Correlation Effects in Itinerant Magnetism

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Abstract

In this contribution we would like to revisit the problems of ferromagnetism (F) and antiferromagnetism (AF) in the pure itinerant model. These methods can be extended later to the superconducting materials. In our model we assume the extended Hubbard Hamiltonian. Transition from the paramagnetic state to the ordered state of magnetic nature is decided by the competition between kinetic and potential energy in which there is an increase in the kinetic energy moderated by the inter-site interactions, and a decrease in the potential energy. The competition between these two energies results in the existence of critical values of interactions for creating magnetic alignment. Only when existing in a given material interaction exceeds the critical value for a given type of ordering we can have the alignment of this type.

The influence of inter-site correlation on F and AF in the presence of Coulomb on-site correlation is investigated. The well known Landau free energy expansion is corrected for both F and AF ordering to reflect the presence of critical interaction in the second order term, which leads to the magnetic alignment.

The numerical results show that the inter-site interactions favor F at the end of the band and AF at the half-filled point. In both cases of F and AF ordering, these interactions lower substantially the Curie and Neel’s temperature towards experimental data. This helps to remove the paradox in magnetism that has persisted for a long time.

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1. INTRODUCTION

In the solids there are many phenomena such as band magnetism, metal-insulator transition, high temperature superconductivity, which are closely related to the Coulomb correlation. To describe this correlation scientists have developed what is known today as the single band Hubbard model [1–3]. In the original version of this model only the on-site Coulomb repulsion, $U = (\langle i, i | 1/r | i, i \rangle$ was included. The use of the simple mean-field approximation for this model led back to the Stoner model [4–6], in which the majority and minority spin bands are shifted with respect to each other for the quantity $\Delta E = m \cdot U$, where $m$ is the magnetization in Bohr’s magnetons, and the on-site Coulomb constant $U$ plays the role of the exchange interaction. The Coulomb constant $U$ resulting from the Stoner condition for creating ferromagnetism is large, i.e. of the order of the bandwidth. On one hand it can be justified by the existing strong Coulomb interaction, but on the other hand for such a strong interaction, one can not use the mean-field approximation.

These limitations of the mean-field approximation started the search for a more realistic ferromagnetic solution using higher order approximations, e.g. the Hubbard I approximation [1], coherent potential approximation (CPA) [7,8]. While the Hubbard I approximation describes correctly the atomic limit ($t = 0$) it is not correct for the intermediate $U/t$. For these values the coherent potential approximation (CPA), which is equivalent to Hubbard III decoupling of the Green functions, is better. Unfortunately, after a thorough analysis it was concluded that the Coulomb repulsion $U$, no matter how strong, does not lead to the ferromagnetic order (see e.g., [9,10]). The reason is that it does not yield the spin dependent band shift or spin dependent band narrowing necessary for a ferromagnetic ordering.

Both Hubbard I and CPA approximation have two types of particles; electrons moving between empty sites and electrons moving between sites occupied by electrons of opposite spin, separated from each other by the energy $U$ and forming lower and upper Hubbard’s sub-bands. This is the two-pole approximation in the language of Green functions. Base on this scheme is the newer model called “spectral density approach” (SDA) [11,12]. The magnetic phase diagrams calculated by this method are more realistic and the values of the Curie temperatures also make sense. The main advantage of SDA is to obtain a spin-dependent band shift necessary to obtain the ferromagnetic ordering. On the other side the SDA method is the linear combination of two $\delta$ functions leading to the real self-energy, and lacking the quasi-particle damping. Therefore, Nolting and co-workers have proposed a combination of
SDA and CPA called “modified alloy analogy” (MAA) [13]. This approximation has brought the self-consistent ferromagnetic solutions, and the complex values of self-energy. The defect of this method is the small range of concentrations for which one has the ferromagnetism and also a slightly unclear derivation of the method.

Another approach to solving the Hubbard model is computer simulation. The initial attempts of the Monte Carlo simulation applied to the basic Hubbard model also did not give the ferromagnetic ground state [14]. More recently, the new dynamical mean-field theory (DMFT) [15,16] has been developed for a direct computational simulation of systems with correlated electrons on a crystal lattice. This method has the exact solution in the non-trivial limit of an infinite coordination number [17]. The results have been obtained by using quantum Monte-Carlo (QMC) simulation [18–20] and the mean-field Green function theory. Use of this dynamical mean field theory (DMFT method), has introduced a significant progress in the theory of ferromagnetism. The results (see e.g. [21,22]) show the existence of ferromagnetism but at much lower temperatures than those coming from the Hartree-Fock approximation. Such results could remove the problem known as a “magnetic paradox”, i.e. the Curie temperature coming from the interaction constant (e.g. $U$) - fitted to obtain the correct magnetic moment at $T = 0$ K - as being much too high. The later attempts along the computational lines (see [16,20,22–25]) are still inconclusive, mainly for the reason of the limited size of the computational systems which seems to be too small too represent the bulk materials.

In recent years there has been a very fruitful analytical development in describing the magnetism by extending the Hubbard model and including into it the band degeneration and the inter-site Coulomb interactions. The influence of inter-site interactions on the band magnetism has been studied by many authors [26–37]. They have shown how different inter-site interactions would affect the ferromagnetism in the presence of the on-site Coulomb repulsion. This also will be the subject of the present chapter.

On the experimental front in the last few years there has been discovery of a triplet superconductivity in $\text{UGe}_2$ [38], $\text{URhGe}$ [39] and $\text{ZrZn}_2$ [40] materials. Although the transition to superconductivity takes place in very low temperatures ($\sim 0.8$ K), the mechanism of this phenomena is very interesting, since the superconducting pairing is (probably) stimulated by the Hund’s interaction (see e.g. [41]), the same one which stimulates weak itinerant ferromagnetism. It was also found that the growing magnetic moment would suppress the superconductivity. The explanation of these facts would be quite simple; the Hund’s interaction stimulates both F and SC ordering, but if the ordering of a given type already takes place then it precludes the other type of ordering.

Another type of new phenomenon which includes the band magnetism is the well documented coexistence between superconducting ordering and itinerant antiferromagnetism in high-$T_C$ cuprates, e.g. $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$, $\text{La}_{2-x}(\text{Sr, Ba})_x\text{CuO}_4$. Since in these compounds the magnetic moment is stronger it suppresses the superconductivity until the moment itself disappears (see [42–44]).

Because of all these reasons of all these theoretical problems and experimental facts we would like in this chapter to revisit the problems of ferromagnetism and antiferromagnetism in the pure itinerant model. These methods can be extended later to the superconducting materials, where the magnetic ordering competes rather than cooperates with superconductivity.
2. THE MODEL

The general model of itinerant magnetic ordering is based on the extended Hubbard quasi-single band Hamiltonian of the following form [33]

\[ H = - \sum_{\langle ij \rangle} t_{ij}^\sigma (c_{i\sigma}^+ c_{j\sigma} + h.c.) - \mu_0 \sum_i \hat{n}_i - F \sum_{i\sigma} n_{i\sigma} \hat{n}_{i\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + V \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j \\
+ J \sum_{\langle ij \rangle} c_{i\sigma}^+ c_{j\sigma} + J' \sum_{\langle ij \rangle} (c_{i\sigma}^+ c_{i\sigma}^+ c_{j\sigma} + h.c. ) \]  

(1)

where \( \mu_0 \) is the chemical potential, \( c_{i\sigma}^+ \) \( (c_{i\sigma}) \) creates (annihilates) the electron with spin \( \sigma \) on the \( i \)-th lattice site, \( \hat{n}_{i\sigma} = c_{i\sigma}^+ c_{i\sigma} \) is the particle number operator for electrons with spin \( \sigma \) on the \( i \)-th lattice site, \( \hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} \) is the charge operator, \( n_{i\sigma} \) is the average number of electrons on sites \( i \) with spin \( \sigma \).

In this Hamiltonian we included not only the dominant on-site Coulomb correlation, \( U \), but also the on-site Hund’s field \( F \). Such a field can exist only as the interaction between different orbitals in a multi-orbital model. We assume the single band, but composed from identical orbitals, which are fully degenerate i.e. have the same density of states and the same electron occupation (see [10]). In such a band the effective exchange field can be expressed as; \( F = (d - 1) \cdot J_{\text{in}} \), where \( J_{\text{in}} \) is the exchange interaction between different orbitals within the same atomic site, and \( d \) is the number of orbitals within the band. As a result our model is a quasi-single band model. The intra-atomic Hund field in Eq. (1) is already expressed in the Hartree-Fock approximation, which will be justified only for small values of this interaction. In addition we have three explicit inter-site interactions [1,45,46]: \( J \)-exchange interaction, \( J' \)-pair hopping interaction, \( V \)-density-density interaction. To avoid a large number of free parameters we will assume later on in the numerical analysis that \( J' = J, V = 0 \), which will leave us with only two parameters; \( J \) and parameter \( S \) representing kinetic interactions (see Eq. (5)).

