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Metallic ferromagnetism in the presence of orbital degeneracy

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Abstract

The effect of orbital degeneracy on metallic ferromagnetism is considered in the strong coupling limit of the Hubbard model within a generalized Roth approximation. For concentrations of less than one electron per lattice site and forbidden double occupancy we find that orbital degeneracy favours magnetic polarization on different lattice structures. The effect is strong enough to induce a ferromagnetic ordering even on frustrated lattices, where polarization is excluded in the absence of degeneracy. We discuss the physical origin of the new results in terms of competition between tendencies towards localization and delocalization.

1. Introduction

Metallic ferromagnetism in narrow band systems has been a controversial issue of condensed matter physics for a long time. This controversy stems from the dual character of the electrons responsible for polarization, i.e. they are itinerant electrons described by band theory showing, at the same time, various properties that have been long attributed to localized moments. When the on-site Coulomb interaction is strong, the electrons can minimize the Coulomb repulsion due to the Pauli principle by preferably occupying the same spin sector, resulting in a spin polarized ground state. The Hubbard model [1] was initially introduced to explain magnetism of correlated itinerant electrons in transition metals; however, it turned out to be particularly difficult to establish the existence of ferromagnetic ordering in approaches beyond mean-field theories. It is well known that for the infinite repulsion and for any dimension $d > 1$ this model has a fully polarized ferromagnetic ground state on a bipartite lattice with exactly one hole (Nagaoka theorem [2]). However, the theorem does not address either the finite hole concentration or the finite repulsion cases, these remaining a matter of debate up to the present, despite a large number of both analytical and numerical works on this topic [3]. A significant progress has been achieved recently in understanding the infinite- U limit of the non-degenerate Hubbard model (NHM), e.g. [4–6]. In [7] exact cluster diagonalization and

quantum Monte Carlo calculation studies have found that the paramagnetic state becomes unstable against a non-saturated ferromagnetic phase at a finite hole density. Although this is a very important proof of the existence of a ferromagnetic ordering in a 2D Hubbard model at finite hole concentration, it is still desirable to clarify the physical mechanisms causing polarization on different lattice structures. In particular, it is known that ferromagnetism of non-bipartite lattices is strongly dependent on the sign of the hopping amplitude. For example, for a face centred cubic lattice (FCC) with negative hopping parameter ($t < 0$) there is a general consensus that ferromagnetic polarization does not occur at all, while for the opposite sign ferromagnetism is expected in a very large region of concentrations [4]. This dependence is attributed to the electron–hole asymmetry of the density of states. It has also been pointed out that unlike antiferromagnetism or superconductivity, metallic ferromagnetism is generally a strong coupling phenomenon as far as the original Hubbard model is concerned [8]. Therefore a great deal of research has been focused on what additional factors should be included to describe the essential physics of ferromagnetism. Among others, it is important to consider different Coulomb interaction matrix elements within a single band model [9] or the orbital degeneracy [10] that allows for intra-atomic ferromagnetic Hund coupling, or take both generalizations into account [11]. Besides being a natural component of many real magnetic systems, orbital physics has recently attracted much research interest motivated by the discovery of materials with new properties related to orbital degrees of freedom, such as colossal magnetoresistance manganites [12], superconductivity in fullerenes [13], spin triplet pairing in ruthenates [14], new types of ordering and elementary excitations [15] and others.

The aim of the present paper is to consider a different aspect of the orbital degeneracy related to the kinetic energy of correlated electrons, which is already present in the first order of perturbation theory. We will consider the case of a relatively small concentration of less than one electron per lattice site and the strong coupling limit with excluded double occupancy. Under these restrictions we may neglect some interactions, such as the Hund coupling, superexchange or double exchange mechanisms, which are responsible for a rich variety of charge, orbital and spin orderings at finite coupling strength [16]. The major role of the Hund parameter in orbitally degenerate systems has been emphasized already in earlier papers [17–19]. For instance, it has been rigorously proved [20] that for the strong coupling limit of the degenerate Hubbard model (DHM) an infinitesimal value of this parameter is sufficient to stabilize metallic ferromagnetism even on a periodic chain, where ordering is strictly excluded in the absence of degeneracy [21]. Instead, our aim is to focus on the effect of an enlarged Hilbert space provided by the degeneracy and to reveal another mechanism for ferromagnetism, independent of those mentioned before. On the one hand, our analysis shows that the presence of orbital degeneracy reinforces ferromagnetism on bipartite lattices, despite the expectation that it would favour a disordered state [22] in the considered limit; on the other hand, degeneracy offers a new route to overcome the geometrical constraints that inhibit ferromagnetism on frustrated lattices. The proposed physical interpretation of these results is rather general and can be useful for a deeper understanding of itinerant magnetism.

To investigate the above issues one cannot rely on the standard weak coupling perturbation theory, and we employ the approach by Roth [23] generalized to the case of orbital degeneracy. This approach is related to the irreducible Green function method [24, 25], the spectral density approach [26], the method of projection operators [27], the composite operator method [28], variational wavefunction [29] and some others. Its reliability in the strong coupling limit of the NHM has been demonstrated in previous papers [30] and resides in conservation of higher spectral moments. As demonstrated in [31], it corresponds to the strong coupling canonical perturbation theory and therefore incorporates the correlation effects in a regular way. In this sense the approach is superior to the coherent potential approximation or to the Hubbard I

and III approximations [32]. The generalized Roth approach can therefore serve as a good mean-field starting point for a proper description of dynamical effects; however, this goes beyond the purpose of the present paper. Inclusion of dynamical corrections requires a further development of the theory and remains an open problem even for the NHM [33]. Nevertheless, we do not expect that our predictions on the behaviour of DHM in the considered limit will be qualitatively changed by dynamical corrections since we find that the Roth approach agrees well with recent numerical studies on the strong coupling limit of NHM (see below) as well as with the extension of the Nagaoka theorem to orbital degeneracy proved in [34]. Comparison with some other approaches is also discussed below.

