

GREEN'S FUNCTION FOR THE STRONG COUPLING LIMIT OF THE DEGENERATE HUBBARD MODEL

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ABSTRACT

The asymptotic expression for the one-particle Green's function in the strong coupling limit of the double degenerate Hubbard model containing multiplet terms is obtained for arbitrary band filling within the irreducible Green's function approach. An explicit analytic expression is obtained for the mean-field Green's function, conserving the sum rules for the first few spectral moments. Stability of homogeneous phases is analysed in terms of a single flip spin and orbital excitations. It is shown that degeneracy has an additional enhancing effect on correlation driven interband transfer of spectral weight.

PACS numbers: 75.10.Lp, 74.20.-z

Discovery of superconductivity in fullerenes and of materials with colossal magnetoresistance during recent years have increased the interest for electron systems with physical properties being essentially dependent on orbital degeneracy and strong correlation effects. In many cases the orbitally degenerate Hubbard model (DHM) incorporates the key features of such materials [1], although there are even fewer exact results established for DHM than for the nondegenerate Hubbard model (NHM). In view of complexity of correlated systems, corrections to the atomic limit of one-particle excitation spectrum and spectral weights of correlated bands found by Harris and Lange for NHM [2] by means of perturbation theory based on canonical transformations provide an important exact result which serves as a test for different approximations. A similar derivation for DHM has not been carried out yet. In the present paper the Green's function for the strong coupling limit of the DHM is obtained by means of irreducible Green's function approach [3] - [6] which is closely related to canonical perturbation theory because of its spectral moment conserving construction. As was explicitly proved in [7] for the NHM, the first couples of spectral moments of correlated bands obtained within mean-field decoupling are identical to those of canonical perturbation theory to first order in t/U (t is the n.n. hopping amplitude and U the Coulomb repulsion).

There are fundamental problems why there is still no established regular many body method available for investigation of such systems. If the electron-electron correlation is strong enough we can rely no more on the well elaborated weak-coupling perturbative treatment and have to consider the two-particle interaction from the very beginning by adopting some kind of localized picture of excitations in a solid as a starting point. Then a qualitatively new complication one has to resolve is the large degeneracy of the ground state of the H_0 Hamiltonian consisting of separate atoms or clusters on a lattice. Factorization of the zero-order density matrix over the lattice sites in the atomic limit, as opposed to its factorization over the quasi-wave vectors in the free electron limit, can not be used to construct a formal expansion with respect to perturbing interaction in terms of Wick's theorem

(regular decomposition of arising many-particle expectation values into zero-order quantities). The correct zero-order wave-functions should have the degeneracy lifted by perturbation in the first or second order by a site-non-diagonal perturbation which, in general, would make the zero-order density matrix nondiagonal. On the other hand, a theoretical treatment should also be able to describe phase transitions, i.e. to contain infinite partial summations of rearranged series. Another problem arising with Wick theorem based expansions over the localized limit at non-zero temperature is the analytic continuation of the thermodynamic (Matsubara, or discrete frequency) GF from imaginary to real frequency axis when the GF has branch cuts (a feature already present in second order). The mentioned difficulties can lead in some cases to violation of spectral sum rules even for the zero order moment [8]. The method of irreducible two-time thermodynamic Green's function allows to dispose of these complications by considering the equations of motion for the full (retarded) GF and employing the quite general principles of orthogonalization and linearization for their regular decoupling. There exist different formulations or variants of this approach sharing the same main idea, such as Roth's pole approximation [9], cumulant expansion and projection technique [10], [11], the spectral density approach [12], spectral moment conserving decoupling of the equations of motion [13], Cluster Mean Field approach [14]. Such a decoupling was shown to be related to the variational principle [15] and can also be put into the framework of Baym-Kadanoff formulation [16]. Relation of the irreducible GF method to diagram perturbation expansion is not straightforward but can be shown to have correspondence in some cases [17].

The Hamiltonian of DHM can be written in the form:

$$\begin{aligned}
 H &= H_0 + H_1 - \mu \sum_{i,\alpha,\sigma} n_{i\alpha\sigma}; \\
 H_0 &= U_{\parallel} \sum_{i,\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + U_{\perp} \sum_{i,\sigma} \sum_{(\alpha,\beta)} n_{i\alpha\sigma} n_{i\beta\bar{\sigma}} + (U_{\perp} - J) \sum_{i,\sigma} \sum_{(\alpha,\beta)} n_{i\alpha\sigma} n_{i\beta\sigma} \\
 &\quad - J \sum_{i,\sigma} \sum_{(\alpha,\beta)} c_{i\alpha\sigma}^+ c_{i\alpha\bar{\sigma}} c_{i\beta\bar{\sigma}}^+ c_{i\beta\sigma} + J \sum_i \sum_{\alpha \neq \beta} c_{i\alpha\uparrow}^+ c_{i\alpha\downarrow}^+ c_{i\beta\downarrow} c_{i\beta\uparrow} \\
 H_1 &= \sum_{\alpha,\sigma} \sum_{(i,j)} t_{ij} c_{i\alpha\sigma}^+ c_{j\alpha\sigma} \tag{1}
 \end{aligned}$$