The spin dependent correlation hopping \( t_{ij}^\sigma \) depends on the occupation of sites \( i \) and \( j \), and in the operator form can be expressed as

\[ t_{ij}^\sigma = t(1 - \hat{n}_{i-\sigma})(1 - \hat{n}_{j-\sigma}) + t_1 [\hat{n}_{i-\sigma}(1 - \hat{n}_{j-\sigma}) + \hat{n}_{j-\sigma}(1 - \hat{n}_{i-\sigma})] + t_2 \hat{n}_{i-\sigma} \hat{n}_{j-\sigma} \]  

(2)

where \( t \) is the hopping amplitude for an electron of spin \( \sigma \) when both sites \( i \) and \( j \) are empty. Parameters; \( t_1, t_2 \), are the hopping amplitudes for an electron of spin \( \sigma \) when one or both of the sites \( i \) or \( j \) are occupied by an electron with opposite spin, respectively. Quite recently, several authors have suggested that the expected relation; \( t > t_1 > t_2 \), may be reversed for large enough inter-atomic distances; \( t < t_1 < t_2 \) (see Refs. [47] and [48]). This concept would fit the results of Gunnarsson and Christensen [49], who for the heavier elements (e.g. 3d or 4f) claim growing hopping integrals with increasing occupation.

Including the occupationally dependent hopping given by Eq. (2) into the Hamiltonian (1) we obtain the following result

\[ H = - \sum_{\langle ij \rangle} [t - \Delta t (\hat{n}_{i-\sigma} + \hat{n}_{j-\sigma}) + 2t_\text{ex}\hat{n}_{i-\sigma}\hat{n}_{j-\sigma} \] \( (c_{i\sigma}^+ c_{j\sigma} + h.c.) - \mu_0 \sum_i \hat{n}_i - F \sum_{i\sigma} n_{i\sigma} \hat{n}_{i\sigma} \\
+ U \sum_i \hat{n}_i \hat{n}_j + V \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j + J \sum_{\langle ij \rangle \sigma,\sigma'} c_{i\sigma}^+ c_{j\sigma} c_{i\sigma} c_{j\sigma} + J' \sum_{\langle ij \rangle} (c_{i\sigma}^+ c_{i\sigma}^+ c_{j\sigma} + h.c.) \]  

(3)
where

\[
\Delta t = t - t_1 \quad , \quad t_{ex} = \frac{t + t_2}{2} - t_1 .
\]  

(4)

In this form it is quite visible that the kinetic interactions: the hopping interaction, \(\Delta t\), and the exchange hopping interaction, \(t_{ex}\), are also the inter-site interactions.

We assume that \(t_1/t = S\) and \(t_2/t = S_1\). In general these parameters are different and they both fulfill the condition \(S < 1\) and \(S_1 < 1\) which is equivalent to \(t > t_1 > t_2\) (see Ref. [47]). For simplicity we will assume now additionally that \(S = S_1\). With this assumption we have the relationships

\[
\Delta t = t - t_1 = t(1 - S) \quad , \quad t_{ex} = \frac{t + t_2}{2} - t_1 = \frac{t}{2} (1 - S)^2 .
\]  

(5)

In the Hamiltonian (3) there are many inter-site interactions: \(\Delta t, t_{ex}, J, J', V\), for which we will use the modified Hartree-Fock (H-F) approximation. For the two- and three-body terms of Hamiltonian we will adopt the procedure introduced by Foglio and Falicov [50], Aligia and co-workers [51], and Hirsch [27]. Neglecting superconductive averages of the type: \(\langle c_{i\sigma}^+ c_{j\sigma'}^+ \rangle, \langle c_{i\sigma} c_{j\sigma'} \rangle\), and the spin-flip terms \(\langle c_{i\sigma}^+ c_{j-\sigma} \rangle\) we obtain

- e.g. for two-body term

\[
\hat{n}_i \hat{n}_j = (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow})(\hat{n}_{j\uparrow} + \hat{n}_{j\downarrow}) \cong \langle \hat{n}_{i\uparrow}\rangle \langle \hat{n}_{j\uparrow}\rangle + \langle \hat{n}_{i\downarrow}\rangle \langle \hat{n}_{j\downarrow}\rangle - \sum_{\sigma}(\langle c_{i\sigma}^+ c_{j\sigma} \rangle c_{j\sigma} + h.c.) + const .
\]  

(6)

- e.g. for three-body term

\[
c_{i\uparrow}^+ c_{j\downarrow}^+ \hat{n}_{i\uparrow} \hat{n}_{j\downarrow} = c_{i\sigma}^+ c_{j\sigma}^+ c_{i\sigma} c_{i\sigma} c_{i\sigma} c_{j\sigma} \cong c_{i\uparrow}^+ c_{j\downarrow}^+ \left( \langle \hat{n}_{i\uparrow}\rangle \langle \hat{n}_{j\downarrow}\rangle - \langle c_{i\uparrow}^+ c_{j\downarrow} \rangle \langle c_{j\downarrow}^+ c_{i\downarrow} \rangle \right)
- c_{i\sigma}^+ c_{j\sigma} \langle c_{i\sigma}^+ c_{j\sigma} \rangle \langle c_{i\sigma} c_{j\sigma} \rangle - c_{i\sigma}^+ c_{j\sigma} \langle c_{i\sigma}^+ c_{j\sigma} \rangle \langle c_{i\sigma} c_{j\sigma} \rangle
+ \hat{n}_{i\uparrow} \langle c_{i\sigma}^+ c_{j\sigma} \rangle \langle \hat{n}_{i\uparrow}\rangle + \hat{n}_{j\downarrow} \langle c_{i\sigma}^+ c_{j\sigma} \rangle \langle \hat{n}_{j\downarrow}\rangle + const .
\]  

(7)

The main point of this approximation is to retain the following inter-site averages: \(I_{\sigma} = \langle c_{i\sigma}^+ c_{j\sigma} \rangle\), in addition to the usual on site averages: \(n_{i\sigma} = \langle \hat{n}_{i\sigma}\rangle\), which contribute to the Stoner field.

After performing this modified Hartree-Fock approximation on all inter-site interactions: \(\Delta t, t_{ex}, J, J', V\), we obtain the following simplified Hamiltonian

\[
H = - \sum_{<i,j>\sigma} t_{eff}^{\sigma} (c_{i\sigma}^+ c_{j\sigma} + h.c.) - \mu_0 \sum_i \hat{n}_i + \sum_{i\sigma} M_i^\sigma \hat{n}_{i\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} ,
\]  

(8)

where \(t_{eff}^{\sigma} = t \cdot b^{\sigma}\) is the effective hopping integral, with \(b^{\sigma}\) given by

\[
b^{\sigma} = 1 - \frac{\Delta t}{t} (n_{i-\sigma} + n_{j-\sigma}) + 2 \frac{t_{ex}}{t} (n_{i-\sigma} n_{j-\sigma} - I_{-\sigma}^2 - 2 I_{\sigma} I_{-\sigma}) - \frac{J - V}{t} I_{\sigma} - \frac{J + J'}{t} I_{-\sigma} .
\]  

(9)

and \(M_i^\sigma\) is the spin-dependent modified molecular field for electrons with spin \(\sigma\) expressed as
\[ M_i^\sigma = -F n_{i\sigma} - J \sum_j n_{j\sigma} + V \sum_j \left( n_{j\sigma} + n_{j-\sigma} \right) + 2z\Delta t I_{-\sigma} - 2t_{ex} I_{-\sigma} \sum_j n_{j\sigma} , \]  

where \( z \) is the number of the nearest neighbors, \( \sum_j \) is the sum over nearest neighbors of the lattice site \( i \). The above molecular field is the sum of the on-site contribution \( F \) and the inter-site contributions, which will be different for \( F \) and \( AF \).

### 2.1 INTER-SITE AVERAGES \( I_\sigma = \langle c_{i\sigma}^+ c_{j\sigma} \rangle \)

Parameter \( I_\sigma \) can be calculated from the average kinetic energy. In the case of ferromagnetism one can write the following expression for the average kinetic energy of \(+\sigma\) electrons \( \langle K^\sigma \rangle \)

\[
\langle K^\sigma \rangle = -t_{eff}^\sigma \sum_{<ij>} \langle c_{i\sigma}^+ c_{j\sigma} \rangle = -zt_{eff}^\sigma I_\sigma = -D_{eff}^\sigma I_\sigma ,
\]  

where \( D_{eff}^\sigma = zt_{eff}^\sigma \) is the half band-width of the \(+\sigma\) electrons.

The kinetic energy can be calculated straightforward as

\[
\langle K^\sigma \rangle = \int_{-D}^D f \left[ \varepsilon^\sigma (\varepsilon^0) \right] \cdot \varepsilon^\sigma (\varepsilon^0) \cdot \rho^0 (\varepsilon^0) d\varepsilon^0 = -D_{eff}^\sigma I_\sigma ,
\]  

with \( \varepsilon^\sigma (\varepsilon^0) = \beta \varepsilon^0 \) being the energy of the deformed band, \( \varepsilon^0 \) is the energy of unperturbed band with all inter-site interactions being equal to zero, and \( f \left[ \varepsilon^\sigma (\varepsilon^0) \right] \) is the Fermi function. Eq. (12) means that we can calculate the average product of two nearest neighbor operators: \( I_\sigma = -\langle K^\sigma \rangle / D_{eff}^\sigma \).