2. The DHM model and the Roth approach

We consider the following Hubbard Hamiltonian for degenerate orbital states:

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

H_0 is the atomic Hamiltonian, where i is the lattice site ($i = 1, \dots, N$), and λ and σ stand for orbital and spin index, respectively ($\lambda = 1, \dots, L$, $\bar{\sigma} = -\sigma$). The parameters U_{\parallel} and U_{\perp} stand for the on-site intra- and inter-orbital Coulomb repulsion, and J is the Hund coupling. The energies are measured with respect to the chemical potential in units of the non-interacting bandwidth W . H_1 is the kinetic term describing hopping of a given spin between identical orbitals on nearest neighbour sites. It is also assumed that $t_{ii} = \frac{1}{N} \sum_{\mathbf{k}} \varepsilon(\mathbf{k}) = 0$. As explained in the introduction, we consider the strong coupling regime with electron concentration $n < 1$, and exclude double occupancy to focus on new effects of the order of W . It will become clear that this scale characterizes a rather non-trivial effective interaction, although in the considered limit H_0 describes a hard core bare interaction.

To calculate the retarded Green function (GF), the matrix propagator of a generalized state-vector $A_{i\sigma} = \{A_i^\alpha\}$, we chose the basis set α of local operators diagonalizing the atomic limit. In the case of a two-fold degeneracy, and neglecting the last two terms in H_0 , the set α has eight components (see the appendix). The local density operators, $n_{i1\bar{\sigma}} \equiv c_{i1\bar{\sigma}}^\dagger c_{i1\bar{\sigma}}$, etc, play the role of projectors onto states with definite occupation numbers. The equation of motion of the generalized state-vector is considered in a split form:

$$i \frac{d}{dt} A^\alpha(t) = [A^\alpha(t); H] = K^{\alpha\gamma} A^\gamma(t) + B^\alpha(t).$$

It is then decoupled according to the orthogonalization and linearization (i.e., neglecting B^α) procedure by requiring that

$$\langle \{ [A^\alpha(t); H] - K^{\alpha\gamma} A^\gamma(t), A^{\beta\dagger}(t) \} \rangle = 0, \tag{2}$$

where $\langle \{ \dots; \dots \} \rangle$ stands for the quantum statistical average of an anticommutator. This allows for obtaining a self-consistent expression for the frequency-dependent Green function in terms of zero-, $M_0^{\alpha\beta}(i, \sigma | i', \sigma') = \langle \{ A_{i\sigma}^\alpha; A_{i'\sigma'}^{\beta\dagger} \} \rangle$, and first-order, $M_1^{\alpha\beta}(i, \sigma | i', \sigma') = \langle \{ [A_{i\sigma}^\alpha; H]; A_{i'\sigma'}^{\beta\dagger} \} \rangle$, spectral moment matrices:

$$G^{\alpha\beta}(\omega) = M_0^{\alpha\gamma_1} (\omega M_0 - M_1)_{\gamma_1 \gamma_2}^{-1} M_0^{\gamma_2 \beta}. \tag{3}$$

Corrections to the Hubbard I approximation [1] are contained in the first-order spectral moment matrix, since the static expectation values are determined self-consistently from the spectral density

$$S_{i\sigma}^{\alpha\beta}(\omega) = -\frac{1}{\pi} \text{Im } G^{\alpha\beta}(i\sigma, i'\sigma' | \omega + i0^+) \quad (4)$$

instead of decoupling the intersite averages into single site products. To describe these corrections it is important to specify first the structure of the Hubbard I approximation that represents an infinite chain of atomic Green functions $G_a(\omega)$ connected by nearest neighbour hopping:

$$\begin{aligned} G^{1,1}(\mathbf{k}, \omega) &= \langle \langle c_{1\sigma} | c_{1\sigma}^\dagger \rangle \rangle_{\mathbf{k}, \omega} = \frac{1}{G_a^{-1}(\omega) - \varepsilon(\mathbf{k})}, \\ G^{2,1}(\mathbf{k}, \omega) &= \langle \langle n_{1\bar{\sigma}} c_{1\sigma} | c_{1\sigma}^\dagger \rangle \rangle_{\mathbf{k}, \omega} = \frac{G_{a2}(\omega)}{G_a(\omega)} \times \frac{1}{G_a^{-1}(\omega) - \varepsilon(\mathbf{k})}, \dots, \\ G^{8,1}(\mathbf{k}, \omega) &= \langle \langle n_{2\sigma} n_{2\bar{\sigma}} n_{1\bar{\sigma}} c_{1\sigma} | c_{1\sigma}^\dagger \rangle \rangle_{\mathbf{k}, \omega} = \frac{G_{a8}(\omega)}{G_a(\omega)} \times \frac{1}{G_a^{-1}(\omega) - \varepsilon(\mathbf{k})}, \dots \end{aligned} \quad (5)$$

where $\varepsilon(\mathbf{k})$ is the Fourier transform of the transfer integral and the atomic Green functions G_a are described in the appendix. The corrections mentioned above can now be described as static energy shifts of the frequency ω and of the band dispersion $\varepsilon(\mathbf{k})$ in the form of the Hubbard I solution given by (5). These shifts are proportional to the transfer integral t_{ij} as their source is the commutation of \vec{A} with the kinetic energy operator. The shifts can be divided into two categories: local and non-local. The local ones are determined by the ‘kinetic motion’ of the projecting operators $(n_{i1\bar{\sigma}}, n_{i2\bar{\sigma}}, n_{i2\sigma}) \rightarrow (c_{i1\bar{\sigma}}^\dagger c_{j1\bar{\sigma}}, c_{i2\bar{\sigma}}^\dagger c_{j2\bar{\sigma}}, c_{i2\sigma}^\dagger c_{j2\sigma})$, i.e. are proportional to the expectation values of terms like $\sum_j t_{ij} c_{i1\bar{\sigma}}^\dagger c_{j1\bar{\sigma}}$. For instance, the diagonal element $M_1^{2,2}(i, \sigma | j, \sigma)$ is identical to the local term obtained by Roth [23] for the NHM ($i = j$):

$$\begin{aligned} & - \sum'_{l(\neq i)} t_{il} [\langle (1 - n_{i\sigma}) c_{i1\bar{\sigma}}^\dagger c_{l1\bar{\sigma}} (1 - n_{l1\sigma}) \rangle - \langle n_{i1\sigma} c_{i1\bar{\sigma}}^\dagger c_{l1\bar{\sigma}} n_{l1\sigma} \rangle] \\ & = - \sum'_{l(\neq i)} t_{il} [\langle (1 - n_{i1\sigma} - n_{l1\sigma}) c_{i1\bar{\sigma}}^\dagger c_{l1\bar{\sigma}} \rangle]. \end{aligned}$$

