = d^\dagger(\sigma/2)d + p^\dagger(\sigma/2)p$$

with $d \equiv \binom{d_\uparrow}{d_\downarrow}$ and $p \equiv \binom{p_\uparrow}{p_\downarrow}$ are conserved quantities, the eigenstates of H_0 can be classified as shown in table 1.

Table 1. Eigenstates of H_0 where $\Delta_1 = \sqrt{(\epsilon_p - \epsilon_d)^2 + 4V^2}$, $\Delta_2 = \sqrt{(\epsilon_p - \epsilon_d + U_p - U_d)^2 + 4V^2}$ $x_i y_i z_i$ $(i = 7, 10, 13)$ are given in the appendix and E_7, E_{10} and E_{13} are the solution of the equation: $x^3 - x^2[3(\epsilon_p + \epsilon_d) + U_p + U_d] - x[4V^2 - 2\epsilon_p^2 - 2\epsilon_d^2 - \epsilon_p U_p - \epsilon_d U_d - 8\epsilon_p\epsilon_d - 3\epsilon_p U_d - 3\epsilon_d U_p - U_p U_d] + 2V^2(2\epsilon_p + 2\epsilon_d + U_p + U_d) - (\epsilon_p + \epsilon_d)[(2\epsilon_p + U_p)(2\epsilon_d + U_d)] = 0$.

Eigenstates	Energies	Number of electrons	Total spin
$\|0\rangle$	$E_{16} = 0$	0	0
$\|d_\sigma\rangle = (\cos\phi d_\sigma^\dagger + \sin\phi p_\sigma^\dagger)\|0\rangle$	$E_8 = E_{12} = (\epsilon_p + \epsilon_d - \Delta_1)/2$	1	$\pm\frac{1}{2}$
$\|p_\sigma\rangle = (\cos\phi p_\sigma^\dagger - \sin\phi d_\sigma^\dagger)\|0\rangle$	$E_{14} = E_{15} = (\epsilon_p + \epsilon_d + \Delta_1)/2$	1	$\pm\frac{1}{2}$
$\|S_\sigma\rangle = d_\sigma^\dagger p_\sigma^\dagger\|0\rangle$	$E_6 = E_{11} = \epsilon_p + \epsilon_d$	2	± 1
$\|S_0\rangle = \sqrt{1/2}(d_\uparrow^\dagger p_\downarrow^\dagger + d_\downarrow^\dagger p_\uparrow^\dagger)\|0\rangle$	$E_4 = \epsilon_p + \epsilon_d$	2	0
$\|T_+\rangle = [x_7 d_\uparrow^\dagger d_\downarrow^\dagger + z_7 p_\uparrow^\dagger p_\downarrow^\dagger - y_7(d_\uparrow^\dagger p_\downarrow^\dagger - d_\downarrow^\dagger p_\uparrow^\dagger)]\|0\rangle$	E_7	2	0
$\|T_0\rangle = [x_{10} d_\uparrow^\dagger d_\downarrow^\dagger + z_{10} p_\uparrow^\dagger p_\downarrow^\dagger - y_{10}(d_\uparrow^\dagger p_\downarrow^\dagger - d_\downarrow^\dagger p_\uparrow^\dagger)]\|0\rangle$	E_{10}	2	0
$\|T_-\rangle = [x_{13} d_\uparrow^\dagger d_\downarrow^\dagger + z_{13} p_\uparrow^\dagger p_\downarrow^\dagger - y_{13}(d_\uparrow^\dagger p_\downarrow^\dagger - d_\downarrow^\dagger p_\uparrow^\dagger)]\|0\rangle$	E_{13}	2	0
$\|D_\sigma\rangle = (\cos\theta d_\sigma^\dagger p_\sigma^\dagger d_{-\sigma}^\dagger + \sin\theta d_\sigma^\dagger p_\sigma^\dagger p_{-\sigma}^\dagger)\|0\rangle$	$E_2 = E_3 = (3\epsilon_p + 3\epsilon_d + U_p + U_d - \Delta_2)/2$	3	$\pm\frac{1}{2}$
$\|P_\sigma\rangle = (-\sin\theta d_\sigma^\dagger p_\sigma^\dagger d_{-\sigma}^\dagger + \cos\theta d_\sigma^\dagger p_\sigma^\dagger p_{-\sigma}^\dagger)\|0\rangle$	$E_5 = E_9 = (3\epsilon_p + 3\epsilon_d + U_p + U_d + \Delta_2)/2$	3	$\pm\frac{1}{2}$
$\|DP\rangle = d_\uparrow^\dagger p_\uparrow^\dagger d_\downarrow^\dagger p_\downarrow^\dagger\|0\rangle$	$E_1 = 2\epsilon_p + 2\epsilon_d + U_p + U_d$	4	0

Knowledge of the energy levels allows us to determine the analytic expression of the n-point Green functions directly from their definitions and, by means of the partition function, all the thermodynamics quantities may be easily computed [10]. However due to the large number of the eigenstates of H_0, this type of computation is very tedious.