In the case of zero temperature, \( T = 0 \) K, and constant density of state (DOS): \( \rho^0 (\varepsilon^0) = \text{const} = \frac{1}{T} \) for \(-D \leq \varepsilon^0 \leq D\) \( (D = zt - \text{unperturbed half-bandwidth}) \), we obtain from Eq. (12) that

\[
I_\sigma = n_\sigma (1 - n_\sigma) .
\]  

This approximation suggests that we can treat the average \( I_\sigma = \langle c_{i\sigma}^+ c_{j\sigma} \rangle \) as the probability of electron with spin \( \sigma \) hopping from the \( i \) to the \( j \) lattice site and back. More precisely, it is given by the average of two products. One is the product of probabilities that there is an electron with spin \( \sigma \) on the \( i \) site and that the \( j \) site has empty states; \( \frac{\tilde{n}_{i\sigma} \tilde{n}_{i\sigma} - \tilde{n}_{i\sigma}}{\tilde{n}_{i\sigma} + (\tilde{n}_{j\sigma} - \tilde{n}_{j\sigma})} \), and the second one is the probability of the opposite jump; \( \frac{\tilde{n}_{j\sigma} (\tilde{n}_{i\sigma} - \tilde{n}_{i\sigma})}{\tilde{n}_{j\sigma} + (\tilde{n}_{i\sigma} - \tilde{n}_{i\sigma})} \). The quantity \( \tilde{n}_{i\sigma} \) is the average number of electrons in the sub-band \( \sigma \) on sites \( i \) and \( \tilde{n}_{i\sigma}^t \) is the total capacity of the sub-band \( \sigma \) on site \( i \). The total hopping probability, called \( I_\sigma \), is given by the average of above probabilities

\[
I_\sigma \equiv \frac{1}{2} \left[ \frac{\tilde{n}_{i\sigma} (\tilde{n}_{j\sigma} - \tilde{n}_{j\sigma})}{\tilde{n}_{i\sigma} + (\tilde{n}_{j\sigma} - \tilde{n}_{j\sigma})} + \frac{\tilde{n}_{j\sigma} (\tilde{n}_{i\sigma}^t - \tilde{n}_{i\sigma})}{\tilde{n}_{j\sigma} + (\tilde{n}_{i\sigma}^t - \tilde{n}_{i\sigma})} \right] .
\]  

For the weak correlation \( (U << D) \), when the band is not split by the Coulomb repulsion, we have \( \tilde{n}_{i\sigma}^t = 1 \) and \( \tilde{n}_{i\sigma} = n_{i\sigma} \).
\[ I_\sigma \equiv \frac{1}{2} \left[ \frac{n_{i\sigma}(1 - n_{j\sigma})}{n_{i\sigma} + (1 - n_{j\sigma})} + \frac{n_{j\sigma}(1 - n_{i\sigma})}{n_{j\sigma} + (1 - n_{i\sigma})} \right] \tag{15} \]

Expressions (14) and (15) give a general form of quantity \( I_\sigma \), which depend on the type of magnetic ordering and on the strength of Coulomb on-site interaction through the mean values \( \bar{n}_{i\sigma} \) and \( \bar{n}_{j\sigma} \).

At first let us consider the quantity \( I_\sigma \) in the ferromagnetic state when one has the obvious relation; \( \bar{n}_{i\sigma} = \bar{n}_{j\sigma} \). In the case of a weak correlation (\( U << D \)) the band is not split and for the electrons with spin \( \sigma \) we have; \( \bar{n}_{i\sigma} = n_{i\sigma} \equiv n_\sigma \), and expression (15) can be simplified to Eq. (13).

In the case of strong correlation (\( U >> D \)) when the band is split into the lower and the upper Hubbard sub-band, quantities \( \bar{n}_{i\sigma} \) and \( \bar{n}_{t\sigma} \), will depend on the location of the chemical potential. When \( n < 1 \) the chemical potential is located in the lower Hubbard sub-band and we have; \( \bar{n}_{i\sigma} = n_\sigma, \bar{n}_{t\sigma} = 1 - n_{-\sigma} \), what gives for \( I_\sigma \) the result

\[ I_\sigma = \frac{n_\sigma (1 - n)}{1 - n_{-\sigma}} \tag{16} \]

-for the upper Hubbard sub-band (\( n > 1 \)) we have: \( \bar{n}_{i\sigma} = n_\sigma - (1 - n_{-\sigma}) = n - 1, \bar{n}_{t\sigma} = n_{-\sigma} \) and \( I_\sigma \) is equal to

\[ I_\sigma = \frac{(n - 1)(1 - n_\sigma)}{n_{-\sigma}} \tag{17} \]

In the antiferromagnetic state the crystal lattice will be divided into two interpenetrating sub-lattices; \( \alpha, \beta \) with opposite spins, and with the average electron numbers equal to

\[ n_{\pm\sigma}^\alpha = n_{\pm\sigma} = \frac{n \pm m}{2}, \quad n_{\pm\sigma}^\beta = n_{\mp\sigma} = \frac{n \mp m}{2} \tag{18} \]

where \( m \) is the antiferromagnetic moment per atom in Bohr's magnetons.

The indices \( i, j \) belong to the neighboring sub-lattices \( \alpha, \beta \) with opposite magnetic moments. In the result for AF ground state the parameter; \( I_\sigma = I_{-\sigma} = I_{AF} \) is spin independent (i.e. it does not depend on the first power of antiferromagnetic moment \( m \)).

The parameter \( I_{AF} \) for the weak correlation is calculated from Eq. (15) using values of \( n_{\alpha(\beta)}^\sigma \) from Eq. (18)

\[ I_{AF} = \frac{2n - n^2 - m^2}{4(1 - m^2)} \tag{19} \]

For the strong correlation and the chemical potential located in the lower sub-band (\( n \leq 1 \)), we obtain from Eq. (14) that

\[ I_{AF} = \frac{(2n - n^2 - m^2)(1 - n)}{(2 - n)^2 - m^2} \tag{20} \]

and for the upper sub-band
\[ I_{AF} = \frac{(n-1)(2n-n^2-m^2)}{n^2-m^2} \]  

After calculating the quantity \( I_\sigma \) for F and \( I_{AF} \) for AF ordering we can find the bandwidth parameter, \( b^\sigma \), and the modified molecular field, \( M^\sigma_i \), which are present in the Hamiltonian of Eq. (8).

### 2.2 Bandwidth, Molecular Field and Electron Occupation

#### 2.2.1 Ferromagnetic State

In the **ferromagnetic** state the electron concentration is the same on each lattice site: \( n_i^\sigma = n_j^\sigma = n^\sigma \), and the spin dependent parameter \( I_\sigma \) in the case of weak Coulomb correlation is given by Eq. (13), and Eqs (16) or (17) in the case of the strong correlation. Inserting those values into Eqs (9) and (10) we have

\[ b^\sigma = 1 - 2\frac{\Delta t}{t} n_{-\sigma} + 2\frac{t_{ex}}{t} \left( n_{-\sigma}^2 - I_{-\sigma}^2 - 2I_{\sigma}I_{-\sigma} \right) - \frac{J-V}{t} I_\sigma - \frac{J+J'}{t} I_{-\sigma} \]  

(22)

\[ M^\sigma_i \equiv M_\sigma = -(F+zJ)n_\sigma + zV n + 2zI_{-\sigma} (\Delta t - t_{ex}n_\sigma) \]  

(23)

Using Eq. (5) we can simplify Eq. (22) to the form

\[ b^\sigma = 1 - 2(1-S) n_{-\sigma} + (1-S)^2 \left( n_{-\sigma}^2 - I_{-\sigma}^2 - 2I_{\sigma}I_{-\sigma} \right) - \frac{J-V}{t} I_\sigma - \frac{J+J'}{t} I_{-\sigma} \]  

(24)

The effective total field in a ferromagnetic state, \( F_{tot}^F \), can be found now from the Weiss assumption that the energy shift between both spin sub-bands, \( \Delta E \), is equal to this field multiplied by the existing magnetic moment

\[ \Delta E = M^-_\sigma - M^\sigma = F_{tot}^F \cdot m \]  

(25)

which after assuming the Eq. (13) for \( I_\sigma \) gives

\[ F_{tot}^F = F + z[J + t_{ex} \frac{n^2-m^2}{2} + 2\Delta t(1-n)] \]  

(26)

In analyzing the Hamiltonian (8) for the appearance of ferromagnetism we will use the level of approximation which will modify the DOS, in addition to its shift by the molecular field.