Indices i ; α and σ stand for a lattice site, orbital and spin respectively ($i=1,\dots, N$; $\alpha=1,\dots, M$), $n_{i\alpha\sigma} \equiv c_{i\alpha\sigma}^+ c_{i\alpha\sigma}$, the sums (α, β) are over non-equivalent pairs and $\bar{\sigma} = -\sigma$. Relation between the coupling parameters $U_{\parallel} = U_{\perp} + 2J$ which follows from the equivalence of the degenerate orbitals with respect to Coulomb interaction is not of significance in the present context. For a bipartite lattice with n.n. hopping the Hamiltonian

has a useful symmetry property with respect to electron-hole canonical transformation :

$$c_{i\alpha\sigma} \rightarrow (-1)^i \times c_{i\alpha\sigma}^+ ; \quad (n_{i\alpha\sigma} \rightarrow 1 - n_{i\alpha\sigma}) \tag{2}$$

$$H(t; \mu; U_{\parallel}; U_{\perp}; J) \rightarrow H(t; U_{\parallel} + (M - 1) \times (2U_{\perp} - J) - \mu; U_{\parallel}; U_{\perp}; J)$$

$$+ \left[\frac{1}{2} (U_{\parallel} + (M-1) \times (2U_{\perp} - J)) - \mu \right] \times \sum_{i, \alpha, \sigma} (1)$$

From the invariance condition we readily obtain the exact value of the chemical potential μ at half-filling (one electron per site and orbital on average: $\frac{1}{N \times M} \sum_{i, \alpha, \sigma} \langle n_{i\alpha\sigma} \rangle = \frac{1}{N \times M} \sum_{i, \alpha, \sigma} (1 - \langle n_{i\alpha\sigma} \rangle) = 1$, or equal number of holes and electrons) which is independent of temperature and transfer integral and stays at the center of mass of the atomic levels' structure:

$$\mu = [U_{\parallel} + (M-1) \times (2U_{\perp} - J)] / 2 \quad (3)$$

The retarded GF to be considered below is defined as a propagator of a generalized state-vector \vec{A} ($\vec{A}_{i\sigma} = \{A_{i\sigma}^{\lambda}\}$):

$$G^{\lambda\mu}(i, \sigma, t | j, \sigma', t') \equiv -i\theta(t-t') \left\langle \left\{ \vec{A}_{i\sigma}^{\lambda}(t) ; \vec{A}_{j\sigma'}^{\mu+}(t') \right\} \right\rangle \equiv \langle \langle A | A^+ \rangle \rangle \quad (4)$$

In (4) operators are in Heisenberg representation, $\theta(t-t')$ is the step function and $\langle \{.,.\} \rangle$ means quantum statistical average of an anticommutator. Adequate choice of \vec{A} is crucial for the method to give sensible results. As for the above model we start from the localized picture the basis set has to give a complete description of the atomic limit. Then for the double DHM \vec{A} can be defined as follows ($a_{i\sigma} \equiv c_{i1\sigma}$, $b_{i\sigma} \equiv c_{i2\sigma}$, $n_{i\sigma} \equiv a_{i\sigma}^+ a_{i\sigma}$, $m_{i\sigma} \equiv b_{i\sigma}^+ b_{i\sigma}$):

$$A_{i\sigma}^1 = a_{i\sigma}, \quad A_{i\sigma}^2 = n_{i\bar{\sigma}} a_{i\sigma}, \quad A_{i\sigma}^3 = m_{i\bar{\sigma}} a_{i\sigma}, \quad A_{i\sigma}^4 = m_{i\sigma} a_{i\sigma}, \quad A_{i\sigma}^5 = n_{i\bar{\sigma}} m_{i\bar{\sigma}} a_{i\sigma},$$

$$A_{i\sigma}^6 = n_{i\bar{\sigma}} m_{i\sigma} a_{i\sigma}, \quad A_{i\sigma}^7 = m_{i\bar{\sigma}} m_{i\sigma} a_{i\sigma}, \quad A_{i\sigma}^8 = n_{i\bar{\sigma}} m_{i\bar{\sigma}} m_{i\sigma} a_{i\sigma},$$

$$A_{i\sigma}^9 = b_{i\sigma}, \quad \dots, \quad A_{i\sigma}^{16} = m_{i\bar{\sigma}} n_{i\bar{\sigma}} n_{i\sigma} b_{i\sigma}. \quad (5)$$

where the density operators $n_{i\sigma}$ and $m_{i\sigma}$ are meant to project the probe excitations $a_{i\sigma}$ and $b_{i\sigma}$ onto all the possible site occupations. The state vector which arises on the r.h.s of the equation of motion for $\vec{A}(t)$ as a result of commutation of A^{λ} with the Hamiltonian

$$i \frac{d}{dt} A^{\lambda}(t) = [A^{\lambda}(t); H] = K^{\lambda\mu} A^{\mu}(t) + B^{\lambda}(t), \quad (6)$$

is split according to Gram-Schmidt orthogonalization procedure into "longitudinal" and "transverse" (or irreducible) components. The latter (vector \vec{B}) describes scattering of states out of the initial set due to inelastic processes and is responsible for lifetime effects of "longitudinal" states. For the retarded GF the appropriate definition of the scalar product required for orthogonalization is the expectation value of an anticommutator. Then the orthogonality condition $\langle \{ \vec{B}(t) ; \vec{A}^+(t) \} \rangle = 0$ defines the matrix elements of $K^{\lambda\mu}$ in terms of static expectation values:

$$K^{\lambda\nu} \langle \{ A^{\nu}(t) ; A^{\mu+}(t) \} \rangle = \left\langle \left\{ [A^{\lambda}(t); H] ; A^{\mu+}(t) \right\} \right\rangle \quad (7)$$