Due to orbital degeneracy new terms appear with the same features but involving the orbital projection operators. For example, in the matrix element $M_1^{7,3}(i, \sigma | i, \sigma) (=M_1^{3,7}(i, \sigma | i, \sigma))$ we have

$$- \sum'_{l(\neq i)} t_{il} [\langle (1 - n_{i1\sigma} - n_{l1\sigma}) n_{i2\sigma} c_{i2\bar{\sigma}}^\dagger c_{l2\bar{\sigma}} \rangle].$$

The non-local corrections are given by the charge, spin, orbital, mixed spin-orbital and pair fluctuations. For example, the non-local corrections contained in $M_1^{2,2}$ and $M_1^{3,7}$ are given respectively by

$$\begin{aligned} & t_{ij} [\langle n_{i1\bar{\sigma}} n_{j1\bar{\sigma}} \rangle - \langle n_{i1\bar{\sigma}} \rangle \langle n_{j1\bar{\sigma}} \rangle \\ & \quad + \langle c_{i1\sigma}^\dagger c_{i1\bar{\sigma}} c_{j1\bar{\sigma}}^\dagger c_{j1\sigma} \rangle - \langle c_{i1\sigma}^\dagger c_{i1\bar{\sigma}} \rangle \langle c_{j1\bar{\sigma}}^\dagger c_{j1\sigma} \rangle], \\ & t_{ij} [\langle n_{i2\sigma} n_{i2\bar{\sigma}} n_{j2\bar{\sigma}} \rangle - \langle n_{i2\sigma} n_{i2\bar{\sigma}} \rangle \langle n_{j2\bar{\sigma}} \rangle \\ & \quad + \langle n_{i2\sigma} (c_{i2\bar{\sigma}}^\dagger c_{i1\sigma}) (c_{j1\sigma}^\dagger c_{j2\bar{\sigma}}) \rangle - \langle (c_{j1\sigma}^\dagger c_{j2\bar{\sigma}}) (c_{i2\bar{\sigma}} c_{i1\sigma}) n_{i2\sigma} \rangle]. \end{aligned}$$

In the following we will mainly consider the local corrections. The non-local ones require lengthy but straightforward calculation and do not alter our main conclusions. Their effect will be briefly discussed in the last section.

To derive the strong coupling limit of the Green function (3) it is useful to rewrite the expression (58) obtained in [23] for NHM in the following form:

$$\begin{aligned} \langle\langle a_{\mathbf{k}\sigma} | a_{\mathbf{k}\sigma}^\dagger \rangle\rangle_\omega &= \frac{1}{G_a^{-1}(\mathbf{k}, \omega + T_R(\mathbf{k}) / (1 - n_{i\bar{\sigma}}) n_{i\bar{\sigma}}) - \varepsilon(\mathbf{k}) - T_R(\mathbf{k}) / (1 - n_{i\bar{\sigma}}) n_{i\bar{\sigma}}} \\ &\simeq \frac{1 - n_{i\bar{\sigma}} - 2[\varepsilon(\mathbf{k}) n_{i\bar{\sigma}} (1 - n_{i\bar{\sigma}}) + T_R(\mathbf{k})] / U + O(t^2 / U^2)}{\omega - \varepsilon(\mathbf{k})(1 - n_{i\bar{\sigma}}) + T_R(\mathbf{k}) / (1 - n_{i\bar{\sigma}}) + O(t^2 / U)} \\ &\quad + \frac{n_{i\bar{\sigma}} + 2[\varepsilon(\mathbf{k}) n_{i\bar{\sigma}} (1 - n_{i\bar{\sigma}}) + T_R(\mathbf{k})] / U + O(t^2 / U^2)}{\omega - U - \varepsilon(\mathbf{k}) n_{i\bar{\sigma}} + T_R(\mathbf{k}) / n_{i\bar{\sigma}} + O(t^2 / U)}. \end{aligned}$$

It then becomes clear that the asymptotic expansion of the one-particle GF for the DHM should have a similar ‘shifted pole’ structure. Indeed, as a result of straightforward calculation, we obtain the following expression:

$$\langle\langle c_{\mathbf{k}\lambda\sigma} | c_{\mathbf{k}\lambda\sigma}^\dagger \rangle\rangle_\omega \simeq \sum_\alpha \frac{P_\alpha + O(t/U)}{\omega - E_\alpha^0 - \varepsilon(\mathbf{k}) P_\alpha + T_\alpha(\mathbf{k}) / P_\alpha + O(t^2 / U)}, \quad (6)$$

where E_α^0 are the resonance energies corresponding to all the transitions between the atomic states and P_α are the respective weight factors (the indices $\lambda\sigma$ have been dropped for simplicity). The poles $E_\alpha(\mathbf{k}) = E_\alpha^0 + \varepsilon(\mathbf{k}) P_\alpha - T_\alpha(\mathbf{k}) / P_\alpha + O(t^2 / U)$ are shifted compared to the atomic counterparts E_α^0 by quantities $T_\alpha(\mathbf{k})$ proportional to the transfer integral (see the appendix). In the strong-coupling limit for concentrations $n = \sum_{\lambda\sigma} \langle n_{\lambda\sigma} \rangle < 1$ double occupancy is excluded and therefore only the lowest band is relevant. We then use the index $\lambda\sigma$ to label the band energy $E_{\lambda\sigma}(\mathbf{k})$:

$$E_{\lambda\sigma}(\mathbf{k}) = \varepsilon_{\mathbf{k}} P_{\lambda\sigma} - \frac{1}{P_{\lambda\sigma}} \left(\frac{1}{N} \sum_{j,v \neq \lambda} t_{ij} \langle c_{jv\sigma}^+ c_{iv\sigma} \rangle + \frac{1}{N} \sum_{j,v} t_{ij} \langle c_{jv-\sigma}^+ c_{iv-\sigma} \rangle \right), \quad (7)$$

where $P_{\lambda\sigma}$ are the band narrowing factors, $P_{\lambda\sigma} = 1 - \sum_{\lambda\sigma \neq v\sigma} \langle n_{v\sigma} \rangle$. The partial densities $\langle n_{\lambda\sigma} \rangle$ and the intersite correlators in (7) are then determined in a self-consistent way from (6). We point out that both band narrowing and band shifts are composed of partial terms representing each possible spin and orbital state. One can also see that the structure of the strong coupling solution (6) and (7) remains unchanged for arbitrary degeneracy L . The expectation values $\langle c_{jv\sigma}^+ c_{iv\sigma} \rangle$ on the rhs can be interpreted as bond charges corresponding to symmetric (bonding) or antisymmetric (antibonding) wavefunctions between sites i and j . Equation (7) shows two relevant aspects, the band narrowing effects related to the factors $P_{\lambda\sigma}$ and the shifting of the band, related to the bond charges that give a measure of the kinetic motion. Both effects depend on L and the spin σ . In a complete form the band narrowing factors are supplemented by dispersion corrections proportional to bond charges, similar to [9, 35]. It is worth mentioning that the bond charge terms, previously introduced by Hirsch in [9] using a more complex model containing intra-atomic exchange interactions or off-diagonal matrix elements of the Coulomb interaction, in this scheme are directly generated by our strong-coupling approach.