After Fourier transform of the kinetic energy the Hamiltonian (8) takes on the following form

\[ H = \sum_{k\sigma} (\varepsilon_k^\sigma + M^\sigma - \mu) \hat{n}_{k\sigma} + U \sum_{i\sigma} \hat{n}_{i\sigma} \hat{n}_{i-\sigma} \]  

(27)

with the spin dependent electron dispersion relation given by
\[ \varepsilon_k^\sigma = \varepsilon_k^0 b^\sigma, \]  

where \( b^\sigma \) and \( M^\sigma \) for the ferromagnetic state are given by Eqs (22) and (23), and \( \varepsilon_k^0 \) is the initial dispersion energy of the electron (without the inter-site interactions)

\[ \varepsilon_k^0 = -t \sum_{<i,j>} \varepsilon^{ik(R_i-R_j)}. \]  

The Hamiltonian (27) is solved in the CPA approximation (see \([8,52]\)), which produces the following equation for the on-site self-energy \( \Sigma_\sigma(\varepsilon) \)

\[ (1 - n^-_\sigma) \frac{-\Sigma_\sigma}{1 + \Sigma_\sigma F_\sigma(\varepsilon)} + n^-_\sigma \frac{U - \Sigma_\sigma}{1 - (U - \Sigma_\sigma) F_\sigma(\varepsilon)} = 0, \]  

with the spin dependent Slater-Koster function \( F_\sigma(\varepsilon) \) which can be written as

\[ F_\sigma(\varepsilon) = \frac{1}{N} \sum_k \frac{1}{\varepsilon - \varepsilon_k^0 - M^\sigma - \Sigma_\sigma + \mu}. \]  

This function \( F_\sigma(\varepsilon) \) can be expressed by the unperturbed function

\[ F_0(\varepsilon) = \frac{1}{N} \sum_k \frac{1}{\varepsilon - \varepsilon_k^0}, \]  

by the help of the following relation

\[ F_\sigma(\varepsilon) = \frac{1}{b^\sigma} F_0 \left( \frac{\varepsilon - M^\sigma + \mu - \Sigma_\sigma}{b^\sigma} \right), \]  

which becomes the standard CPA relation: \( F_\sigma(\varepsilon) = F_0(\varepsilon - M^\sigma + \mu - \Sigma_\sigma) \), when all the inter-site interactions are zero and as a result \( b^\sigma = 1 \). The above defined Slater-Koster function was obtained from the solution of the CPA equation and depends on the spin orientation and on the on-site interaction, \( U \), and the inter-site interactions.

For the unperturbed Slater-Koster function we have the relation [8]

\[ \rho(\varepsilon) = -\frac{1}{\pi} \text{Im} F_0(\varepsilon). \]  

Using the identity

\[ \rho_\sigma(\varepsilon) = -\frac{1}{\pi} \text{Im} F_\sigma(\varepsilon), \]  

one can calculate the perturbed DOS depending on the on-site Coulomb correlation \( U \) through the self-energy \( \Sigma_\sigma \), and on the inter-site interactions through the band-width parameter \( b^\sigma \).

Using this DOS one can write the expression for electron occupation in the ferromagnetic state

\[ n_{\pm\sigma} = \int_{-\infty}^{\infty} \rho_{\pm\sigma}(\varepsilon) \frac{d\varepsilon}{1 + e^{(\varepsilon - \mu + M_{\pm\sigma})/kT}}, \]  

\[ \text{(36)} \]
where $\rho_{\sigma}(\varepsilon)$ is the spin dependent density of states given by Eq. (35), and the previous CPA equations.

The electron occupation number and the magnetization are given by

$$n = n_{\sigma} + n_{-\sigma} \quad ,$$  

$$m = n_{\sigma} - n_{-\sigma} \quad .$$  



\[2.2.2 \text{ ANTIFERROMAGNETIC STATE, DIAGONALIZATION}\]

In the antiferromagnetic state the magnetic moment on the nearest lattice sites is opposite with respect to each other (see Eqs (18)), the quantity $I_{\sigma} = I_{-\sigma} = I_{AF}$, and the bandwidth reduction parameter $b^\sigma$ from Eq. (9) is spin independent

$$b^\sigma = b_{-\sigma} = b^{AF} = 1 - \frac{\Delta t}{t} n + 2\frac{t_{ex}}{t} \left( \frac{n^2 - m^2}{4} - 3I_{AF}^2 \right) - \frac{2J + J' - V}{t} I_{AF} \quad .$$  

(39)

After expressing the kinetic terms by a factor $S$ defined in Eq. (5) it takes on the form

$$b^{AF} = 1 - (1 - S) n + (1 - S)^2 \left( \frac{n^2 - m^2}{4} - 3I_{AF}^2 \right) - \frac{2J + J' - V}{t} I_{AF} \quad .$$  

(40)

The generalized (modified) molecular field from Eq. (10) depends on the spin and on the sub-lattice index: $\alpha$ or $\beta$. For the sub-lattice $\alpha$ we have

$$M_{\sigma}^\alpha = -F n_{\sigma} - z \left( J + 2t_{ex} I_{AF} \right) n_{-\sigma} + zV n + 2z\Delta t I_{AF} \quad ,$$  

(41)

and for the sub-lattice $\beta$

$$M_{\sigma}^\beta = -F n_{-\sigma} - z \left( J + 2t_{ex} I_{AF} \right) n_{\sigma} + zV n + 2z\Delta t I_{AF} \quad .$$  

(42)

Now, we can calculate the effective total field on the sites $\alpha, \beta$ in a similar way to the case of ferromagnetism

$$F^{AF}_{tot} = \frac{M_{\sigma}^\alpha - M_{\sigma}^\beta}{m} = \frac{M_{\sigma}^\beta - M_{\sigma}^\alpha}{m} = F - z \left( J + 2t_{ex} I_{AF} \right) \quad .$$  

(43)

This equation shows that the positive inter-site exchange interaction, $J$, and exchange-hopping interaction, $t_{ex}$, are opposing AF. It is contrary to the case of ferromagnetism (see Eq. (26)), where both these interactions (when positive) are helping the ferromagnetism.

As mentioned above we assume the type of the crystal lattice, which can be divided into two interpenetrating sub-lattices: $\alpha, \beta$, with the average electron numbers given by Eqs (18).

For the AF ground state we use the diagonalization of Plischke & Mattis [53], Brouers [54] and Mizia [55]. The Hamiltonian (8), after taking into account Eqs (39)-(42), will take on the following form
\[ H = -t_{eff} \sum_{i\sigma} \left( \alpha_{i\sigma}^+ \beta_{i\sigma} + \beta_{i\sigma}^+ \alpha_{i\sigma} \right) + \sum_{i, \gamma, \sigma} \left( M_{\gamma} - \mu_0 + U \hat{n}_{i\sigma}^\gamma \right) \hat{n}_{i\sigma}^\gamma , \]  

(44)

where \( \alpha_{i\sigma}^+ (\alpha_{i\sigma}) \) and \( \beta_{i\sigma}^+ (\beta_{i\sigma}) \) are the creation (annihilation) operators for an electron of spin \( \sigma \) on the sub-lattice \( \alpha \) and \( \beta \) respectively, \( \hat{n}_{i\sigma}^\gamma = \gamma_{i\sigma}^+ \gamma_{i\sigma} \) is the electron number operator for electrons with spin \( \sigma \) on the sub-lattice \( \gamma = \alpha, \beta \), \( t_{eff} = t \cdot b_{AF} \) is the effective hopping integral.

Now we will derive the equations for dispersion relation, particle number and magnetization in the antiferromagnetic state using Hamiltonian (44) and the Green function technique. For the on-site interaction, \( U \), we use the standard CPA approximation, which for simplicity, in further analysis, is treated in the weak and strong correlation limits. For the weak correlation we use a first order approximation in interaction constant over the bandwidth. This is equivalent to the Hartree-Fock approximation. The second case is the high correlation approximation, \( U >> D \), which will be easy to extend for the arbitrary strength of the on-site interaction later on.

The main idea of the CPA formalism [8] is used now. We split the above stochastic Hamiltonian (44) into a homogeneous part

\[ H_0 = -t_{eff} \sum_{i\sigma} \left( \alpha_{i\sigma}^+ \beta_{i\sigma} + \beta_{i\sigma}^+ \alpha_{i\sigma} \right) - \mu \sum_{i\sigma} (\hat{n}_{i\sigma}^\alpha + \hat{n}_{i\sigma}^\beta) + \sum_{i\sigma} \Sigma_{\sigma}^\alpha \hat{n}_{i\sigma}^\alpha + \sum_{i\sigma} \Sigma_{\sigma}^\beta \hat{n}_{i\sigma}^\beta , \]  

(45)

and a stochastic part

\[ H_I = \sum_{i\sigma} (\tilde{V}^\alpha_{\sigma} - \Sigma_{\sigma}^\alpha) \hat{n}_{i\sigma}^\alpha + \sum_{i\sigma} (\tilde{V}^\beta_{\sigma} - \Sigma_{\sigma}^\beta) \hat{n}_{i\sigma}^\beta , \]  

(46)

where

\[ \mu = \mu_0 - zVn - 2z\Delta tI_{AF} \]  