The equation of motion for the GF resulting from (5) and (6) is

$$i \frac{d}{dt} G^{\lambda\mu}(i, \sigma, t | i', \sigma', t') = \delta(i, i') \delta(\sigma, \sigma') \times \left\langle \left\{ A^\nu ; A^{\mu+} \right\} \right\rangle + \sum_{j, \nu, \sigma''} K^{\lambda\nu}(i, \sigma | j, \sigma'') G^{\nu\mu}(j, \sigma'', t | i', \sigma', t') + \left\langle \left\langle B | A^+ \right\rangle \right\rangle \quad (8)$$

The mean-field approximation is obtained by linearization of (8) and self-consistent determination of static averages in $K^{\lambda\nu}$. If we would have restricted our operator space to one-particle components only (A^l and A^p) the mean-field solution would lead to the usual Hartree-Fock approximation. In general, as is known for the NHM too, not all of the static expectation values can be determined self-consistently within the linearized equation (8) and one has to consider the equation of motion for the irreducible GF, i.e. the last term, or decouple these averages by, e.g. HF to fit into the initial operator space (details can be found in [Zubarev],[Kuzemsky]). In the frequency representation the linearized equation of motion takes the form

$$G^{\lambda\mu}(\omega) = M_0^{\lambda\nu_1} (\omega M_0 - M_1)_{\nu_1 \nu_2}^{-1} M_0^{\nu_2\mu} \quad (9)$$

where $M_0^{\lambda\mu}(i, \sigma | i', \sigma') = \left\langle \left\{ A_{i\sigma}^\lambda ; A_{i'\sigma'}^{\mu+} \right\} \right\rangle$ is the zero-order spectral moment matrix (or "susceptibility" matrix) and $M_1^{\lambda\mu}(i, \sigma | i', \sigma') = \left\langle \left[\left[A_{i\sigma}^\lambda ; H \right] ; A_{i'\sigma'}^{\mu+} \right] \right\rangle$ is the first-order spectral moment (or "energy") matrix, lattice and spin summations are implicit. The generalized spectral density function has the matrix form too

$$S_{ij}^{\lambda\mu}(\omega) = -\frac{1}{\pi} \text{Im} G_{ij}^{\lambda\mu}(\omega + i0^+) \quad (10)$$

The formal solution (9) looks very complicated and physically not transparent, but one can expect to find a more revealing representation for it in the strong coupling limit. To simplify the discussion we assume a uniform spin and orbital ordering which allow a simple diagonalization over lattice space variables by the Fourier transform and we also neglect the last two terms in the Hamiltonian (1) (spin-flip and orbital pair excitation). First we note that the structure of the atomic GF ($t_{ij} = 0$) shown in (11) below is quite simple: the spectral weights of atomic resonances P_λ are just the probabilities of having the site occupation corresponding to the respective resonance energy E_λ .

$$\frac{1}{F_1^{(0)}(\omega)} \equiv \left\langle \left\langle a_{i\sigma} | a_{i\sigma}^+ \right\rangle \right\rangle = \sum_{\lambda=1}^8 P_\lambda / (\omega + \mu - E_\lambda);$$

$$\frac{1}{F_2^{(0)}(\omega)} \equiv \left\langle \left\langle n_{i-\sigma} a_{i\sigma} | a_{i\sigma}^+ \right\rangle \right\rangle = P_4 (\omega + \mu - E_4) + P_6 (\omega + \mu - E_6)$$

$$+ P_7 (\omega + \mu - E_7) + P_8 (\omega + \mu - E_8);$$

...

$$\frac{1}{F_8^{(0)}(\omega)} \equiv \left\langle \left\langle n_{i-\sigma} m_{i-\sigma} m_{i\sigma} a_{i\sigma} \left| a_{i\sigma}^+ \right. \right\rangle \right\rangle = P_8 (\omega + \mu - E_8). \quad (11)$$

Where

$$P_1 = \langle (1 - n_{i\bar{\sigma}})(1 - m_{i\bar{\sigma}})(1 - m_{i\sigma}) \rangle, \quad E_1 = 0; \quad P_2 = \langle (1 - n_{i\bar{\sigma}})(1 - m_{i\bar{\sigma}})m_{i\sigma} \rangle, \quad E_2 = U_{\perp} - J;$$

$$P_3 = \langle (1 - n_{i\bar{\sigma}})m_{i\bar{\sigma}}(1 - m_{i\sigma}) \rangle, \quad E_3 = U_{\perp}; \quad P_4 = \langle n_{i\bar{\sigma}}(1 - m_{i\bar{\sigma}})(1 - m_{i\sigma}) \rangle, \quad E_4 = U_{\parallel};$$

$$P_5 = \langle (1 - n_{i\bar{\sigma}})m_{i\bar{\sigma}}m_{i\sigma} \rangle, \quad E_5 = 2U_{\gamma} - J; \quad P_6 = \langle n_{i\bar{\sigma}}(1 - m_{i\bar{\sigma}})m_{i\sigma} \rangle, \quad E_6 = U_{\parallel} + U_{\perp} - J;$$

$$P_7 = \langle n_{i\bar{\sigma}}m_{i\bar{\sigma}}(1 - m_{i\sigma}) \rangle, \quad E_7 = U_{\parallel} + U_{\perp}; \quad P_8 = \langle n_{i\bar{\sigma}}m_{i\bar{\sigma}}m_{i\sigma} \rangle, \quad E_8 = 2U_{\perp} + U_{\parallel} - J;$$