3. Ordering in the limit of no double occupancy

To study the possible ordering we begin with the low density limit, where the disordered, fully paramagnetic (PM), phase is known to be the ground state of the system. By considering the possible instabilities of this state we take into account several criteria, which include the calculation of various types of longitudinal susceptibilities, single spin and/or orbital flip and a direct calculation of the total energy (see [6] for the NHM case):

$$E_{\text{GS}} = \frac{1}{2N} \sum_{\mathbf{k} \in \text{B.Z.}} \sum_{\sigma, \lambda} \int_{-\infty}^{\varepsilon_{\text{F}}} S_{\lambda\sigma}(\mathbf{k}, \omega) [\omega + \varepsilon(\mathbf{k})] d\omega. \quad (8)$$

The second criterion considers a process of ‘flipping’ an electron with momentum \mathbf{k}_F , at the top of the occupied band, into the bottom of the one of unoccupied bands [31]. This process generally involves a non-zero momentum transfer and, as shown in [29] for NHM, results in the same instability criterion as the RPA transverse susceptibility (see also [36]). In the PM phase at $T = 0$ the partial densities and the band narrowing factors are given by $\langle n_{\lambda\sigma} \rangle = n/2L = \int_{W_B}^{\epsilon_F} \rho(\epsilon) d\epsilon$, where $\rho(\epsilon)$ is the non-interacting density of states, and $P_{\lambda\sigma} = P = 1 - n + n/2L$. From the knowledge of the band energies and the partial densities, we have analysed the instability of the paramagnetic state towards a spin and/or orbital order at varying electron concentration by calculating the susceptibility for different types of lattices. By adding a Zeeman term $hM = h \sum_{i,\lambda,\sigma} \sigma n_{i\lambda\sigma}$ to the Hamiltonian, we find the static paramagnetic susceptibility $\chi = \left(\frac{\delta M}{\delta h}\right)_{h \rightarrow 0}$. To calculate χ we have to determine the excitation energies $E_{\lambda\sigma}(\mathbf{k})$ and the partial densities $\langle n_{\lambda\sigma} \rangle = P_{\lambda\sigma} \frac{1}{N} \sum_{\mathbf{k}} n_F(E_{\lambda\sigma}(\mathbf{k}))$ from (6) in a self-consistent way up to the first-order terms in the field h . After straightforward calculations we find

$$\chi = \frac{2LP\rho(\epsilon_F)}{(1-n) + \rho(\epsilon_F)\epsilon_F [P + (1-n)/P] + 2LK\rho(\epsilon_F)}, \quad (9)$$

where the Fermi energy ϵ_F is fixed by the self-consistency equation $n = 2L \langle n_{\lambda\sigma} \rangle$. The kinetic energy for a single band K is proportional to the sum over bond charges:

$$K = \frac{1}{N} \sum_j t_{ij} \langle c_{jv\sigma}^\dagger c_{iv\sigma} \rangle = P \int_{W_B}^{\epsilon_F} \rho(\epsilon) \epsilon d\epsilon. \quad (10)$$

We have first considered the case extremely unfavourable to polarization, that of frustrated lattices with $t < 0$, FCC and triangular [4]. As a criterion for the instability towards magnetic ordering, we have searched for the zeros of the denominator in (9) starting from the region of low densities.

The susceptibility (9) contains several contributions. The Hubbard I approximation corresponds to the first two terms in the denominator. It is easy to see that the latter is strictly less than the former, even in the presence of a van Hove singularity. The same drawback is shared by the coherent potential approximation [37]. Consequently these approximations are unable to describe a polarized state even for simple bipartite lattices. The second term in the square brackets corresponds to the one-loop approximation of the diagrammatic approach [38]. Also in this approximation the susceptibility remains finite for the FCC lattice in the whole region of concentrations for any value of L . The last term generalizes Roth correction to the degenerate case and, as will be shown below, is responsible for the phase transition into a polarized state. In agreement with previous studies on NHM ($L = 1$), we find that for the frustrated lattices the susceptibility never diverges and has only a weak peak when the band filling reaches the energy corresponding to the van Hove singularity. However, already for $L = 2$ the inverse susceptibility for the FCC lattice crosses zero at some finite concentration $n_c(L)$, as shown in figure 1. This signals an instability towards transition into a polarized state at a critical concentration lower than the one corresponding to the van Hove singularity. A similar behaviour is observed for the triangular lattice. By increasing L the critical value n_c decreases further, reducing the region of the PM state on the phase diagram. The same behaviour is also found for a bipartite square lattice, where the transition is already present at $L = 1$. The critical concentration we find in this case, $n_c \simeq 0.6$, is in complete agreement with the QMC results of [7]. The calculation of the critical concentration n_c within the slave boson approach for NHM [39] gives $n_c \simeq 0.67$; however, this critical value turns out to be independent of the dimensionality of the lattice. Similar calculations for the DHM [22] in the considered concentration range require finite values of Coulomb parameters and Hund

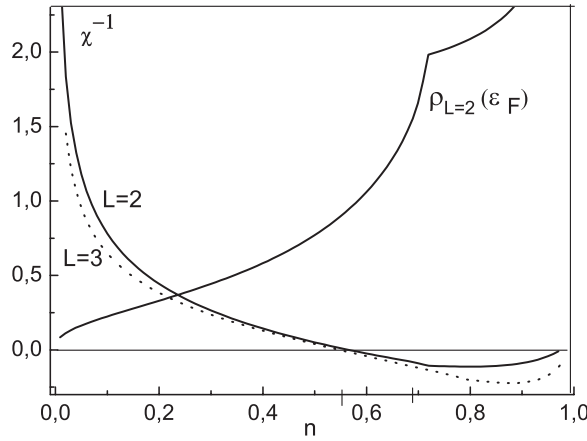


Figure 1. Inverse static paramagnetic susceptibility for values of orbital degeneracy $L > 1$ (FCC lattice, $t < 0$) versus electron concentration. The critical concentration, $\chi^{-1}(n_c) = 0$, is not related to the van Hove singularity, as seen for $L = 2$.