Motivated by this fact we here present a solution of the model in a compact form by using the path-integral formalism and we give an explicit expression for two-point Green functions.

The generating functional for temperature Green functions is

$$Z[J,K] = \mathrm{Tr}\left\{ \exp(-\beta H_0) T_\tau \exp\left[\int_0^\beta \mathrm{d}\tau \, (J^\dagger(\tau) d(\tau) + d^\dagger(\tau) J(\tau) + K^\dagger(\tau) p(\tau) + p^\dagger(\tau) K(\tau))\right]\right\} \tag{4}$$

where T_τ orders the operators according to their value of τ, with the smallest at right, and $J \equiv \binom{J_\uparrow}{J_\downarrow}$ and $K \equiv \binom{K_\uparrow}{K_\downarrow}$ are the external sources associated with d and p, respectively and $\beta = 1/K_B T$.

By dividing the interval $0 \leqslant \tau \leqslant \beta$ into N parts, $Z[J,K]$ can be written as

$$Z[J,K] = \lim_{N\to\infty} Z^{(N)}[J,K] \tag{5}$$

where

$$\begin{aligned} Z^{(N)}[J,K] = \exp&\left[\sum_{k=1}^{N} \left(\frac{\partial}{\partial J_k}\right)\left(\frac{\partial}{\partial J_{k+1}^\dagger}\right) + \left(\frac{\partial}{\partial K_k}\right)\left(\frac{\partial}{\partial K_{k+1}^\dagger}\right)\right] \\ &\times \exp\left[\sum_{m=1}^{N} \left(\frac{\beta^V}{N}\right)\left(\frac{\partial}{\partial J_m}\right)\left(\frac{\partial}{\partial K_m^\dagger}\right) + \left(\frac{\partial}{\partial K_m}\right)\left(\frac{\partial}{\partial J_m^\dagger}\right)\right] \\ &\times \omega^N \Omega^N \prod_{i=1}^{N} Z_S^{(N)}[J_i, K_i] \end{aligned} \tag{6}$$

with

$$\begin{aligned} &\Omega = (1 - \beta\epsilon_d/N)^2 - \beta U_d/N \\ &\omega = (1 - \beta\epsilon_p/N)^2 - \beta U_p/N \\ &J_i \equiv J(\tau_i) \qquad K_i \equiv K(\tau_i) \qquad (\tau_i = i\beta/N) \end{aligned}$$

and

$$Z_S^{(N)}[J_i, K_i] = Z_d^{(N)}[J_i] Z_p^{(N)}[K_i]$$

Here $Z_d^{(N)}[J_i]$ and $Z_p^{(N)}[K_i]$ denote respectively

$$\begin{aligned} Z_d^{(N)}[J] &= 1 + \Omega^{-1}(1 - \beta\epsilon_d/N)(J_\uparrow J_\uparrow^\dagger + J_\downarrow J_\downarrow^\dagger) + \Omega^{-1}(J_\uparrow J_\uparrow^\dagger J_\downarrow J_\downarrow^\dagger) \\ Z_p^{(N)}[K] &= 1 + \omega^{-1}(1 - \beta\epsilon_p/N)(K_\uparrow K_\uparrow^\dagger + K_\downarrow K_\downarrow^\dagger) + \omega^{-1}(K_\uparrow K_\uparrow^\dagger K_\downarrow K_\downarrow^\dagger). \end{aligned} \tag{7}$$

In equation (6) we have assumed the periodic conditions:

$$\frac{\partial}{\partial J_{N+1}^\dagger} = -\frac{\partial}{\partial J_1^\dagger} \qquad \frac{\partial}{\partial K_{N+1}^\dagger} = -\frac{\partial}{\partial K_1^\dagger}$$

Table 2. Non-vanishing elements of the matrix $\mathbf{Q}[0,0]$ where $u = \beta V/N$, $a = (1-\beta\epsilon_d/N)\Omega^{-1}$, $\hat{a} = (1-\beta\epsilon_p/N)\omega^{-1}$, $b = \Omega^{-1}$ and $\hat{b} = \omega^{-1}$.