The remaining functions ($\lambda = 9, \dots, 16$) are obtained from (11) by interchanging orbitals according to the definitions in (5). The neglected flip-terms of the Hamiltonian (1) would lead to additional excitation energy splittings bringing their number to 12 as well as to more complicated weight factors. The simplest approximation describing the formation of correlated bands (a generalization of the Hubbard I approximation [18]) can be obtained from (9) by decoupling intersite averages in $M_1^{\lambda\mu}$ into single site products. This solution can also be cast into a physically transparent form reflecting the formation of correlated bands out of respective atomic transitions (we make use of Hubbard's notations):

$$G^{1,1}(\mathbf{k}, \omega) = \left\langle \left\langle a_{\mathbf{k}\sigma} \left| a_{\mathbf{k}\sigma}^+ \right. \right\rangle \right\rangle_{\omega} = \frac{1}{F_1(\omega) - \varepsilon(\mathbf{k})},$$

$$G^{2,1}(\mathbf{k}, \omega) = \frac{F_1(\omega)}{F_2(\omega)} \times \frac{1}{F_1(\omega) - \varepsilon(\mathbf{k})},$$

...

$$G^{8,1}(\mathbf{k}, \omega) = \frac{F_1(\omega)}{F_8(\omega)} \times \frac{1}{F_1(\omega) - \varepsilon(\mathbf{k})}. \quad (12)$$

where $\varepsilon(\mathbf{k})$ is the Fourier transform of the transfer integral. Excitation spectrum is determined by the poles of the one-particle GF $G^{1,1}(\mathbf{k}, \omega)$. With the higher order propagators which are modulated by the ratio of respective atomic GF equations (12) allow to determine all the static expectation values and the chemical potential selfconsistently:

$$\langle n_{i\sigma} \rangle = \int_{-\infty}^{\mu} S_{ii}^{1,1}(\omega) d\omega,$$

$$\langle n_{i-\sigma} n_{i\sigma} \rangle = \int_{-\infty}^{\mu} S_{ii}^{2,1}(\omega) d\omega, \quad (13)$$

...

Then the ground state energy per lattice site is determined by the expression:

$$E_{GS} = \frac{1}{2N} \sum_{\mathbf{k} \in \text{B.Z.}} \sum_{\sigma, \alpha} \int_{-\infty}^{\mu} S_{\sigma}^{\alpha}(\mathbf{k}, \omega) [\omega + \varepsilon(\mathbf{k})] d\omega,$$

where $S_{\sigma}^{\alpha}(\mathbf{k}, \omega)$ is the spectral density for spin σ and orbital α .

As follows from (12) the middle of each sub-band coincides with the respective atomic level. This is, of course, a drawback of the decoupling which introduces errors of order $O(t)$ as will be seen below. Nevertheless we expect that corrections to this approximation contained in (9), which is consistent with the first order of the strong coupling perturbation theory, will follow some regular pattern. First, we note that as compared to Hubbard I solution the new terms entering the $M_1^{\lambda\mu}$ - matrix are proportional to the transfer integral and can be divided in two categories: local and nonlocal. The local corrections can be described as pairs of differences between the correlated kinetic energies in the electron ($n_{i\sigma}$) and hole ($1 - n_{i\sigma}$) states of the probe excitation $a_{i\sigma}^+$. The intersite hopping within each term of a pair is determined by motion of the projecting density operators ($n_{i\bar{\sigma}}, m_{i\bar{\sigma}}, m_{i\sigma}$) associated to the probe excitation and which are present in both A^{λ} and A^{μ} - components of the energy matrix $M_1^{\lambda\mu}$ (see (5)). The associated projecting density operators present only in A^{λ} or A^{μ} enter unchanged in both expectation values. The described structure of corrections follows from the hermiticity of $M_1^{\lambda\mu}$ and commutation of \bar{A} with kinetic energy term. For instance, the diagonal element $M_1^{2,2}(i, \sigma | j, \sigma)$ is identical to the familiar local term obtained by Roth for the NHM ($i = j$) and we show here only those responsible for the correction to Hubbard I:

$$-\sum_{l(\neq i)} t_{il} \left[\langle (1 - n_{i\sigma}) \times a_{i\bar{\sigma}}^+ a_{l\bar{\sigma}} \times (1 - n_{l\sigma}) \rangle - \langle n_{i\sigma} \times a_{i\bar{\sigma}}^+ a_{l\bar{\sigma}} \times n_{l\sigma} \rangle \right] =$$

$$-\sum_{l(\neq i)} t_{il} \left[\langle (1 - n_{i\sigma} - n_{l\sigma}) a_{i\bar{\sigma}}^+ a_{l\bar{\sigma}} \rangle \right]. \tag{14}$$

To exemplify the orbital degeneracy related features described above we show the local correction to $M_1^{7,3}(i, \sigma | i, \sigma)$ ($= M_1^{3,7}(i, \sigma | i, \sigma)$) :

$$-\sum_{l(\neq i)} t_{il} \left[\langle (1 - n_{i\sigma} - n_{l\sigma}) m_{i\sigma} b_{i\bar{\sigma}}^+ b_{l\bar{\sigma}} \rangle \right].$$