coupling in order to obtain an instability of the fully disordered state. For triangular and square lattices we find that as $L \rightarrow \infty$, the critical concentration $n_c(L)$ reaches saturation at values 0.38 and 0.32 respectively. The spin polarization, however, is not the only possible instability in a degenerate system since the disordered phase can become unstable with respect to orbital ordering as well. This can be probed by calculating a generalized susceptibility, which instead of the Zeeman term considered above introduces fictitious fields coupled to different possibilities to repopulate the orbital and spin states with respect to the initial equal distribution of the PM phase. For instance, if $L = 2$ we may consider a spin-orbital term

$$-H \sum_i \left\langle n_{i1\sigma} - \frac{1}{3} (n_{i1-\sigma} + n_{i2\sigma} + n_{i2-\sigma}) \right\rangle.$$

After carrying out this analysis we find the same critical value n_c as for the spin channel discussed above, that signals the onset of a spin-orbital order at this concentration.

A further insight into the instability of the PM phase comes from the analysis of the ground state energy (8):

$$E_{\text{PM}} = -|K|(P+1)L + |K|(1-P)L/P. \quad (11)$$

The first term is the contribution of the band narrowing (see the first term in the rhs of equation (7)), while the other one accounts for bond charge effects (corresponding to the second term of (7)). The evolution of E_{PM} with orbital degeneracy is shown in figure 2. At small concentrations we find that degeneracy lowers the energy of the PM state, as expected. However, for an intermediate concentration the behaviour is reversed, indicating the onset of a new phase near the crossing point. To analyse which ordered state is realized at the critical point, we have performed extensive calculations of the ground state energies corresponding to different occupations of spin and orbital states mentioned earlier. We find that the lowest energy state is polarized in such a way that a single spin and orbital state is preferred over the others, $\langle n_{\lambda=1,\sigma} \rangle$, while the remaining ones are equally populated (or disordered), e.g. for $L = 2$ we have $\langle n_{\lambda=1,\bar{\sigma}} \rangle = \langle n_{\lambda=2,\sigma} \rangle = \langle n_{\lambda=2,\bar{\sigma}} \rangle < \langle n_{\lambda=1,\sigma} \rangle$. The energy corresponding to this configuration decreases with orbital degeneracy, while the magnetization increases. The behaviour of the magnetization for the FCC lattice is shown in figure 3 for $L = 2, 3$. Calculations have been carried out also for the triangular lattice and for the bipartite (simple

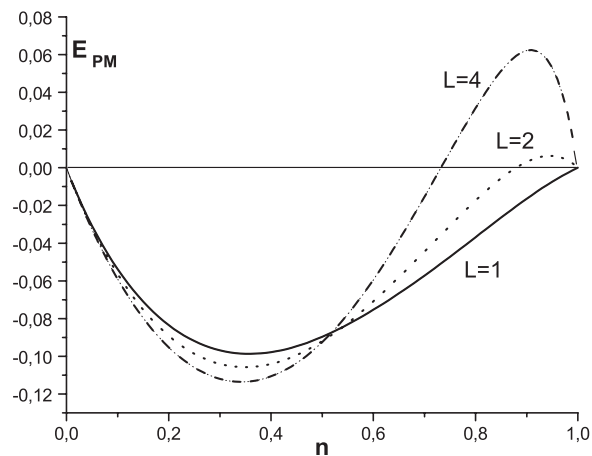


Figure 2. Energy of the fully disordered phase for the FCC lattice with $t < 0$ versus electron concentration at different values of orbital degeneracy L .

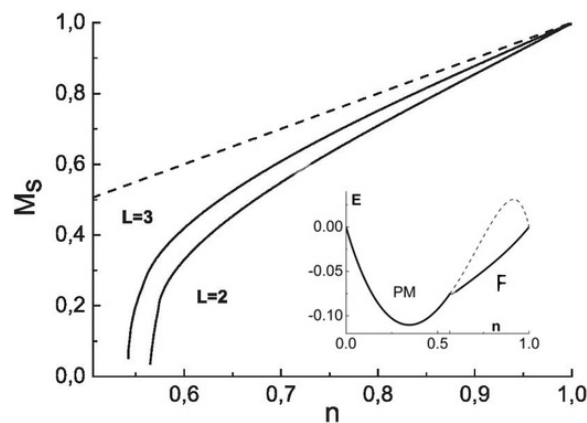


Figure 3. Magnetization of the lowest energy polarized state at $L = 2, 3$. The dashed line corresponds to saturation. The inset shows the energies of the PM and polarized ground states at $L = 2$.

cubic and square) lattices, which all share the above features. For frustrated lattices with $t < 0$ the magnetization never reaches saturation, in contrast to the bipartite lattices, which acquire a saturated moment at certain finite concentration larger than n_c . We mention that the effect of the non-local corrections to the band energy (7), that requires more complicated but straightforward calculations, is essentially to enhance the tendency towards the polarized state without changing the qualitative picture (e.g., n_c is slightly shifted towards lower values). The reason for this behaviour is that the non-local corrections describe different types of fluctuations or inter-site correlation functions, which are the more significant, the more disordered is the ground state. As has already been mentioned, these corrections contribute to the renormalization of the band narrowing factors leading to an enhanced frustration of the disordered configurations. In other words, their main effect is to favour polarization.

It should be noted that the well known electron-hole transformation [40] allows for establishing a simple correspondence between the region of electron concentrations $n < 1$