(47)

is the effective chemical potential, \( \Sigma_{\sigma}^\gamma \) are the self energies on sites \( \gamma = \alpha, \beta \) for electrons with spin \( \sigma \) and \( \tilde{V}^{\alpha (\beta)}_{\sigma} \) are the stochastic potentials given by

\[ \tilde{V}^{\alpha (\beta)}_{\sigma} = \begin{cases} \tilde{V}^{\alpha (\beta)}_{1\sigma} = -F_{n_{\sigma}^{\alpha (\beta)}} - z (J + 2t_{ex}I_{AF}) n_{\sigma}^{\alpha (\beta)} \\
\tilde{V}^{\alpha (\beta)}_{2\sigma} = U - F_{n_{\sigma}^{\alpha (\beta)}} - z (J + 2t_{ex}I_{AF}) n_{\sigma}^{\alpha (\beta)} \end{cases} \]

with probabilities \( P_{1\sigma}^{\alpha (\beta)} = 1 - n_{-\sigma}^{\alpha (\beta)} \) \( P_{2\sigma}^{\alpha (\beta)} = n_{-\sigma}^{\alpha (\beta)} \)

(48)

The self-energies \( \Sigma_{\sigma}^\gamma \) fulfill the CPA equations

\[ \sum_{i=1}^{2} P_{i\sigma}^{\gamma} \frac{\tilde{V}_{i\sigma}^{\gamma} - \Sigma_{\sigma}^{\gamma}}{1 - (\tilde{V}_{i\sigma}^{\gamma} - \Sigma_{\sigma}^{\gamma}) F_{\sigma}^{\gamma}(\varepsilon)} = 0 \quad \text{for} \quad \gamma = \alpha (\beta), \]  

(49)

with the Slater-Koster function \( F_{\sigma}^{\gamma}(\varepsilon) \) for the sub-lattice \( \gamma \) in the following form

\[ F_{\sigma}^{\gamma}(\varepsilon) = \frac{1}{N} \sum_{k} G_{\sigma}^{\gamma}(\varepsilon, k) \]  

(50)
and $G^\gamma_\sigma(\varepsilon, k)$ given by Eq. (55) below.

After dropping the paramagnetic part the stochastic potential (48) takes on the following form

$$
\tilde{V}_\sigma^{\alpha(\beta)} = \begin{cases} 
\tilde{V}_{1\sigma}^{\alpha(\beta)} = \mp \Delta 
\tilde{V}_{2\sigma}^{\alpha(\beta)} = U \mp \Delta 
\end{cases}, \text{ with } F^{\alpha(\beta)}_{1\sigma} = 1 - n_{\mp}\sigma, 
$$

where

$$
n_{\pm}\sigma = \frac{n \pm m}{2}, \quad \Delta = F_{tot}^{AF} \frac{m}{2}, \text{ and } F_{tot}^{AF} = F - z (J + 2t_{ex}I_{AF}).
$$

This simplification of the Eq. (49) allows to see that the self-energies fulfill the relations; $\Sigma_{\sigma}^\alpha = \Sigma_{\sigma}^{\beta+}\equiv \Sigma_+,$ and $\Sigma_{\sigma}^{\alpha-} = \Sigma_{\sigma}^{\beta-} \equiv \Sigma_-.$ Therefore the solution of the problem can be reduced to finding only the self-energies, $\Sigma_{\pm}.$ The interpretation of the parameter $\Delta$ as the antiferromagnetic energy gap will be given below.

We transform Hamiltonian (45) into the momentum space, and use it in the equations of motion for the Green functions

$$
\varepsilon \langle \langle A ; B \rangle \rangle_{\varepsilon} = \langle \langle [A, B]_+ \rangle \rangle_{\varepsilon} + \langle \langle [A, H_0]_+ ; B \rangle \rangle_{\varepsilon},
$$

where $(A, B) \in (\alpha^+_{k\sigma}, \beta_{k\sigma}, \beta_{k\sigma}^+, \beta_{k\sigma}).$ As a result the following equations are obtained

$$
\begin{bmatrix} 
\varepsilon + \mu - \Sigma_{\sigma}^\alpha & -\varepsilon_k \\
-\varepsilon_k & \varepsilon + \mu - \Sigma_{\sigma}^\beta 
\end{bmatrix}
\begin{bmatrix} 
G_{\sigma}^{\alpha\alpha}(\varepsilon, k) \\
G_{\sigma}^{\beta\alpha}(\varepsilon, k)
\end{bmatrix} = 
\begin{bmatrix} 
1 & 0 \\
0 & 1 
\end{bmatrix},
$$

with e.g. $G_{\sigma}^{\alpha\alpha}(\varepsilon, k) = \langle \langle \alpha_{k\sigma}^+ \rangle \rangle,$ $G_{\sigma}^{\beta\alpha}(\varepsilon, k) = \langle \langle \beta_{k\sigma}^+ \rangle \rangle.$

Solving this set of equations we arrive at the following expressions for the Green functions

$$
G_{\sigma}^{\alpha(\beta)}(\varepsilon, k) = \frac{1}{2} \sqrt{\frac{\varepsilon + \mu - \Sigma_{\sigma}^{\beta(\alpha)}}{\varepsilon + \mu - \Sigma_{\sigma}^{\alpha(\beta)}}}
\begin{bmatrix} 
G(\varepsilon_{eff}, k) - G(-\varepsilon_{eff}, k) \\
G(\varepsilon_{eff}, k)
\end{bmatrix},
$$

with

$$
\varepsilon_{eff} = \sqrt{(\varepsilon + \mu - \Sigma_+)(\varepsilon + \mu - \Sigma_-)},
$$

and $G(\varepsilon_{eff}, k)$ given by

$$
G(\varepsilon_{eff}, k) = \frac{1}{\varepsilon_{eff} - \varepsilon_k} , \quad \varepsilon_k = \varepsilon^0_k b^{AF} .
$$

Remembering that

$$
\rho_{\sigma}^\gamma(\varepsilon) = -\frac{1}{\pi} \text{Im} [F_{\sigma}^\gamma(\varepsilon)]
$$

we obtain

$$
\rho_{\sigma}^{\alpha(\beta)} = -\frac{1}{\pi} \text{Im} \left[ \frac{\varepsilon + \mu - \Sigma_{\sigma}^{\beta(\alpha)}}{\varepsilon + \mu - \Sigma_{\sigma}^{\alpha(\beta)}} \right] \frac{1}{b^{AF}} F_0 \left( \varepsilon_{eff} / b^{AF} \right) \equiv -\frac{1}{\pi} \text{Im} F^{\pm} .
$$
where $F_0(\varepsilon)$ is the unperturbed Slater-Koster function given by Eq. (32).

Using Eq. (50) we obtain the expressions for electron numbers

$$n_\gamma = \int_{-\infty}^{\infty} \frac{1}{1 + e^{\varepsilon/kT}} \left( -\frac{1}{\pi} \right) \text{Im} [F_\sigma^\gamma (\varepsilon)] d\varepsilon = \frac{1}{N} \sum_k \int_{-\infty}^{\infty} \frac{1}{1 + e^{\varepsilon/kT}} \left( -\frac{1}{\pi} \right) \text{Im} [G_\sigma^\gamma (\varepsilon, k)] d\varepsilon .$$

(60)

Treating the self-energies $\Sigma_\gamma^\sigma$ as the solutions of Eq. (49), and using it only in the first order approximation with respect to the Coulomb on-site repulsion, $U$, we obtain

$$\Sigma_{\pm \sigma} = \Sigma_\pm \approx 2 \sum_{i=1}^{2} P_{i \pm \sigma}^{\alpha} \tilde{V}_{i \pm \sigma}^\alpha = [U - F - z(J + 2t_{ex} I_{AF})] \frac{n}{2} \mp \Delta .$$

(61)

where the antiferromagnetic energy gap $\Delta$ is given by the expression

$$\Delta = \left[ U + F_{AF} \right] \frac{m}{2} .$$

(62)

This expression is different from Eq. (52) by adding to the effective field the Coulomb repulsion, $U$, which in the case of the weak interaction is also treated in the Hartree-Fock approximation.

Neglecting the paramagnetic part in self-energies we have

$$\Sigma_\pm = \mp \Delta .$$

(63)

Inserting these self-energies into Eq. (55) and redefining $\varepsilon + \mu$ as $\varepsilon$ we obtain

$$G_\sigma^{\alpha(\beta)}(\varepsilon, k) = \frac{1}{2} \sqrt{\frac{\varepsilon \pm \Delta}{\varepsilon \pm \Delta}} [G(\varepsilon_{eff}, k) - G(-\varepsilon_{eff}, k)] .$$

(64)

From this equation using Eqs (50) and (58) one can obtain the following relation for the DOS on sites $\alpha, \beta$

$$\rho_\sigma^{\alpha(\beta)}(\varepsilon) = \sqrt{\frac{\varepsilon \pm \Delta}{\varepsilon \pm \Delta}} \rho(\varepsilon_{eff}) \equiv \rho_{\pm}(\varepsilon) .$$

(65)

In this form it is evident that the AF DOS will vanish between energies $-\Delta$ and $+\Delta$ (zero energy was assumed in the center of the atomic band or approximately at the atomic level). Hence, the quantity $\Delta$ is the AF energy gap. The schematic shape of the DOS is shown in Fig. 1.
FIG. 1. Schematic DOS in the antiferromagnetic state. The energy gap extends from $-\Delta$ to $+\Delta$.