The non-local corrections are determined by charge, spin, pseudospin (orbital), mixed spin-pseudospin and pair fluctuations. The respective terms for $M_1^{2,2}$ and $M_1^{7,3}$ are shown below:

$$t_{ij} \left[\langle n_{i\bar{\sigma}} n_{j\bar{\sigma}} \rangle - \langle n_{i\bar{\sigma}} \rangle \langle n_{j\bar{\sigma}} \rangle + \langle a_{i\sigma}^+ a_{i\bar{\sigma}} a_{j\bar{\sigma}}^+ a_{j\sigma} \rangle - \langle a_{i\sigma}^+ a_{i\bar{\sigma}}^+ a_{j\bar{\sigma}} a_{j\sigma} \rangle \right], \tag{15}$$

$$t_{ij} \left[\langle m_{i\sigma} m_{i\bar{\sigma}} m_{j\bar{\sigma}} \rangle - \langle m_{i\sigma} m_{i\bar{\sigma}} \rangle \langle m_{j\bar{\sigma}} \rangle + \right.$$

$$\langle m_{i\sigma} (b_{i\bar{\sigma}}^+ a_{i\sigma}) (a_{j\sigma}^+ b_{j\bar{\sigma}}) \rangle - \langle (a_{j\sigma}^+ b_{j\bar{\sigma}}^+) (b_{i\bar{\sigma}} a_{i\sigma}) m_{i\sigma} \rangle].$$

Naturally, if only one orbital is considered (9) reduces to Roth's solution which is known to agree with the exact result of Harris and Lange[Harris] mentioned above. For the purpose of comparison we rewrite the strong coupling expression which follows from[Roth] as:

$$\begin{aligned} \langle \langle a_{\mathbf{k}\sigma} | a_{\mathbf{k}\sigma}^+ \rangle \rangle_{\omega} &= \frac{1}{F^{(0)}(\mathbf{k}, \omega + T_R(\mathbf{k}) / (1 - n_{i\bar{\sigma}}) n_{i\bar{\sigma}}) - \varepsilon(\mathbf{k}) - T_R(\mathbf{k}) / (1 - n_{i\bar{\sigma}}) n_{i\bar{\sigma}}} \\ &= \frac{1 - n_{i\bar{\sigma}} - 2\varepsilon(\mathbf{k}) n_{i\bar{\sigma}}(1 - n_{i\bar{\sigma}}) - 2 T_R(\mathbf{k}) / U + O(t^2 / U^2)}{\omega + \mu - \varepsilon(\mathbf{k}) (1 - n_{i\bar{\sigma}}) + T_R(\mathbf{k}) / (1 - n_{i\bar{\sigma}}) + O(t^2 / U)} \\ &\quad + \frac{n_{i\bar{\sigma}} + 2\varepsilon(\mathbf{k}) n_{i\bar{\sigma}}(1 - n_{i\bar{\sigma}}) + 2 T_R(\mathbf{k}) / U + O(t^2 / U^2)}{\omega - U + \mu - \varepsilon(\mathbf{k}) n_{i\bar{\sigma}} + T_R(\mathbf{k}) / n_{i\bar{\sigma}} + O(t^2 / U)}; \end{aligned} \quad (16)$$

where $(F^{(0)})^{-1}$ is the atomic Green function and $T_R(\mathbf{k})$ is the Fourier transform of the correction terms in $M_1^{2,2}(i, \sigma | j, \sigma)$. Then for the double DHM in the limit of large Coulomb parameters ($U_{\parallel}, U_{\perp}, |J| \gg |t|$) the asymptotic form of the solution can be reduced to a rather simple one which is a generalization of (16) for the double degenerate case:

$$\langle \langle a_{\mathbf{k}\sigma} | a_{\mathbf{k}\sigma}^+ \rangle \rangle_{\omega} = \sum_{\lambda=1}^8 \frac{\tilde{P}_{\lambda} + O(t^2 / U^2)}{\omega + \mu - E_{\lambda} - \varepsilon(\mathbf{k})P_{\lambda} + T_{\lambda}(\mathbf{k}) / P_{\lambda} + O(t^2 / U)}. \quad (17)$$

One can see that the resonance energies and weight factors are shifted compared to the atomic, "bare", counterparts of $F_1^{(0)}(\omega)$ in (11) by quantities proportional to the hopping amplitude t . By defining the cumulants as

$$\langle A_i B_j \rangle_c \equiv \langle A_i B_j \rangle - \langle A_i \rangle \langle B_j \rangle,$$

the energy shifts are

$$T_1(\mathbf{k}) =$$

$$\sum_{l(\neq i)} t_{il} \exp(-i\mathbf{k}\mathbf{R}_{il}) \langle (1 - n_{i\bar{\sigma}})(1 - m_{i\bar{\sigma}})(1 - m_{i\sigma})(1 - n_{l\bar{\sigma}})(1 - m_{l\bar{\sigma}})(1 - m_{l\sigma}) \rangle_c$$

$$- \sum_{l(\neq i)} t_{il} \langle (1 - 2n_{i\sigma})(1 - m_{i\bar{\sigma}})(1 - m_{i\sigma}) a_{i\bar{\sigma}}^+ a_{l\bar{\sigma}} \rangle$$

$$- \sum_{l(\neq i)} t_{il} \exp(-i\mathbf{k}\mathbf{R}_{il}) \langle (1 - m_{i\bar{\sigma}})(1 - m_{i\sigma}) a_{i\bar{\sigma}}^+ a_{i\bar{\sigma}} a_{l\bar{\sigma}}^+ a_{l\sigma} (1 - m_{l\bar{\sigma}})(1 - m_{l\sigma}) \rangle$$