and that with $n' = 2L - n$: equivalent results hold for the latter if holes are used instead of electrons (for a non-bipartite lattice the sign of hopping should be reversed). One can see from the analytic form of the generalized Roth approximation that this symmetry is conserved. The limit of excluded double occupancy, which amounts to a hard core interaction ($n < 1$, U , $U - J \rightarrow \infty$), has allowed us to reveal some important aspects of the correlated electron motion. Beyond this limit the magnitudes of Hund and Hubbard U -parameters become important (generally, $U > J$ by physical arguments). The Hund exchange interaction favours atomic polarization also in the case when the last two terms in the Hamiltonian (1) are neglected (Ising-type truncation). Then using the full basis set chosen in the present paper (see the appendix) allows for considering the possibility of a global polarization for arbitrary parameters. For instance, in a recent paper [41] the case of strong but finite interaction in the two-fold DHM has been studied within the slave boson approach for the truncated version of (1) with $L = 2$. In agreement with arguments of earlier works (e.g., [42]) based on kinetic exchange between degenerate orbitals, it has been found that ferromagnetic spin polarization exists in an extended region of concentrations on a simple cubic lattice and is accompanied by antiferromagnetic orbital ordering. We have investigated the possibility of such a superstructure in our strong coupling limit and have found that the homogeneous ferromagnetic phase has a lower total energy. As already mentioned, the superstructure is strictly excluded also for the Nagaoka regime [34]. This result implies that a further investigation for large but finite coupling will establish a critical line of transition between the two phases, or the existence of phase separated regions. The rich variety of possible spin and orbital orderings of the DHM due to interplay of different physical parameters reflects the situation observed in real materials, e.g. manganites. However, this model also contains the possibility of describing anomalously large transfer of spectral weight between excitations which is observed in spectroscopic measurements [43]. This effect is determined by the correlated nature of the energy bands of strongly interacting electrons and depends on different factors. The simplest one is already contained in the Hubbard I approximation (5) via the Gutzwiller-like weights of the atomic GF (A.1). In our approach the additional contributions appear due to interplay of the kinetic energy projected onto a separate band and the Coulomb parameters U and J , as shown in (A.2). It can be seen that these contributions are increased as the interaction parameters are decreased. Although the truncation of the Hamiltonian mentioned above is often used in the literature, the role of ‘transverse terms’ is generally not negligible and can be studied by such a generalization of the basis set, which diagonalizes the complete Hamiltonian. This would generally result in a more complicated form of the matrix Green function. The transparent structure we have described in terms of frequency and dispersion shifts with respect to the Hubbard I approximation indicates that it should be possible to identify an analogous one for the complete Hamiltonian too. On the other hand, the existence of such a structure opens a possibility to generalize the dynamical approach proposed in [44]. to the DHM. For the NHM, dynamical effects have been introduced via a modified alloy analogy approximation by replacing the atomic energy levels with those derived from the spectral density approach. Given that the simplest version of DHM with $L = 2$ already results in an eight-pole GF, an important advantage of the present mean-field solution is that it allows an equivalent and totally self-consistent description, while, as is well known, there does not exist an algebraic solution which would allow for resolving the eight sub-bands within the spectral density approach itself.

4. Discussion

The results described in the present paper can be understood in terms of competition between itinerancy and localization. Indeed, one can notice that the latter is present in various scenarios

of ferromagnetism and can be associated with strong coupling, van Hove singularities, flat bands, asymmetric density of states with a peak in the vicinity of the band's bottom or with band narrowing effects, including the mechanism due to depletion of bond charges [35]. These factors are known to favour transition from a disordered to a polarized state. Our strong coupling analysis has shown that the enlargement of the Hilbert space of states due to the inclusion of orbital degeneracy enhances the tendency to ferromagnetic polarization irrespective of the lattice structure. The effect turns out to be strong enough to induce the transition on non-bipartite lattices or to significantly reduce the critical concentration for bipartite lattices, shifting it away from the van Hove singularity, as in the case of a square lattice. At very small concentrations the enlargement of the Hilbert space allows electrons to gain more kinetic energy by delocalizing over a larger number of orbital and spin states on the empty lattice sites, leading to a fully disordered ground state. As the concentration is increased and the number of available empty sites is diminished, the fully disordered state becomes inconvenient due to the enhancement of scattering processes. In other words, the additional degrees of freedom introduce more frustration in the disordered configuration and, as a result, favour polarization. These tendencies are described in our approach by the two competing contributions to the total energy (11). The negative term in equation (11) describes the kinetic energy gain due to the occupation of a larger number of spin and orbital states, while the positive term accounts for the loss of energy due to scattering. The latter depends on the magnitude of the bond charges, which in turn are related to the kinetic energy ($\sim L|K|$). This contribution starts to prevail at intermediate concentrations, giving rise to the typical behaviour of E_{PM} shown in figure 2. Orbital degeneracy affects in a positive manner both the band narrowing (see the first term in the rhs of equation (7)) and the bond charges, increasing the number of channels for kinetic motion (or the magnitude of the total bond charge). At intermediate concentrations the increased bond charge associated with bonding states results in an enhanced scattering. To reduce this energy loss, the system has to decrease the number of bond charges associated with bonding states and increase those associated to antibonding states. This, by virtue of the Pauli principle, implies a spin and orbital polarization. Indeed, by taking a constant single particle density of states $\rho(\varepsilon) = W^{-1}$ one can easily calculate the bond charge corresponding to different phases $B = \sum_{\lambda\sigma} |K_{\lambda\sigma}| / W$. Let us compare the fully disordered (PM), fully spin ordered and orbitally disordered (OD), and fully polarized (F) phases:

$$B_{\text{PM}} = \frac{B_{\text{F}}}{1 - n + n/(2L)} > B_{\text{OD}} = \frac{B_{\text{F}}}{1 - n + n/L} > B_{\text{F}} = \frac{n}{2} (1 - n). \quad (12)$$

One clearly sees a decrease of the total bond charge as the degree of polarization is increased. From figure 4 one can also notice that in the fully disordered phase (PM) the largest increase of the bond charge with L is achieved at $L = 2$. This naturally explains why the largest drop in $n_c(L)$ takes place when L is increased from 1 to 2. The above arguments indicate that polarization is associated not to a gain, but to a loss in kinetic energy, which allows the system to gain more in potential energy by adopting a more localized state. This mechanism of ordering caused by increased disorder in PM phase is not related to the lattice structure and does not contradict the Nagaoka theorem, that finds the ground state corresponding to zero loss in potential energy. Moreover, it is particularly pronounced for non-bipartite lattices where geometrical frustration strongly opposes polarization. Indeed, when $t < 0$ these lattices favour the formation of bonding states, as can be illustrated by the example of a single electron on a triangle. The frustrated geometry thus leads to larger bond charges and respectively to a larger scattering. In this case, the orbital degeneracy promotes a non-saturated ferromagnetism with larger values of magnetization corresponding to larger values of L .