$Q_{11} = 1 - 2u^2 a\hat{a} + u^4 b\hat{b}$
$Q_{22} = Q_{33} = \hat{a} - u^2 a\hat{b}$
$Q_{25} = Q_{52} = Q_{39} = Q_{93} = u(a\hat{a} - u^2 b\hat{b})$
$Q_{44} = \hat{b}$
$Q_{47} = Q_{74} = -Q_{4,10} = -Q_{10,4} = ua\hat{b}$
$Q_{4,13} = Q_{13,4} = -Q_{7,10} = -Q_{10,7} = u^2 b\hat{b}$
$Q_{55} = Q_{99} = a - u^2\hat{a}b$
$Q_{66} = Q_{11,11} = a\hat{a} - u^2 b\hat{b}$
$Q_{77} = Q_{10,10} = a\hat{a}$
$Q_{88} = Q_{12,12} = a\hat{b}$
$Q_{7,13} = Q_{13,7} = u\hat{a}b$
$Q_{8,14} = Q_{14,8} = -ub\hat{b}$
$Q_{10,13} = Q_{13,10} = -u\hat{a}b$
$Q_{12,15} = Q_{15,12} = -ub\hat{b}$
$Q_{13,13} = b$
$Q_{14,14} = Q_{15,15} = \hat{a}b$
$Q_{16,16} = b\hat{b}$

After some easy but tedious calculations [8] we can rewrite $Z^{(N)}[J,K]$ in the form

$$Z^{(N)}[J,K] = \omega^{(N)}\Omega^{(N)} \prod_{i=1}^{N} \Gamma^i \Delta^{i,i+1}\hat{\Delta}^{i,i+1} \prod_{i=1}^{N} R^i \hat{R}^i \tag{8}$$

where

$$\Gamma^i = \left[1 + \left(\frac{\beta V}{N}\right)\left(\frac{\partial}{\partial J_{\uparrow i}}\right)\left(\frac{\partial}{\partial K^\dagger_{\uparrow i}}\right)\right]\left[1 + \left(\frac{\beta V}{N}\right)\left(\frac{\partial}{\partial J_{\downarrow i}}\right)\left(\frac{\partial}{\partial K^\dagger_{\downarrow i}}\right)\right]$$
$$\times \left[1 + \left(\frac{\beta V}{N}\right)\left(\frac{\partial}{\partial J^\dagger_{\uparrow i}}\right)\left(\frac{\partial}{\partial K_{\uparrow i}}\right)\right]\left[1 + \left(\frac{\beta V}{N}\right)\left(\frac{\partial}{\partial J^\dagger_{\downarrow i}}\right)\left(\frac{\partial}{\partial K_{\downarrow i}}\right)\right]$$

$$\Delta^{i,i+1} = \left[1 + \left(\frac{\partial}{\partial J_{\uparrow i}}\right)\left(\frac{\partial}{\partial J^\dagger_{\uparrow i+1}}\right)\right]\left[1 + \left(\frac{\partial}{\partial J_{\downarrow i}}\right)\left(\frac{\partial}{\partial J^\dagger_{\downarrow i+1}}\right)\right]$$

$$\hat{\Delta}^{i,i+1} = \left[1 + \left(\frac{\partial}{\partial K_{\uparrow i}}\right)\left(\frac{\partial}{\partial K^\dagger_{\uparrow i+1}}\right)\right]\left[1 + \left(\frac{\partial}{\partial K_{\downarrow i}}\right)\left(\frac{\partial}{\partial K^\dagger_{\downarrow i+1}}\right)\right]$$

$$R^i = 1 + \Omega^{-1}(1-\beta\epsilon_d/N)(J_{\uparrow i}J^\dagger_{\uparrow i} + J_{\downarrow i}J^\dagger_{\downarrow i}) + \Omega^{-1}(J_{\uparrow i}J^\dagger_{\uparrow i}J_{\downarrow i}J^\dagger_{\downarrow i})$$

$$\hat{R}^i = 1 + \omega^{-1}(1-\beta\epsilon_p/N)(K_{\uparrow i}K^\dagger_{\uparrow i} + K_{\downarrow i}K^\dagger_{\downarrow i}) + \omega^{-1}(K_{\uparrow i}K^\dagger_{\uparrow i}K_{\downarrow i}K^\dagger_{\downarrow i}).$$

Following the same procedure as that outlined in [8] it is easy to derive the expression

$$Z^{(N)}[J,K] = \omega^N \Omega^N \operatorname{Tr} \mathbf{Q}^1 \mathbf{Q}^2 \ldots \mathbf{Q}^N \tag{9}$$

where $\mathbf{Q}^i[J,K]$ are 16×16 matrices.

In the limit $J = K = 0$ the matrices $\mathbf{Q}^i$ do not depend on i; the non-vanishing elements of $\mathbf{Q}$ are reported in table 2.

Let us define

$$\mathbf{P} = \mathbf{S}\mathbf{Q}[0,0]\mathbf{S}^{-1}$$

where the matrix $\mathbf{S}$ is such that $\mathbf{P}$ is diagonal. From equation (9) we have

$$Z^{(N)}[0,0] = \omega^N \Omega^N \operatorname{Tr}(\mathbf{P}[0,0])^N = \omega^N \Omega^N \sum_{i=1}^{16} [P_{ii}]^N \tag{10}$$

so that, once the diagonalization of $\mathbf{Q}[0,0]$ is performed, the partition function $Z[0,0]$ is calculated from equation (5).