$$+ \sum_{l(\neq i)} t_{il} \exp(-i\mathbf{k}\mathbf{R}_{il}) \langle (1 - m_{i\bar{\sigma}})(1 - m_{i\sigma}) a_{i\bar{\sigma}}^+ a_{i\bar{\sigma}} a_{l\bar{\sigma}}^+ a_{l\sigma} (1 - m_{l\bar{\sigma}})(1 - m_{l\sigma}) \rangle$$

$$- \sum_{l(\neq i)} t_{il} \langle (1 - 2n_{i\sigma})(1 - n_{i\bar{\sigma}})(1 - m_{i\bar{\sigma}}) b_{i\sigma}^+ b_{l\sigma} \rangle$$

$$- \sum_{l(\neq i)} t_{il} \exp(-i\mathbf{k}\mathbf{R}_{il}) \langle (1 - n_{i\bar{\sigma}})(1 - m_{i\bar{\sigma}}) a_{i\bar{\sigma}}^+ b_{i\sigma} b_{l\sigma}^+ a_{l\sigma} (1 - n_{l\bar{\sigma}})(1 - m_{l\bar{\sigma}}) \rangle$$

$$+ \sum_{l(\neq i)} t_{il} \exp(-i\mathbf{k}\mathbf{R}_{il}) \langle (1 - n_{i\bar{\sigma}})(1 - m_{i\bar{\sigma}}) a_{i\bar{\sigma}}^+ b_{i\sigma} b_{l\sigma}^+ a_{l\sigma} (1 - n_{l\bar{\sigma}})(1 - m_{l\bar{\sigma}}) \rangle$$

$$\begin{aligned}
 & -\sum_{l(\neq i)}' t_{il} \langle (1-2n_{i\sigma})(1-n_{i\bar{\sigma}})(1-m_{i\sigma}) b_{i\bar{\sigma}}^{\dagger} b_{l\bar{\sigma}} \rangle \\
 & -\sum_{l(\neq i)}' t_{il} \exp(-i\mathbf{k}\mathbf{R}_{il}) \langle (1-n_{i\bar{\sigma}})(1-m_{i\sigma}) a_{i\sigma}^{\dagger} b_{i\bar{\sigma}}^{\dagger} b_{l\bar{\sigma}}^{\dagger} a_{l\sigma} (1-n_{l\bar{\sigma}})(1-m_{l\sigma}) \rangle \\
 & +\sum_{l(\neq i)}' t_{il} \exp(-i\mathbf{k}\mathbf{R}_{il}) \langle (1-n_{i\bar{\sigma}})(1-m_{i\sigma}) a_{i\sigma}^{\dagger} b_{i\bar{\sigma}}^{\dagger} b_{l\bar{\sigma}}^{\dagger} a_{l\sigma} (1-n_{l\bar{\sigma}})(1-m_{l\sigma}) \rangle.
 \end{aligned}$$

Below only the local corrections are given, while the structure of the nonlocal corrections is explained in the text.

$$\begin{aligned}
 T_2 = & -\sum_{l(\neq i)}' t_{il} \langle (1-2n_{i\sigma}) [m_{i\sigma}(1-m_{i\bar{\sigma}}) a_{i\sigma}^{\dagger} a_{l\bar{\sigma}} + \\
 & m_{i\sigma}(1-n_{i\bar{\sigma}}) b_{i\bar{\sigma}}^{\dagger} b_{l\bar{\sigma}} + (1-n_{i\bar{\sigma}})(1-m_{i\bar{\sigma}}) b_{i\sigma}^{\dagger} b_{l\sigma}] \rangle;
 \end{aligned}$$

...

$$T_8 = -\sum_{l(\neq i)}' t_{il} \langle (1-2n_{i\sigma}) [m_{i\bar{\sigma}} m_{i\sigma} a_{i\bar{\sigma}}^{\dagger} a_{l\bar{\sigma}} +$$

$$n_{i\bar{\sigma}} m_{i\bar{\sigma}} b_{i\sigma}^{\dagger} b_{l\sigma} + n_{i\bar{\sigma}} m_{i\sigma} b_{i\bar{\sigma}}^{\dagger} b_{l\bar{\sigma}}] \rangle;$$

and the spectral weights (see the remark above concerning the dispersion correction terms):

$$\begin{aligned}
 \tilde{P}_1 = & P_1 - 2 \times \left[\frac{1}{U_{\square}} \sum_{l(\neq i)}' t_{il} \langle (1-2n_{i\sigma})(1-m_{i\bar{\sigma}})(1-m_{i\sigma}) a_{i\bar{\sigma}}^{\dagger} a_{l\bar{\sigma}} \rangle \right. \\
 & + \varepsilon_k \langle (1-n_{i\bar{\sigma}}) (1-m_{i\bar{\sigma}})(1-m_{i\sigma}) \rangle \langle n_{i\bar{\sigma}} (1-m_{i\bar{\sigma}})(1-m_{i\sigma}) \rangle \\
 & + \frac{1}{U_{\perp}} \sum_{l(\neq i)}' t_{il} \langle (1-2n_{i\sigma})(1-n_{i\bar{\sigma}})(1-m_{i\sigma}) b_{i\bar{\sigma}}^{\dagger} b_{l\bar{\sigma}} \rangle \\
 & \quad \left. + \varepsilon_k \langle (1-n_{i\bar{\sigma}}) (1-m_{i\bar{\sigma}})(1-m_{i\sigma}) \rangle \langle (1-n_{i\bar{\sigma}}) (1-m_{i\sigma}) m_{i\bar{\sigma}} \rangle \right. \\
 & \left. + \frac{1}{U_{\perp} - J} \sum_{l(\neq i)}' t_{il} \langle (1-2n_{i\sigma})(1-n_{i\bar{\sigma}})(1-m_{i\bar{\sigma}}) b_{i\sigma}^{\dagger} b_{l\sigma} \rangle \right] \\
 & + \varepsilon_k \langle (1-n_{i\bar{\sigma}}) (1-m_{i\bar{\sigma}})(1-m_{i\sigma}) \rangle \langle (1-n_{i\bar{\sigma}}) (1-m_{i\bar{\sigma}}) m_{i\sigma} \rangle];
 \end{aligned}$$