One can prove that if the old distribution is normalized to unity;

$$\int_{-D}^{D} \rho(\varepsilon^0) d\varepsilon^0 = 1,$$

(66)

then the new one given by Eq. (65) is also normalized.

Since $\rho_+(\varepsilon) = \rho_-(-\varepsilon)$, one can write that

$$\frac{1}{2} \int_{-\sqrt{D^2_{eff} + \Delta^2}}^{\sqrt{D^2_{eff} + \Delta^2}} \rho_+(\varepsilon) d\varepsilon = \frac{1}{2} \int_{-\sqrt{D^2_{eff} + \Delta^2}}^{\sqrt{D^2_{eff} + \Delta^2}} \frac{1}{2} [\rho_+(\varepsilon) + \rho_-(-\varepsilon)] d\varepsilon = \frac{1}{2} \int_{-\sqrt{D^2_{eff} + \Delta^2}}^{\sqrt{D^2_{eff} + \Delta^2}} [\rho_+(\varepsilon) + \rho_-(-\varepsilon)] d\varepsilon,$$

(67)

where $D_{eff} = zt \cdot b^{AF}$. Inserting

$$\rho_+(\varepsilon) + \rho_-(-\varepsilon) = \left( \sqrt{\frac{\varepsilon - \Delta}{\varepsilon + \Delta}} + \sqrt{\frac{\varepsilon + \Delta}{\varepsilon - \Delta}} \right) \rho(\varepsilon_{eff}) \equiv \frac{2\varepsilon}{\varepsilon_{eff}} \rho(\varepsilon_{eff})$$

(68)
and using the identity obtained from Eq. (56); $d\varepsilon = \varepsilon_{eff} d\varepsilon_{eff}$, one obtains from Eq. (67)

$$\sqrt{D_{eff}^2 + \Delta^2} \int_{-\sqrt{D_{eff}^2 + \Delta^2}}^D \rho_+ (\varepsilon) d\varepsilon = \int_{-D_{eff}}^{D_{eff}} \rho(\varepsilon_{eff}) d\varepsilon_{eff} = 1.$$  \hspace{1cm} (69)

Restricting as before only to the first order approximation for the self-energies (Eq. (63)) in Eq. (60) we obtain the following expressions for electron numbers

$$n_{\pm \sigma} = n_{\mp \sigma} = \frac{1}{2N} \sum_k \left[ P_k^{\pm \sigma} f(E_k) + P_k^{\mp \sigma} f(-E_k) \right],$$  \hspace{1cm} (70)

where $f(E_k)$ is the Fermi function

$$f(E_k) = \frac{1}{1 + e^{(E_k - \mu)/kT}},$$  \hspace{1cm} (71)

$$E_k = \sqrt{\varepsilon_k^2 + \Delta^2}, \quad S_k^{\pm \sigma} = \sqrt{\frac{E_k + \Delta}{E_k - \Delta}},$$  \hspace{1cm} (72)

and

$$P_k^{\pm \sigma} = \frac{\varepsilon_k S_k^{\pm \sigma}}{E_k},$$  \hspace{1cm} (73)

is the occupation probability of state $(k, \pm \sigma)$.

The expression for electron occupation in the antiferromagnetic state in the presence of external field $H$ will be different from Eq. (36), which was suitable for ferromagnetism. Now, the external field will act differently on both spins $\pm \sigma$ in two sub-lattices $\alpha$ and $\beta$. Therefore its energy has to be included into the energy of the internal exchange field in the process of diagonalization. It will result in the following formula for the electron occupation on the sub-lattice $\alpha$

$$n_{\sigma}^\alpha = \int_{-\infty}^\infty \rho_\sigma^{\alpha} (\varepsilon, x^\sigma) \frac{d\varepsilon}{1 + e^{(\varepsilon - \mu)/kT}}$$  \hspace{1cm} (74)

where $x^\sigma = \sigma \Delta + \sigma \mu_B H$.

The precise form of the density of states $\rho_\sigma^{\alpha(\beta)} (\varepsilon)$ comes from Eq. (59) (or (65) in the case of the Hartree-Fock approximation). As it can be seen, it depends on the initial DOS and on the result of the diagonalization of two sub-lattices Hamiltonian.

3. **FREE ENERGY, STATIC MAGNETIC SUSCEPTIBILITY**

For a simple magnetic material, the free energy can be written

$$F_m = F_0 + a_2 m^2 + a_4 m^4 + \ldots = F_0 + \mu_B^2 m^2 / \chi + a_4 m^4 + \ldots$$  \hspace{1cm} (75)
with $\chi$ being the magnetic susceptibility.

The electron occupation of the ferromagnetic state in the presence of an external magnetic field $H$ is given by the expression (36) with added shift from the magnetic field

$$n_\sigma = \int_{-\infty}^{\infty} \rho_\sigma(\varepsilon) \frac{d\varepsilon}{1 + e^{(\varepsilon - \mu + M^\sigma - \sigma \mu_B H)/kT}},$$

(76)

where $\mu_B$ is the Bohr magneton.

The magnetic susceptibility is given by

$$\chi = \mu_B \left( \frac{\partial (n_\sigma - n_{-\sigma})}{\partial H} \right)_{H=0},$$

(77)

As a result of inserting Eq. (76) into it we arrive at the following equation for the static ferromagnetic susceptibility

$$\chi = \frac{2\mu_B^2 I_T}{1 - K - F^F_{tot} I_T},$$

(78)

where $K$ is the correlation factor defined mathematically by the following equation

$$K = \int_{-\infty}^{\infty} \frac{\partial \rho_\sigma(\varepsilon)}{\partial m} \frac{d\varepsilon}{1 + e^{(\varepsilon - \mu + M^\sigma)/kT}} - \int_{-\infty}^{\infty} \frac{\partial \rho_{-\sigma}(\varepsilon)}{\partial m} \frac{d\varepsilon}{1 + e^{(\varepsilon - \mu + M^{-\sigma})/kT}},$$

(79)

$F^F_{tot}$ is the total Stoner exchange field, which on the base of Eq. (25) can be written as

$$F^F_{tot} = -\left( \frac{\partial M^\sigma}{\partial m} \bigg|_{m \to 0} - \frac{\partial M^{-\sigma}}{\partial m} \bigg|_{m \to 0} \right) = -2 \frac{\partial M^\sigma}{\partial m} \bigg|_{m \to 0},$$

(80)

and

$$I_T = \int_{-\infty}^{\infty} \rho_{m=0}(\varepsilon) P_T(\varepsilon) d\varepsilon, \quad P_T(\varepsilon) = -\frac{\partial f(\varepsilon)}{\partial \varepsilon} = f^2(\varepsilon) e^{(\varepsilon - \mu)/kT} \frac{1}{kT},$$

(81)

$f(\varepsilon)$ is a Fermi function.

Returning with the expression (78) to Eq. (75) we arrive at a new form of Landau expansion which is

$$F_m = F_0 + m^2 \frac{1 - K - F^F_{tot} I_T}{2I_T} + a_4 m^4 + \ldots.$$

(82)

The critical (minimum) value of the total Stoner field creating ferromagnetism; $(F^F_{tot})_{\text{min}} = F^{cr}_{tot}$, is obtained from the zero of susceptibility denominator (Eq. (78)) or zero of the numerator in Eq. (82), around which changes the sign of the second order term. Hence, we arrive at the well-known Stoner criterion (see [56,57])

$$F^{cr}_{tot} = \frac{1 - K}{I_T},$$

(83)
which is modified here by including the correlation factor $K$.

Using the Stoner condition $F_{\text{tot}}^{cr} = (1 - K)/I_T$, back in the expression for susceptibility, Eq. (78), and in Landau expansion (82) we arrive at their corrected forms

$$\chi = \frac{2\mu_B^2}{F_{\text{tot}}^{cr} - F_{\text{tot}}} , \quad (84)$$

$$F_m = F_0 + \frac{m^2}{2} (F_{\text{tot}}^{cr} - F_{\text{tot}}) + a_4m^4 + \ldots \quad (85)$$

since $a_4 > 0$, the existence of the minimum in the above equation for $F_m$ will depend on the sign of $a_2 = \frac{1}{2}(F_{\text{tot}}^{cr} - F_{\text{tot}})$ or equivalently on the sign of the difference: $F_{\text{tot}}^{cr} - F_{\text{tot}}$. As a result, the simple Stoner criterion (Eq. (83)) will lead to the ferromagnetic instability with nonzero magnetic moment being given by the minimum of $F_m$ curve in Fig. 2. This minimum appears only when existing in a given material, $F_{\text{tot}}^{F} > F_{\text{tot}}^{cr}$, the $F_{\text{tot}}^{cr}$ being given by condition of Eq. (83). It is not mistake that in Eqs (84) and (85) we have $F_{\text{tot}}$ without the upper-script $F$, since as we will see below those two equations are valid without any changes for both $F$ and AF ordering.