Since $\mathbf{Q}[0,0]$ is a real and symmetric matrix, the eigenvalues $P_{ii} \equiv P^i$ are real and the 16×16 matrix $\mathbf{S}$ is orthogonal. In the continuous limit (i.e. $N \to \infty$) it can be shown that equation (5) takes the form

$$Z[0,0] = \lim_{N\to\infty} Z^{(N)}[0,0] = \sum_{a=1}^{16} \mathrm{e}^{(-\beta E_a)}$$

where the energies E_a are given in table 1.

We now pass to the evaluation of the n-point thermal Green functions and equation (9) provides us with a general formula with which to compute them. The analytic expression for these functions is given by

$$\begin{aligned}\langle \psi_{m_n}(\tau_n)\psi_{m_{n-1}}(\tau_{n-1})\dots\psi_{m_1}(\tau_1)\rangle &= \operatorname{Tr}[\exp(-\beta H)\psi_{m_n}(\tau_n)\psi_{m_{n-1}}(\tau_{n-1})\dots\psi_{m_1}(\tau_1)] \\ &= Z[0,0]^{-1}\exp[-\beta(2\epsilon_p + U_p)]\exp[-\beta(2\epsilon_d + U_d)] \\ &\quad \times \operatorname{Tr}[X^{m_1}(\tau_1 - \tau_n + \beta)\dots X^{m_{n-1}}(\tau_{n_1} - \tau_{n_2})X^{m_n}(\tau_n - \tau_{n-1})]\end{aligned} \tag{11}$$

where we have considered the chronological ordering

$$\tau_k < \tau_{k+1} \qquad (k = 1, \dots, n-1)$$

and $m_k = 1, 2, \dots, 8$ with

$$\begin{aligned}\psi_1(\tau) &= d_\uparrow(\tau) & \psi_5(\tau) &= p_\uparrow(\tau) \\ \psi_2(\tau) &= d_\uparrow^\dagger(\tau) & \psi_6(\tau) &= p_\uparrow^\dagger(\tau) \\ \psi_3(\tau) &= d_\downarrow(\tau) & \psi_7(\tau) &= p_\downarrow(\tau) \\ \psi_4(\tau) &= d_\downarrow^\dagger(\tau) & \psi_8(\tau) &= p_\downarrow^\dagger(\tau).\end{aligned}$$

We have also intoduced the 16×16 matrices $\mathbf{X}^i(\tau)$ whose elements are

$$\mathbf{X}^i(\tau)_{nm} = \lim_{N\to\infty} \sum_k A_{nk}(N\tau/\beta)B^i_{km} \tag{12}$$

with

$$A(N\tau/\beta) = (\mathbf{Q}[0,0])^{N\tau/\beta} \qquad B^i_{km} = (-)^{j+1}\frac{\partial \mathbf{Q}[J,K]_{km}}{\partial w_i}\bigg|_{J=K=0}.$$

The quantities w_i are defined as

$$\begin{aligned} w_1 &= J_\uparrow^\dagger \qquad & w_5 &= K_\uparrow^\dagger \\ w_2 &= J_\uparrow & w_6 &= K_\uparrow \\ w_3 &= J_\downarrow^\dagger & w_7 &= K_\downarrow^\dagger \\ w_4 &= J_\downarrow & w_8 &= K_\downarrow . \end{aligned}$$

We have

$$\begin{aligned} \lim_{N\to\infty} (\mathbf{Q}[0,0]^{N\tau/\beta})_{ik} &= \sum_{k=1}^{16} \underline{\mathbf{S}}_{ik}\underline{\mathbf{S}}_{kj} \lim_{N\to\infty} (\mathbf{P}^k)^{N\tau/\beta} \\ &= \mathrm{e}^{[\tau(2\epsilon_p+U_p)]}\mathrm{e}^{[\tau(2\epsilon_d+U_d)]} \sum_{k=1}^{16} \underline{\mathbf{S}}_{ik}\underline{\mathbf{S}}_{kj}\mathrm{e}^{-\tau E_k} \end{aligned} \tag{13}$$

where the elements of the matrix $\underline{\mathbf{S}} = \lim_{N\to\infty} \mathbf{S}$ are listed in the appendix. Besides, the only non-zero elements of the matrices $\underline{\mathbf{B}}^i = \lim_{N\to\infty} \underline{\mathbf{B}}^i$ are