$$\tilde{P}_2 = P_2 - 2 \times \left[\frac{1}{U_{\square}} \sum_{l(\neq i)}' t_{il} \langle (1-2n_{i\sigma})(1-m_{i\bar{\sigma}}) m_{i\sigma} a_{i\bar{\sigma}}^{\dagger} a_{l\bar{\sigma}} \rangle \right.$$

$$\left. + \frac{1}{U_{\perp}} \sum_{l(\neq i)}' t_{il} \langle (1-2n_{i\sigma})(1-n_{i\bar{\sigma}}) m_{i\sigma} b_{i\bar{\sigma}}^{\dagger} b_{l\bar{\sigma}} \rangle \right]$$

$$\begin{aligned}
 & + \frac{-1}{U_{\perp} - J} \sum'_{l(\neq i)} t_{il} \langle (1 - 2n_{i\sigma}) (1 - n_{i\bar{\sigma}})(1 - m_{i\bar{\sigma}}) b_{i\sigma}^+ b_{l\sigma} \rangle \Big]; \\
 & \dots ; \\
 \tilde{P}_8 = P_8 - 2 \times & \left[\frac{-1}{U_{\parallel}} \sum'_{l(\neq i)} t_{il} \langle (1 - 2n_{i\sigma}) m_{i\bar{\sigma}} m_{i\sigma} a_{i\bar{\sigma}}^+ a_{l\bar{\sigma}} \rangle \right. \\
 & + \frac{-1}{U_{\perp}} \sum'_{l(\neq i)} t_{il} \langle (1 - 2n_{i\sigma}) n_{i\bar{\sigma}} m_{i\sigma} b_{i\bar{\sigma}}^+ b_{l\bar{\sigma}} \rangle \\
 & \left. + \frac{-1}{U_{\perp} - J} \sum'_{l(\neq i)} t_{il} \langle (1 - 2n_{i\sigma}) n_{i\bar{\sigma}} m_{i\bar{\sigma}} b_{i\sigma}^+ b_{l\sigma} \rangle \right].
 \end{aligned} \tag{18}$$

The structure of the strong coupling solution for the one-particle GF (17) and (18) from the point of view of perturbation theory is an infinite chain of renormalized atomic GF connected by intersite hopping. As can be seen from the above expressions, the excitation energy shifts of the atomic GF contain both local and nonlocal additive parts. The local parts are determined by kinetic motion of each projecting operator contributing to the site occupation, or spectral weight, of the respective atomic resonance. The nonlocal parts contain the obvious charge-charge cumulant corresponding to the respective atomic resonance as well as all the possible "transverse" correlation functions (double occupation, spin-spin, orbit-orbit and mixed) constructed by combining the "moving", intersite, operator from the respective local correction term with the operator $a_{i\sigma}^+ a_{l\sigma}$. Renormalization of the spectral weight of atomic excitations is determined by the same partial shift components divided by the Coulomb parameter corresponding to the interaction of the probe excitation density ($n_{i\sigma}$) and the respective density of the moving electron (+1) or hole (-1) (18) projecting operator. The above equations also explicitly exhibit the symmetry properties of the GF under the electron-hole transformation which are important to preserve when considering self-consistent solutions at finite values of parameters as, for instance, the exact vanishing of the sum of all spectral weight corrections. Comparison to the Roth's solution suggests a general trend for the renormalizations in the strong coupling limit for higher degeneracy. Therefore we have performed analogous calculations for triple degenerate HM which indeed have the same structure.

Stability of the saturated ferromagnetism in the NHM at finite doping away from the Nagaoka single hole (electron) doping has been studied in numerous papers (see, e.g.[19]). In this respect it is clear that orbital degrees of freedom are irrelevant provided there is less than one electron per lattice site, as only one spin and orbital state is occupied. On the contrary, for larger hole (electron) qualitatively different behaviour is to be expected. For instance, due to the Hund coupling term, as soon as double occupancy becomes possible, the electrons would prefer to occupy local triplet states. As was rigorously proved in [20] for the double degenerate HM, this would lead to a global saturated spin and orbital ferromagnetic state for $N_e = N + 1$, where N_e is the number of electrons, and moreover, that this state is the ground state for the one dimensional lattice as well, in contrast to the NHM. It has been conjectured

that this remains valid for the whole doping region $N < N_e < 2N$. We show however that there exists a critical electron concentration, where the orbital saturation breaks down due to instability with respect to orbital flipping. Indeed, let us consider the spectral density function of a saturated state at an electron concentration $c = n_\sigma + m_\sigma > 1$ with $n_\sigma = 1$. The orbital flip, $b_\sigma^+ a_\sigma$, creates a hole in the initially filled a_σ band and an electron at the Fermi energy in the b_σ band. The stability criterion means that the energy of such an excitation is positive. The critical concentration is reached as soon as the inequality is violated, i.e., for the hole created at the top of the a_σ band the excitation energy vanishes, signalling an instability with respect to orbital density wave state with a wave vector $k_F - k_T$, where k_T corresponds to the top of the band. Keeping only the relevant terms in the above expressions, we can write the spectral densities for the chosen states:

$$S_\sigma^a(\mathbf{k}, \omega) = \langle (1 - n_{i\bar{\sigma}})(1 - m_{i\bar{\sigma}})m_{i\sigma} \rangle \delta(\omega - E^a)$$

$$E^a = U_\perp - J + \varepsilon(\mathbf{k}) \langle m_{i\sigma} \rangle - T^a(\mathbf{k}) / \langle m_{i\sigma} \rangle$$

$$\begin{aligned} T^a(\mathbf{k}) &= - \sum_{l(\neq i)} t_{il} \langle (1 - 2n_{i\sigma}) (1 - n_{i\bar{\sigma}})(1 - m_{i\bar{\sigma}})b_{i\sigma}^+ b_{l\sigma} \rangle \\ &\quad + \sum_{l(\neq i)} t_{il} \exp(-i\mathbf{k}\mathbf{R}_{il}) \langle (1 - n_{i\bar{\sigma}})(1 - m_{i\bar{\sigma}})m_{i\sigma}m_{l\sigma} (1 - n_{l\bar{\sigma}})(1 - m_{l\bar{\sigma}}) \rangle_c \\ &= \sum_{l(\neq i)} t_{il} \langle b_{i\sigma}^+ b_{l\sigma} \rangle + \varepsilon(\mathbf{k}) \langle m_{i\sigma}m_{l\sigma} \rangle_c \end{aligned}$$

$$\begin{aligned} S_\sigma^b(\mathbf{k}, \omega) &= \langle (1 - n_{i\bar{\sigma}})(1 - m_{i\bar{\sigma}})n_{i\sigma} \rangle \delta(\omega - E^b) \\ &= \delta(\omega - E^b) \end{aligned}$$

$$\begin{aligned} E^b &= U_\perp - J + \varepsilon(\mathbf{k}) \langle n_{i\sigma} \rangle - T^b(\mathbf{k}) / \langle n_{i\sigma} \rangle \\ &= U_\perp - J + \varepsilon(\mathbf{k}) \end{aligned}$$

The expectation values can be expressed in terms of the spectral densities and provide the selfconsistency:

$$\begin{aligned} \langle m_{i\sigma} \rangle &= \int_{-WB}^{E_F} \rho(E) dE \\ \sum_{l(\neq i)} t_{il} \langle b_{i\sigma}^+ b_{l\sigma} \rangle &= \int_{-WB}^{E_F} E \rho(E) dE \\ \langle m_{i\sigma}m_{l\sigma} \rangle_c &= 4 \left(\int_{-WB}^{E_F} E \rho(E) dE \right)^2 \end{aligned}$$

where W_B (W_T) are respectively the bottom and the top of the $\varepsilon(\mathbf{k})$ band with the respective density $\rho(E)$. The band width $W = ET - WB = 2z|t|$, where z is the number of nearest neighbour sites. We have also adopted the energy units with $W = 1$. Thus, for a bipartite lattice the critical concentration $c = \langle m_{i\sigma} \rangle_{critical}$ is determined from the equation

$$E_F - cW_T \left(1 - \frac{4}{c^2} \left(\int_{-WB}^{E_F} E \rho(E) dE \right)^2 \right) + \frac{1}{c} \int_{-WB}^{E_F} E \rho(E) dE = 0$$

The nonlocal correction, given by the second term in the brackets, represents a band narrowing effect which reduces the kinetic energy gain of the flipped orbital state b_{σ}^+ , thus favoring the stability of the saturated state. The last term, representing the local correction, or rigid energy shift, describes the loss of kinetic energy by the majority occupation state a_{σ} due to orbital flipping and is the main driving force for the stability at low c . For a square lattice we find $E_F = 0.003$ and $c = 0.49$ (without nonlocal correction: $E_F = 0.068$ and $c = 0.38$). For a simple cubic lattice: $E_F = 0.103$ and $c = 0.323$ (without nonlocal correction: $E_F = 0.159$ and $c = 0.226$). For the frustrated fcc lattice and $t > 0$ the fully saturated state is not possible for this concentration since the instability occurs at $c = 0$, however for $t < 0$ the fully saturated state is stable up to $c = 1$.

One of most striking effects of strong correlations which has direct implications for the electron density of states related spectroscopies consists in transfer of a large amount of states between the correlated bands upon doping. The static part of this effect is already present in the atomic limit: if, e.g., a hole is introduced into a half-filled non-degenerate orbital, there are two states available to add an electron on the low energy level and no states for an electron to be added on high energy level. In this way one state has been transferred from high to low energy upon hole doping. If the orbital is degenerate, the number of transferred states increases [21]. The kinetic enhancement of spectral weight transfer is due to perturbation (t) induced interference between the ground and the excited states which leads to redistribution of surrounding charges on a lattice upon removal (or addition) of an electron from a site [2], [21]. As follows from the expressions obtained above, the kinetic contribution to this effect for degenerate systems is proportional to the number of degenerate orbitals upon which the charges are being redistributed to increase the number of states in the low energy at the expense of high energy region of the spectrum.

ACKNOWLEDGEMENTS.

Financial support from the Supreme Council for Scientific and Technological Development of Moldova is acknowledged.

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