To calculate the static antiferromagnetic susceptibility we will apply Eq. (77) to the susceptibility of the sub-lattice $^1$

$$\chi = \mu_B \left( \frac{\partial \left( n_\sigma^\alpha - n_{-\sigma}^\alpha \right)}{\partial H} \right)_{H=0} , \quad (86)$$

and we will use expression (74) for the electron occupation on sub-lattice $\alpha$ in the presence of an external field, arriving at the following equation for the static antiferromagnetic susceptibility

$$\chi = \frac{2\mu_B^2 K_x}{1 - K_x F_{\text{AF}}^{\text{tot}}} , \quad (87)$$

where the correlation factor $K_x$ in the antiferromagnetic case can be written as

$$K_x = \frac{1}{2} \left( \frac{\partial n_\sigma^\alpha}{\partial x^\alpha} - \frac{\partial n_{-\sigma}^\alpha}{\partial x^{-\sigma}} \right) = \frac{1}{2} \int_{-\infty}^{\infty} \left( \frac{\partial \rho_\sigma^\alpha (\varepsilon)}{\partial x^\alpha} - \frac{\partial \rho_{-\sigma}^\alpha (\varepsilon)}{\partial x^{-\sigma}} \right) \frac{d\varepsilon}{1 + e^{(\varepsilon - \mu)/kT}} = \int_{-\infty}^{\infty} \frac{\partial \rho_\sigma^\alpha (\varepsilon)}{\partial x^\alpha} f (\varepsilon) \, d\varepsilon . \quad (88)$$

Using the condition for the zero of susceptibility denominator we arrive at the critical value of the total field

$$F_{\text{tot}}^{cr} = \frac{1}{K_x (n)} \quad (89)$$

$^1$This susceptibility is a susceptibility of one sub-lattice. To find its relation with the total experimental susceptibility one has to take into consideration the direction of the external field with respect to the easy magnetic axis (see e.g. [58], [59])
After inserting this value into the sub-lattice susceptibility (Eq. (87)) and next to the formula for Landau expansion (Eq. (75)) we obtain again the same form of the susceptibility as for ferromagnetism (Eq. (84)), and of the free energy expansion as given by Eq. (85) for ferromagnetism. Thus the susceptibility of Eq. (84) and the energy expansion of Eq. (85) are the same for F and AF. The difference between these two orderings lies in the different values of critical (minimum) field. For F this field is given by Eq. (83) and for AF by Eq. (89). In both cases when existing in a given material $F^{F}_{tot} > F^{AF}_{tot}$, then the second order term in energy expansion vs. magnetization becomes negative and we have a nonzero equilibrium value of the ordering parameter $m$, see Fig. 2.

![Diagram](image)

**FIG. 2.** Dependence of Landau free energy on the magnetization $m$ for various values of $a_2 = \frac{1}{2} \left( F^{AF}_{tot} - F^{AF}_{tot} - F^{AF}_{tot} \right)$. Curve (a)- $F^{F}_{tot} < F^{AF}_{tot}$, curve (b)- $F^{F}_{tot} = F^{AF}_{tot}$, curve (c)- $F^{F}_{tot} > F^{AF}_{tot}$.

## 4 FERROMAGNETISM

### 4.1 ONSET OF FERROMAGNETISM

To compute the ferromagnetic criterion from Eq. (83) we have to calculate the correlation factor, $K$, defined in Eq. (79). We will calculate it now in the CPA approximation, assuming that we know the self-energy $\Sigma_a$. The total change of the DOS with magnetization, $K$, which enhances the possibility of creating magnetic ordering, is given from Eq. (79) as

$$ K = K_U + K_b \quad , $$

where
\[
K_U = 2 \int_{-\infty}^{+\infty} \frac{\partial \rho_\sigma(\varepsilon)}{\partial \Sigma_\sigma} \frac{\partial \Sigma_\sigma}{\partial m} f(\varepsilon) d\varepsilon \quad (91)
\]

and

\[
K_b = 2 \int_{-\infty}^{+\infty} \frac{\partial \rho_\sigma(\varepsilon)}{\partial b^\sigma} \frac{\partial b^\sigma}{\partial m} f(\varepsilon) d\varepsilon . \quad (92)
\]

Factor \(K_U\) describes the role of on-site interaction \(U\), and \(K_b\) the role of inter-site interactions in creating magnetization.

The schematic depiction of the DOS deformed by the on-site correlation \(U\) is shown in Fig. 3.

![Diagram of DOS showing influence of strong on-site Coulomb correlation, \(U\).](image)

The paramagnetic DOS for both spins, \(\pm \sigma\), are solid lines. At \(U\) which is strong enough to split the band into two sub-bands, lower sub-bands have the capacity of \(1 - n^{-\sigma}\) for \(+\sigma\) electrons, and \(1 - n^{\sigma}\) for \(-\sigma\) electrons. The changes in the spin electron densities integrated over energy are the shaded areas in this figure, and they are equal to the correlation factor \(K_U\). The shift between \(+\sigma\) and \(-\sigma\) electrons is created by the assumed exchange field.

The schematic depiction of the DOS deformed by the inter-site correlation is shown in Fig. 4.
Comparing Figs 3 and 4 one can see that the on-site correlation causes an increase in capacity of the majority spin band (or lower sub-band in the case of split band), while the inter-site correlation causes a decrease in width of the majority spin band. There is an important difference between these two effects. The situation from Fig. 3 can not lead by itself, without the exchange field, to ferromagnetism (see [9,10]), while the majority spin bandwidth decrease (see Fig 4) can. However, there is the problem with the magnitude of the interaction constants, which can lead to this ordering. There is also a difference in the order of approximation necessary to obtain different correlations. The band shape change shown in the Fig. 3 can be obtained only in the approximations higher than the 1st order in $U/D$, while the change shown in Fig. 4 is obtained already in the 1st order approximation (Hartree-Fock).

After inserting Eq. (90) into Eq. (78) one can write for the static ferromagnetic susceptibility
\[ \chi = \frac{2\mu_B^2 I_T}{1 - K_U - K_b - F_{tot}^F I_T} \].

(93)

At zero temperature we obtain from Eq. (81) that; \( I_T = \rho^0(\varepsilon_F^0)/b^0 \), where \( \varepsilon_F^0 \) is the Fermi level for the system without inter-site interactions and \( b^0 \) is the bandwidth change parameter in the paramagnetic state due to the inter-site interactions. This will modify the last relations into the following form

\[ \chi = \frac{2\mu_B^2 \rho^0(\varepsilon_F^0)}{(1 - K_U - K_b) b^0 - F_{tot}^F \rho^0(\varepsilon_F^0)} \].

(94)

Comparing the above equation with the equation for susceptibility when there is only the Hartree-Fock exchange field

\[ \chi = \frac{2\mu_B^2 \rho^0(\varepsilon_F^0)}{1 - F_{tot}^F \rho^0(\varepsilon_F^0)} \]

one can see that the ferromagnetic state will be favored by both positive correlation factors: \( K_U \) and \( K_b \), and by a decrease in the bandwidth \( b^0 < 1 \) due to the inter-site interactions.

From the zero of the susceptibility denominator (Eq. (94)) and Eqs (80), (23), one can calculate the critical on-site exchange interaction.

\[ F_{cr} = \frac{(1 - K_U - K_b) b^0}{\rho(\varepsilon_F)} - zJ - 4D \frac{\partial}{\partial m} \left[ \frac{(1-S)^2}{2} I_{-\sigma} n_{-\sigma} - I_{-\sigma} (1-S) \right] \],

(96)

where the kinetic interactions were expressed by the common factor \( S \), see Eq. (5).

The inter-site correlation factor given by Eq. (92) can be written as

\[ K_b = -2 \int_{-D}^{D} \rho_{m=0}(\varepsilon) P_T(\varepsilon) \varepsilon \frac{\partial b^\sigma}{\partial m} d\varepsilon. \]

(97)

At zero temperature we have \( P_T(\varepsilon) \Rightarrow \delta(\varepsilon - \varepsilon_F^0) \rho^0 \), which produces the following expression

\[ K_b = -2 \varepsilon_F^0 \rho^0(\varepsilon_F^0) \frac{\partial b^\sigma}{\partial m}. \]

(98)

In further analysis we will use two limiting cases for the on-site Coulomb repulsion-weak and strong correlation.

In the case of weak correlation the Coulomb correlation factor \( K_U = 0 \), and the critical on-site exchange interaction depends only on the inter-site interactions through the inter-site correlation factor \( K_b \). Using \( I_{-\sigma} \) expressed by Eq. (13) one obtains

\[ F_{cr} = \frac{(1 - K_b) b^0}{\rho^0(\varepsilon_F^0)} - zJ - 2D \left[ \frac{(1-S)^2}{2} n_{-\sigma}^2 + (1-S) (1-n) \right] \],

(99)

where the bandwidth change parameter in the paramagnetic state \( b^0 \), is given by
\[ b^0 = 1 - (1 - S) n + (1 - S)^2 \left[ \frac{n^2}{4} - 3 \left( \frac{n(2 - n)}{4} \right)^2 \right] - \frac{2J + J' - V n(2 - n)}{4t} \] . (100)

To illustrate the dependence of the critical on-site Stoner field, \( F^{cr} \) on electron concentration (at zero temperature) we will use the above equations and the initial semi-elliptic DOS given by

\[ \rho^0 (\varepsilon^0) = \frac{2}{\pi D} \sqrt{1 - \left( \frac{\varepsilon^0}{D} \right)^2} \] . (101)

Mathematically this is the simplest possible DOS which can be used for itinerant ferromagnetism. The rectangular DOS does not have a unique relationship between the Stoner field and the magnetization, and the parabolic DOS does not take into account the inter-site interactions, since it does not have a finite width and is not centered on the atomic level.