$$\begin{aligned} &\underline{B}^1_{15} = \underline{B}^1_{26} = \underline{B}^1_{37} = \underline{B}^1_{48} = \underline{B}^1_{9,13} = \underline{B}^1_{10,14} = \underline{B}^1_{11,15} = \underline{B}^1_{12,16} = 1 \\ &\underline{B}^3_{19} = \underline{B}^3_{2,10} = \underline{B}^3_{3,11} = \underline{B}^3_{4,12} = -\underline{B}^3_{5,13} = -\underline{B}^3_{6,14} = -\underline{B}^3_{7,15} = -\underline{B}^3_{8,16} = 1 \\ &\underline{B}^5_{12} = \underline{B}^5_{34} = -\underline{B}^5_{56} = -\underline{B}^5_{78} = -\underline{B}^5_{9,10} = -\underline{B}^5_{11,12} = \underline{B}^5_{13,14} = \underline{B}^5_{15,16} = 1 \\ &\underline{B}^7_{13} = -\underline{B}^7_{24} = -\underline{B}^7_{57} = \underline{B}^7_{68} = -\underline{B}^7_{9,11} = \underline{B}^7_{10,12} = \underline{B}^7_{13,15} = -\underline{B}^7_{14,16} = 1. \end{aligned} \tag{14}$$

Because of the relations

$$\underline{\mathbf{B}}^1 = (\underline{\mathbf{B}}^2)^t \qquad \underline{\mathbf{B}}^3 = (\underline{\mathbf{B}}^4)^t \qquad \underline{\mathbf{B}}^5 = (\underline{\mathbf{B}}^6)^t \qquad \underline{\mathbf{B}}^7 = (\underline{\mathbf{B}}^8)^t$$

it is easy to deduce the non-vanishing elements of $\underline{\mathbf{B}}^2\underline{\mathbf{B}}^4\underline{\mathbf{B}}^6\underline{\mathbf{B}}^8$. Combining equations (11)–(14), the thermal n-point Green functions can be computed.

We first note that the spin-up and spin-down terms are independent and the Green functions do not depend on the spin. Therefore it is sufficient to compute the n-point Green functions for a fixed value of the spin. Using equation (11) we compute the exact two-point Green function for d electrons; we have

$$\begin{aligned} G^0_{\sigma d>}(\tau_2-\tau_1) = \langle d_\sigma(\tau_2)d^\dagger_\sigma(\tau_1)\rangle &= Z[0,0]^{-1}\mathrm{e}^{[-\beta(2\epsilon_p+U_p)]}\mathrm{e}^{[-\beta(2\epsilon_d+U_d)]} \\ &\times \Big\{ \mathrm{e}^{(-\beta e_2)}\sin^2\theta\mathrm{e}^{(\tau e_2)} + \mathrm{e}^{(-\beta e_5)}\cos^2\theta\mathrm{e}^{(\tau e_5)} \\ &+ (\tfrac{3}{2})\mathrm{e}^{(-\beta e_4)}\sin^2\theta\mathrm{e}^{[\tau(e_4-e_5)]} + (\tfrac{3}{2})\mathrm{e}^{(-\beta e_4)}\cos^2\theta\mathrm{e}^{[\tau(e_4-e_2)]} \\ &+ \mathrm{e}^{(-\beta e_{16})}\cos^2\phi\mathrm{e}^{[\tau(e_{16}-e_8)]} + \mathrm{e}^{(-\beta e_{16})}\sin^2\phi\mathrm{e}^{[\tau(e_{16}-e_{14})]} \\ &+ (\tfrac{3}{2})\mathrm{e}^{(-\beta e_8)}\sin^2\phi\mathrm{e}^{[\tau(e_8-e_4)]} + (\tfrac{3}{2})\mathrm{e}^{(-\beta e_{14})}\cos^2\phi\mathrm{e}^{[\tau(e_{14}-e_4)]} \\ &+ \sum_k \mathrm{e}^{(-\beta e_k)}(y_k\cos\theta + z_k\sin\theta)^2\mathrm{e}^{[\tau(e_k-e_2)]} \end{aligned}$$

$$+\sum_k e^{(-\beta e_k)}(y_k\sin\theta - z_k\cos\theta)^2 e^{[\tau(e_k-e_5)]}$$

$$+\sum_k e^{(-\beta e_8)}(x_k\cos\phi - y_k\sin\phi)^2 e^{[\tau(e_8-e_k)]}$$

$$+\sum_k e^{(-\beta e_{14})}(x_k\sin\phi + y_k\cos\phi)^2 e^{[\tau(e_{14}-e_k)]}\Bigg\} \tag{15}$$

where $\tau(>0) = \tau_2 - \tau_1$, $e_n = E_n - 2\epsilon_p - U_p - 2\epsilon_d - U_d$ and $k = 7, 10, 13$.