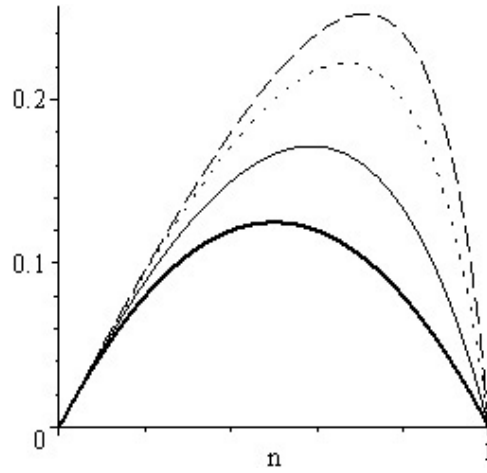


Figure 4. Increase of the total bond charge with orbital degeneracy ($L = 1, 2, 3$) for the constant single particle density of states in the fully disordered phase as compared to the fully polarized phase (lowest curve).

The predicted effects of the orbital degeneracy suggest an extension of the numerical analysis undertaken in [7] for finite dimensional lattices and a generalization of the exact results of [5] for infinite dimensions. These effects are of the first order in bandwidth W and should therefore be important also at finite coupling, where a number of other mechanisms are important for an adequate description of real materials [3, 45, 46]. Nevertheless, the described mechanism sheds a new light on the physics of metallic ferromagnets, most of which belong to the class of materials with degenerate orbital states. Classical examples are the 3d elements Ni, Co, Fe and their alloys [17, 47] or the rare earth molybdates $R_2Mo_2O_7$ [48] with a t_{2g} conduction band, manganites [12] or the series of disulfide compounds $Fe_xCo_{1-x}S_2$ [49] characterized by e_{2g} orbitals and known to support ferromagnetism in a broad range of concentrations. For instance, it is known that magnetization of Ni, which has an FCC structure and a concentration of holes about 0.6, is close to saturation [50]. At present, the enhancement of metallic ferromagnetism in orbitally degenerate systems has become a topic of more intensive study in view of prospective applications in spintronics [51]. The discussed connection between the kinetic energy and the symmetry of the wavefunction can also be useful in understanding the close relation between degeneracy, strong electron correlations, itinerant ferromagnetism and triplet superconductivity observed in some recently discovered materials [52].

In conclusion, we have proposed a generalization of the Roth approach for the degenerate Hubbard model, providing a fairly reliable description of itinerant ferromagnetism in the strong coupling regime. The mechanism we have described allows a better understanding of the phenomenon of metallic ferromagnetism and could be useful to qualitatively understand some properties of systems with degenerate electron states.

Appendix. The atomic Green function

In the double degenerate case, the choice of the basis set is the following:

$$\begin{aligned} A_{i\sigma}^1 &= c_{i1\sigma}, & A_{i\sigma}^2 &= n_{i1\bar{\sigma}} c_{i1\sigma}, & A_{i\sigma}^3 &= n_{i2\bar{\sigma}} c_{i1\sigma}, \\ A_{i\sigma}^4 &= n_{i2\sigma} c_{i1\sigma}, & A_{i\sigma}^5 &= n_{i1\bar{\sigma}} n_{i2\bar{\sigma}} c_{i1\sigma}, & A_{i\sigma}^6 &= n_{i1\bar{\sigma}} n_{i2\sigma} c_{i1\sigma}, \\ A_{i\sigma}^7 &= n_{i2\bar{\sigma}} n_{i2\sigma} c_{i1\sigma}, & A_{i\sigma}^8 &= n_{i1\bar{\sigma}} n_{i2\bar{\sigma}} n_{i2\sigma} c_{i1\sigma}. \end{aligned}$$

The structure of the atomic GF ($t_{ij} = 0$) shown below describes the transitions between different occupation levels of energy E_α and with spectral weights P_α :

$$\begin{aligned}
 G_a(\omega) &\equiv \langle\langle c_{i1\sigma} | c_{i1\sigma}^\dagger \rangle\rangle = \sum_{\alpha=1}^8 P_\alpha / (\omega - E_\alpha); \\
 G_{a2}(\omega) &\equiv \langle\langle n_{i1-\sigma} c_{i1\sigma} | c_{i1\sigma}^\dagger \rangle\rangle = P_4 / (\omega - E_4) + P_6 / (\omega - E_6) \\
 &\quad + P_7 / (\omega - E_7) + P_8 / (\omega - E_8); \dots \\
 G_{a8}(\omega) &\equiv \langle\langle n_{i1-\sigma} n_{i2-\sigma} n_{i2\sigma} c_{i1\sigma} | c_{i1\sigma}^\dagger \rangle\rangle = P_8 / (\omega - E_8), \tag{A.1}
 \end{aligned}$$

where

$$\begin{aligned}
 P_1 &= \langle(1 - n_{i1\bar{\sigma}})(1 - n_{i2\bar{\sigma}})(1 - n_{i2\sigma})\rangle, & E_1 &= 0; \\
 P_2 &= \langle(1 - n_{i1\bar{\sigma}})(1 - n_{i2\bar{\sigma}})n_{i2\sigma}\rangle, & E_2 &= U_\perp - J; \\
 P_3 &= \langle(1 - n_{i1\bar{\sigma}})n_{i2\bar{\sigma}}(1 - n_{i2\sigma})\rangle, & E_3 &= U_\perp; \\
 P_4 &= \langle n_{i1\bar{\sigma}}(1 - n_{i2\bar{\sigma}})(1 - n_{i2\sigma})\rangle, & E_4 &= U_\parallel; \\
 P_5 &= \langle(1 - n_{i1\bar{\sigma}})n_{i2\bar{\sigma}}n_{i2\sigma}\rangle, & E_5 &= 2U_\perp - J; \\
 P_6 &= \langle n_{i1\bar{\sigma}}(1 - n_{i2\bar{\sigma}})n_{i2\sigma}\rangle, & E_6 &= U_\parallel + U_\perp - J; \\
 P_7 &= \langle n_{i1\bar{\sigma}}n_{i2\bar{\sigma}}(1 - n_{i2\sigma})\rangle, & E_7 &= U_\parallel + U_\perp; \\
 P_8 &= \langle n_{i1\bar{\sigma}}n_{i2\bar{\sigma}}n_{i2\sigma}\rangle, & E_8 &= 2U_\perp + U_\parallel - J.
 \end{aligned}$$

The energy shifts corresponding to the Green function (6) (see discussion following (5)).