Using the same procedure we can calculated $G^0_{\sigma p>}(\tau)$ and $G^0_{\sigma pd>}(\tau)$:

$$G^0_{\sigma p>}(\tau_2-\tau_1) = \langle p_\sigma(\tau_2)p^\dagger_\sigma(\tau_1)\rangle = Z[0,0]^{-1}e^{[-\beta(2\epsilon_p+U_p)]}e^{[-\beta(2\epsilon_d+U_d)]}$$

$$\times\Bigg\{e^{(-\beta e_2)}\cos^2\theta e^{(\tau e_2)} + e^{(-\beta e_5)}\sin^2\theta e^{(\tau e_5)}$$

$$+(\tfrac{3}{2})e^{(-\beta e_4)}\cos^2\theta e^{[\tau(e_4-e_5)]} + (\tfrac{3}{2})e^{(-\beta e_4)}\sin^2\theta e^{[\tau(e_4-e_2)]}$$

$$+e^{(-\beta e_{16})}\sin^2\phi e^{[\tau(e_{16}-e_5)]} + e^{(-\beta e_{16})}\cos^2\phi e^{[\tau(e_{16}-e_{14})]}$$

$$+(\tfrac{3}{2})e^{(-\beta e_{14})}\sin^2\phi e^{[\tau(e_{14}-e_4)]} + (\tfrac{3}{2})e^{(-\beta e_8)}\cos^2\phi e^{[\tau(e_8-e_4)]}$$

$$+\sum_k e^{(-\beta e_k)}(y_k\cos\theta - x_k\sin\theta)^2 e^{[\tau(e_k-e_5)]}$$

$$+\sum_k e^{(-\beta e_k)}(y_k\sin\theta + x_k\cos\theta)^2 e^{[\tau(e_k-e_2)]}$$

$$+\sum_k e^{(-\beta e_8)}(z_k\sin\phi - y_k\cos\phi)^2 e^{[\tau(e_8-e_k)]}$$

$$+\sum_k e^{(-\beta e_{14})}(z_k\cos\phi + y_k\sin\phi)^2 e^{[\tau(e_{14}-e_8)]}\Bigg\} \tag{16}$$

and

$$G^0_{\sigma pd>}(\tau_2-\tau_1) = \langle p_\sigma(\tau_2)d^\dagger_\sigma(\tau_1)\rangle = Z[0,0]^{-1}e^{[-\beta(2\epsilon_p+U_p)]}e^{[-\beta(2\epsilon_d+U_d)]}$$

$$\times\Bigg\{\sin\theta\cos\theta[e^{[-(\beta-\tau)e_2]} - e^{[-(\beta-\tau)e_5]}]$$

$$+\sum_k e^{[-(\beta-\tau)e_k]}y_k z_k\{\sin^2\theta e^{(-\tau e_2)} + \cos^2\theta e^{(-\tau e_5)}\}$$

$$+\sum_k e^{[-(\beta-\tau)e_k]}x_k y_k\{\cos^2\theta e^{(-\tau e_2)} + \sin^2\theta e^{(-\tau e_5)}\}$$

$$+\sum_k e^{[-(\beta-\tau)e_k]}x_k z_k\sin\theta\cos\theta\{e^{(-\tau e_2)} - e^{(-\tau e_5)}\}$$

$$-\Bigg\{\tfrac{3}{2}e^{[-(\beta-\tau)e_4]} - \sum_k e^{[-(\beta-\tau)e_k]}y_k^2\Bigg\}\sin\theta\cos\theta\{e^{(-\tau e_2)} - e^{(-\tau e_5)}\}$$

$$+ e^{[-(\beta-\tau)e_{16}]} \sin\phi\cos\phi\{e^{(-\tau e_8)} - e^{(-\tau e_{14})}\}$$
$$- \{\sin^2\phi e^{[-(\beta-\tau)e_8]} + \cos^2\phi e^{[-(\beta-\tau)e_{14}]}\} \sum_k e^{(-\tau e_k)} y_k z_k$$
$$- \{\cos^2\phi e^{[-(\beta-\tau)e_8]} + \sin^2\phi e^{[-(\beta-\tau)e_{14}]}\} \sum_k e^{(-\tau e_k)} x_k y_k$$
$$- \sin\phi\cos\phi\{e^{[-(\beta-\tau)e_8]} - e^{[-(\beta-\tau)e_{14}]}\} \left\{ \frac{3}{2} e^{(-\tau e_4)} - \sum_k e^{(-\tau e_k)} y_k^2 \right\}$$
$$+ \sin\phi\cos\phi\{e^{[-(\beta-\tau)e_8]} - e^{[-(\beta-\tau)e_{14}]}\} \sum_k e^{(-\tau e_k)} x_k z_k \Bigg\}. \qquad (17)$$

We only mention that the computation of two-point Green function determined here may also be performed using the diagram method introduced in [11]. The causal temperature Green function for d, p and pd electrons can be easily calculated using equations (15)–(17) and the well known formula

$$G(\tau) = -[\Theta(\tau)G_>(\tau) - \Theta(-\tau)G_>(\tau+\beta)].$$

3. Spectral functions for p and d electrons

In order to solve the model perturbatively we consider the hopping terms between different sites H_I as the pertubation. Due to the presence in H_0 of the two-particle correlations U_p and U_d the Wick theorem cannot be applied in this case. However by neglecting the fluctuations one can decouple the 'time'-ordered products of p and d electrons operators by means of a Wick-like factorization and an approximate Dyson equation for the full Green functions of the Hamiltonian H can be written.

Nevertheless in such an approach the contributions coming from the Coulomb correlations U_p and U_d, which play a crucial role in the HTS, are exactly evaluated so that we are confident that the effects of fluctuations are really negligible.

We want to point out that when there are no electronic correlations ($U_p = U_d = 0$) the Wick theorem can be applied and then the corresponding Dyson equation for the full Green functions is exact. In our case, where electronic on-site correlations are present, the Wick theorem no longer applies; therefore the Dyson equation is approximate. This approximation corresponds to the hypothesis that the interactions of the electrons on the same site are the most important and that the interactions of electrons on other sites may be neglected. This implies that all Green functions involving more than two sites are approximated in terms of Green functions involving not more than two sites [9, 13]. In this sense, this approximation represents a generalization of the Hubbard I [13] approximation because in our model there is also a hybridization term V_{ij}.

The density of states for p and d electrons may be easily calculated by using the well known relationships

$$\rho_p(E) = -(1/N\pi)\sum_k \operatorname{Im} G_{pp}(k, E)$$

$$\rho_d(E) = -(1/N\pi)\sum_k \operatorname{Im} G_{dd}(k, E)$$

where G_{pp} and G_{dd} are the full Green functions for p and d electrons respectively. These Green functions have been deduced from the following Dyson equation [9, 12]:

$$\hat{G}_\sigma(k,\omega_n) = \hat{G}^0_\sigma(k,\omega_n) + \hat{G}^0_\sigma(k,\omega_n)\hat{\Sigma}_{\sigma\sigma}(k,\omega_n)\hat{G}_\sigma(k,\omega_n) \tag{18}$$

where

$$\hat{G}_\sigma(k,\omega_n) = \begin{pmatrix} G_{dd}(k,\omega_n) & G_{dp}(k,\omega_n) \\ G_{pd}(k,\omega_n) & G_{pp}(k,\omega_n) \end{pmatrix} \tag{19}$$

is the full matrix propagator, $G_{ab}(k,\omega_n)$ being the Fourier tranform of

$$G_{ab,ij}(\tau-\tau') = -\langle T_\tau[a_{\sigma i}(\tau)b^\dagger_{\sigma j}(\tau')]\rangle$$

$\hat{G}^0_\sigma(k,\omega_n) = \hat{G}^0_\sigma(\omega_n)$ is the unpertubed one and

$$\hat{\Sigma}_{\sigma\sigma}(k,\omega_n) = \hat{\Sigma}_{\sigma\sigma}(k) = \begin{pmatrix} \epsilon_k & V_k \\ V_k & E_k \end{pmatrix} \tag{20}$$

with

$$\epsilon_k = (1/N)\sum_{i\neq j} t^d_{ij} e^{-ik\times(R_i-R_j)}$$

$$E_k = (1/N)\sum_{i\neq j} t^p_{ij} e^{-ik\times(R_i-R_j)}$$

and

$$V_k = (1/N)\sum_{i\neq j} V_{ij} e^{-ik\times(R_i-R_j)}.$$

We stress that $G^0_\sigma(\omega_n)$ does not depend on k because of the absence of a finite band width in the unperturbed Hamiltonian H_0.

From (18)–(20) we obtain the equations

$$G_{dd} = \frac{[G^0_d + (V_k G^0_d + E_k G^0_{dp})G_{pd}]}{[1-\epsilon_k G^0_d - V_k G^0_{dp}]} \tag{21a}$$

$$G_{dp} = \frac{[G^0_{dp} + (V_k G^0_d + E_k G^0_{dp})G_{pp}]}{[1-\epsilon_k G^0_d - V_k G^0_{dp}]} \tag{21b}$$

$$G_{pd} = \frac{[G^0_{pd} + (V_k G^0_p + \epsilon_k G^0_{pd})G_{dd}]}{[1-E_k G^0_p - V_k G^0_{pd}]} \tag{21c}$$

$$G_{pp} = \frac{[G^0_p + (V_k G^0_p + \epsilon_k G^0_{pd})G_{dp}]}{[1-E_k G^0_p - V_k G^0_{pd}]} \tag{21d}$$

where we have dropped the dummy subscript σ near the free Green function. By using the results of the previous section, the full propagators (19) are easily obtained from equations (21).

From full Green functions G_{pp} and G_{dd} we calculate the density of states ρ_p and ρ_d.

In order to compute these quantities explicitly we must specify the form of the hopping terms ϵ_k, E_k and V_k.

The analysis of specific situation such as nearest-neighbours hopping correlation and/or more complicated cases will be the subject of a forthcoming article.