$$\begin{aligned}
 T_1(\mathbf{k}) &= - \sum'_{l(\neq i)} t_{il} \exp(-i\mathbf{k}\mathbf{R}_{il}) \langle(1 - n_{i1\bar{\sigma}})(1 - n_{i2\bar{\sigma}})(1 - n_{i2\sigma}) \\
 &\quad \times (1 - n_{l1\bar{\sigma}})(1 - n_{l2\bar{\sigma}})(1 - n_{l2\sigma})\rangle_c \\
 &\quad + \sum'_{l(\neq i)} t_{il} \langle(1 - 2n_{i1\sigma})(1 - n_{i2\bar{\sigma}})(1 - n_{i2\sigma})c_{i1\bar{\sigma}}^\dagger c_{l1\bar{\sigma}}\rangle \\
 &\quad - \sum'_{l(\neq i)} t_{il} \exp(-i\mathbf{k}\mathbf{R}_{il}) \langle(1 - n_{i2\bar{\sigma}})(1 - n_{i2\sigma})c_{i1\sigma}^\dagger c_{i1\bar{\sigma}} c_{l1\bar{\sigma}}^\dagger \\
 &\quad \times c_{l1\sigma}(1 - n_{l2\bar{\sigma}})(1 - n_{l2\sigma})\rangle \\
 &\quad + \sum'_{l(\neq i)} t_{il} \exp(-i\mathbf{k}\mathbf{R}_{il}) \langle(1 - n_{i2\bar{\sigma}})(1 - n_{i2\sigma})c_{i1\sigma}^\dagger c_{i1\bar{\sigma}}^\dagger \\
 &\quad \times c_{l1\bar{\sigma}} c_{l1\sigma}(1 - n_{l2\bar{\sigma}})(1 - n_{l2\sigma})\rangle \\
 &\quad + \sum'_{l(\neq i)} t_{il} \langle(1 - 2n_{i1\sigma})(1 - n_{i1\bar{\sigma}})(1 - n_{i2\bar{\sigma}})c_{i2\sigma}^\dagger c_{l2\sigma}\rangle \\
 &\quad - \sum'_{l(\neq i)} t_{il} \exp(-i\mathbf{k}\mathbf{R}_{il}) \langle(1 - n_{i1\bar{\sigma}})(1 - n_{i2\bar{\sigma}})c_{i1\sigma}^\dagger c_{i2\sigma} \\
 &\quad \times c_{l2\sigma}^\dagger c_{l1\sigma}(1 - n_{l1\bar{\sigma}})(1 - n_{l2\bar{\sigma}})\rangle \\
 &\quad + \sum'_{l(\neq i)} t_{il} \exp(-i\mathbf{k}\mathbf{R}_{il}) \langle(1 - n_{i1\bar{\sigma}})(1 - n_{i2\bar{\sigma}})c_{i1\sigma}^\dagger c_{i2\sigma}^\dagger \\
 &\quad \times c_{l2\sigma} c_{l1\sigma}(1 - n_{l1\bar{\sigma}})(1 - n_{l2\bar{\sigma}})\rangle \\
 &\quad + \sum'_{l(\neq i)} t_{il} \langle(1 - 2n_{i1\sigma})(1 - n_{i1\bar{\sigma}})(1 - n_{i2\sigma})c_{i2\bar{\sigma}}^\dagger c_{l2\bar{\sigma}}\rangle \\
 &\quad - \sum'_{l(\neq i)} t_{il} \exp(-i\mathbf{k}\mathbf{R}_{il}) \langle(1 - n_{i1\bar{\sigma}})(1 - n_{i2\sigma})c_{i1\sigma}^\dagger c_{i2\bar{\sigma}} c_{l2\bar{\sigma}}^\dagger \\
 &\quad \times c_{l1\sigma}(1 - n_{l1\bar{\sigma}})(1 - n_{l2\sigma})\rangle
 \end{aligned}$$

$$+ \sum'_{l(\neq i)} t_{il} \exp(-i\mathbf{k}\mathbf{R}_{il}) \langle (1 - n_{i1\bar{\sigma}})(1 - n_{i2\sigma}) c_{i1\sigma}^+ c_{i2\bar{\sigma}}^+ c_{l2\bar{\sigma}} \rangle \\ \times c_{l1\sigma} (1 - n_{l1\bar{\sigma}})(1 - n_{l2\sigma}).$$

The notation $\langle \dots \rangle_c$ stands for the cumulant average (compare with the non-degenerate case in [23]). Below only the local, \mathbf{k} -independent, shifts are shown:

$$T_2 = \sum'_{l(\neq i)} t_{il} \langle (1 - 2n_{i1\sigma}) [n_{i2\sigma} (1 - n_{i2\bar{\sigma}}) c_{i1\bar{\sigma}}^+ c_{l1\bar{\sigma}} \\ + n_{i2\sigma} (1 - n_{i1\bar{\sigma}}) c_{i2\bar{\sigma}}^+ c_{l2\bar{\sigma}} + (1 - n_{i1\bar{\sigma}})(1 - n_{i2\sigma}) c_{i2\sigma}^+ c_{l2\sigma}] \rangle; \\ \dots \\ T_8 = \sum'_{l(\neq i)} t_{il} \langle (1 - 2n_{i1\sigma}) [n_{i2\bar{\sigma}} n_{i2\sigma} c_{i1\bar{\sigma}}^+ c_{l1\bar{\sigma}} + n_{i1\bar{\sigma}} n_{i2\bar{\sigma}} c_{i2\sigma}^+ c_{l2\sigma} + n_{i1\bar{\sigma}} n_{i2\sigma} c_{i2\bar{\sigma}}^+ c_{l2\bar{\sigma}}] \rangle.$$

First-order corrections to the spectral weight of the lowest energy sub-bands (non-local terms are not shown):

$$\tilde{P}_1 = P_1 - 2 \left[\frac{1}{U_{\parallel}} \sum'_{l(\neq i)} t_{il} \langle (1 - 2n_{i\sigma})(1 - m_{i\bar{\sigma}})(1 - m_{i\sigma}) a_{i\bar{\sigma}}^{\dagger} a_{l\bar{\sigma}} \rangle \right. \\ + \frac{1}{U_{\perp}} \sum'_{l(\neq i)} t_{il} \langle (1 - 2n_{i\sigma})(1 - n_{i\bar{\sigma}})(1 - m_{i\sigma}) b_{i\bar{\sigma}}^{\dagger} b_{l\bar{\sigma}} \rangle \\ \left. + \frac{1}{U_{\perp} - J} \sum'_{l(\neq i)} t_{il} \langle (1 - 2n_{i\sigma})(1 - n_{i\bar{\sigma}})(1 - m_{i\bar{\sigma}}) b_{i\bar{\sigma}}^{\dagger} b_{l\sigma} \rangle \right]. \quad (\text{A.2})$$

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