Appendix

Non-vanishing elements of the matrix **S**

$$S_{11} = S_{66} = S_{11,11} = S_{16,16} = 1$$
$$S_{22} = S_{33} = S_{55} = S_{99} = \cos\theta$$
$$S_{25} = -S_{52} = S_{39} = -S_{93} = \sin\theta$$
$$S_{88} = S_{12,12} = S_{14,14} = S_{15,15} = \cos\phi$$
$$S_{8,14} = -S_{14,8} = S_{12,15} = -S_{15,12} = \sin\phi$$

where

$$\sin\theta = \sqrt{(1/2)\left[1 - (Q_{22} - Q_{55})/\sqrt{[(Q_{22} - Q_{55})^2 + 4Q_{25}^2}\right]}$$

$$\sin\phi = -\sqrt{(1/2)\left[1 - (Q_{88} - Q_{14,14})/\sqrt{[(Q_{88} - Q_{14,14})^2 + 4Q_{8,14}^2}\right]}.$$

In the limit $N \to \infty$ these functions become

$$\lim_{N\to\infty} \sin\theta = \sqrt{(1/2)\left[1 - (\epsilon_p + U_p - \epsilon_d - U_d)/\sqrt{[(\epsilon_p + U_p - \epsilon_d - U_d) + 4V^2]}\right]}$$

$$\lim_{N\to\infty} \sin\phi = -\sqrt{(1/2)\left[1 - (\epsilon_p - \epsilon_d)/\sqrt{[(\epsilon_p - \epsilon_d) + 4V^2]}\right]}$$

$$S_{47} = S_{4,10} = \sqrt{2}/2$$
$$S_{i4} = x_i$$
$$S_{i7} = -S_{i,10} = y_i$$
$$S_{i,13} = z_i \qquad i = 7, 10, 13$$

where x_i, y_i, z_i are the solutions of the system:

$$(\hat{b} - E_i)x_i + 2ua\hat{b}y_i + u^2b\hat{b}z_i = 0$$
$$ua\hat{b}x_i + (a\hat{a} + u^2b\hat{b} - E_i)y_i + u\hat{a}bz_i = 0$$
$$u^2b\hat{b}x_i + 2u\hat{a}by_i + (b - E_i)z_i = 0$$
$$x_ix_j + 2y_iy_j + z_iz_j = \delta_{ij}$$

and E_i are the solutions of the cubic equation

$$\det \begin{vmatrix} \hat{b} - x & -2ua\hat{b} & u^2b\hat{b} \\ -ua\hat{b} & a\hat{a} + u^2b\hat{b} - x & -u^2\hat{a}b \\ u^2b\hat{b} & -2u\hat{a}b & b - x \end{vmatrix} = 0.$$

In the limit $N \to \infty$ the solutions of the system takes the form:

$$(x_i)^2 = 4V^2(2\epsilon_p + U_p - E_i)^2/D_i$$
$$(y_i)^2 = (2\epsilon_p + U_p - E_i)^2(2\epsilon_d + U_d - E_i)^2/D_i$$
$$(z_i)^2 = 4V^2(2\epsilon_d + U_d - E_i)^2/D_i$$

where

$$D_i = 4V^2[(2\epsilon_p + U_p - E_i)^2 + (2\epsilon_d + U_d - E_i)^2] + 2(2\epsilon_p + U_p - E_i)^2(2\epsilon_d + U_d - E_i)^2.$$

References

[1] 1987 *Physica* B+C **148**; 1988 *Physica* C **153–5**; 1989 *Physica* C **162–4**
[2] Lundqvist S, Tosatti E, Tosi M P and Lu Yu (eds) 1988 *Towards the Theoretical Understanding of High T_c Superconductors* (Singapore: World Scientific)
[3] Matsumoto H, Sasaki M, Tachiki M 1989 *Solid State Commun.* **71** 829
[4] Becker K W and Fulde P 1989 *Phys. Scr.* T **27** 109
[5] Oles A M, Zaanen J and Fulde P 1987 *Physica* B+C **148** 260
[6] Balseiro C A, Avignon M, Rojo A G, Alascio B 1989 *Phys. Rev. Lett.* **62** 2624
[7] Castellani C, Di Castro C, Grilli M 1988 *Physica* C **153–5** 1659
Kotliar G, Lee P A and Read N 1988 *Physica* C **153–5** 538
[8] Mancini F, Marinaro M and Nakano Y 1989 *Physica* B **159** 330
Noce C and Romano A 1989 *J. Phys.: Condens. Matter* **1** 8347
[9] Anda E V 1981 *J. Phys. C: Solid State Phys.* **14** L1037
[10] Noce C and Romano A 1990 *Physica* B **160** 304
[11] Noce C 1989 *PhD Thesis* Università di Napoli
Mancini F, Marinaro M, Nakano Y, Noce C and Romano A 1989 *Nuovo Cimento* D **11** 1709
[12] Marinaro M, Noce C and Romano A 1991 *J. Phys.: Condens. Matter* **3** 3719
[13] Hubbard J 1963 *Proc. R. Soc.* A **276** 238