Electron concentration in the paramagnetic state (at T=0K) is calculated from the simple condition

\[ \frac{1}{2}n = \int_{-D}^{\varepsilon^0_F(n)} \rho^0 (\varepsilon^0) d\varepsilon^0 \] , (102)

with expression (101) inserted for the DOS. This will allow to calculate \( \varepsilon^0_F(n) \) and \( \rho^0(\varepsilon^0_F) \) for a given electron occupation \( n \). Finally, we calculate \( F^{cr}(n) \) from Eq. (99) with \( K_b \) estimated from Eq. (98), with the help of the derivative \( \frac{\partial \sigma}{\partial m} \) calculated from Eq. (22).

Calculated in this way the dependence of critical on-site Stoner field on electron concentration is shown in the Fig. 5 for the case of weak Coulomb correlation \( U \) and various parameters of inter-site interaction \( J \) and \( S \), at \( J' = J \) and \( V = 0 \). Parameters \( S = 1 \) and \( J = 0 \) describe the classic Stoner model.

We can see from this Figure that the decreasing factor \( S \) and increasing interaction, \( J \), decrease the on-site Stoner field required to create ferromagnetism, even to zero, at some electron concentrations (solid line). Including only the inter-site exchange interaction (dashed line) lowers the critical field symmetrically with respect to \( n = 1 \). The kinetic interactions: \( t_{ex} \) and \( \Delta t \), described by the hopping inhibiting factor \( S < 1 \) (dotted line) lower the on-site Stoner field, but now there is no symmetry with respect to the half-filled point \( n = 1 \).
FIG. 5. The dependence of the critical on-site Stoner field, $F^{cr}$, on the electron occupation, for different values of $S$ and $J$: $S = 1$ and $J = 0$ (the Stoner model) – dot-dashed line, $S = 0.6$ and $J = 0.5t$ – solid line, $S = 1$ and $J = 0.5t$ – dashed line, $S = 0.6$ and $J = 0$ – dotted line. This is the case of the weak Coulomb correlation, $U$.

In the case of strong correlation ($U >> D$) the band is split into two sub-bands. For the initial semi-elliptic DOS given by Eq. (101) we obtain from Eq. (30) in this limit (see [10]) the following densities

- for the lower Hubbard sub-band

$$
\rho_\sigma (\epsilon) = \frac{2}{\pi D_{ef}} \sqrt{1 - n_\sigma - \left( \frac{\epsilon}{D_{ef}} \right)^2},
$$

(103)

- for the upper Hubbard sub-band

$$
\rho_\sigma (\epsilon) = \frac{2}{\pi D_{ef}} \sqrt{n_\sigma - \left( \frac{\epsilon}{D_{ef}} \right)^2},
$$

(104)

with $\epsilon = \epsilon_0^\sigma b^0$, and $D_{ef} = D b^0$.

The parameter $I_\sigma$ is given by Eqs (16) and (17), which after inserting into Eq. (96) give the following values of the critical on-site exchange interaction

- for the lower Hubbard sub-band

$$
F^{cr} = \frac{(1 - K_U - K_b) b^0}{\rho^0(\epsilon_F^0)} - zJ - 2D \frac{(1 - n)}{(2 - n)^2} \left[ \frac{(1 - S)^2}{2} n^2 + 4 (1 - S) (1 - n) \right],
$$

(105)

- for the upper Hubbard sub-band

$$
F^{cr} = \frac{(1 - K_U - K_b) b^0}{\rho^0(\epsilon_F^0)} - zJ - 2D (n - 1) \left[ \frac{(1 - S)^2}{2} - 4 (1 - S) \frac{(n - 1)}{n^2} \right],
$$

(106)
where $\rho^0(\varepsilon_F) = \lim_{m \to 0} \rho_\sigma(\varepsilon)/b^0$, with $\rho_\sigma(\varepsilon)$ given by Eqs (103), (104) with $n_{-\sigma} = n/2$, and $\varepsilon_F(n)$ calculated from Eq. (102) as $\varepsilon_F(n) = \varepsilon^0_0 b^0$. The correlation factor $K_U$ is calculated from Eq. (91), which at $T=0K$ is reduced to the simple condition

$$K_U = \int_{-D_{eff}}^{\varepsilon_F} \frac{\partial \rho_\sigma(\varepsilon)}{\partial \varepsilon} d\varepsilon - \int_{-D_{eff}}^{\varepsilon_F} \frac{\partial \rho_{-\sigma}(\varepsilon)}{\partial \varepsilon} d\varepsilon = 2 \int_{-D_{eff}}^{\varepsilon_F} \frac{\partial \rho_\sigma(\varepsilon)}{\partial \varepsilon} d\varepsilon,$$

(107)
in which we will use the DOS given by Eqs (103) and (104).

We calculate $F^{cr}(n)$ from Eq. (106), with $K_b$ given by Eq. (98). The bandwidth $b^0$ is calculated from Eq. (22) with $I_\sigma$ given by the $m = 0$ limit of Eqs (20) and (21), for the lower and upper sub-band, respectively.

Fig. 6 shows that in the presence of the on-site strong correlation $U$, the inter-site interactions: $J$, $S$, decrease the critical Stoner field dramatically. The increase of $J$ causes the decrease of $F^{cr}$ for concentrations nearly half-filled and also at small concentrations and concentrations close to completely filled. The decrease of $S$ from 1 to 0 causes a drop of the critical Stoner field, $F^{cr}$, especially for small $n < 0.5$, and for $1 < n < 1.5$, where both Hubbard sub-bands begin to fill. As we know the strong Coulomb repulsion causes the split of the band. This split causes the change in sign of the inter-site correlation factor $K_b$ when the Fermi level moves from the lower to the upper Hubbard sub-band. For $S \neq 1$ the ratio $\frac{K_b b^0}{\rho^0(\varepsilon_F)} \neq 0$. This is why the curves with $S < 1$ will have a discontinuity at half filling, when the Fermi energy jumps from the lower to the upper sub-band.

FIG. 6. Dependence of the on-site critical Stoner field, $F^{cr}$ (in the units of half bandwidth), on the electron occupation. The curves show the influence of inter-site interactions, $J = J'$, $V = 0$, and of the hopping interactions, $\Delta t$, $t_{ex}$, represented by the hopping ‘inhibiting’ factor $S$ on $F^{cr}$ in the presence of strong on-site correlation, $U = \infty$.

To justify the use in this chapter of the rather academic limit of $U >> D$ for F ordering we compare on the next graph the three cases; $U = 0$, $U = 3D$, and $U >> D$. All the curves
were calculated on the base of Eqs (101), (30) and (102). One can see that the difference between the curves $U = 3D$, and $U \gg D$ is small. This justifies the use in numerical calculations (for simplicity) of the strong correlation limit $U \gg D$.

![Diagram showing dependence of critical Stoner field on occupation number](image)

**FIG. 7**. Dependence of the on-site critical Stoner field, $F_{cr}$ (in the units of half bandwidth), on the electron occupation, which shows the influence of on-site correlation, $U$. The inter-site interactions are zero ($J = 0, S = 1$)

### Enhancement of magnetic susceptibility

The susceptibility given by Eq. (93) for $T \neq 0$ K or Eq. (94) for $T = 0$ K is not divergent for most of the pure elements, as only few of them are magnetic. But for many pure elements the denominator of susceptibility is significantly decreased, which produces the experimentally observed increase of susceptibility. This phenomenon was extensively studied in the past. From Eq. (94) in the H-F approximation for $U$, and in the absence of the inter-site interactions, when $K_U = 0$, $K_b = 0$, and $b^0 = 1$ (see e.g. [57]) one can write

$$
\chi = \frac{2\mu_B^2 \rho(\varepsilon_F^0)}{1 - F_{tot}^F \rho(\varepsilon_F^0)} = \chi PA,
$$

where the bare Pauli term $\chi_P = 2\mu_B^2 \rho(\varepsilon_F^0)$ is enhanced by the factor $A = 1/ \left[1 - F_{tot}^F \rho(\varepsilon_F^0) \right]$ the Stoner enhancement factor. This enhancement in the case of nonzero correlations is given by

$$
A = 1/ \left[ (1 - K_U - K_b) b^0 - F_{tot}^F \rho(\varepsilon_F^0) \right].
$$

In the past the CPA approximation describing the on-site repulsion $U$; $K_U \neq 0$, $b^0 = 1$, was used to calculate this enhancement (see [9] for the general model of pure elements and e.g. [60–62] for susceptibility of disordered binary alloys). Experimental data and theoretical results from the local density functional method were collected more recently for pure
transition elements by [56]. In this chapter the factor $A$ (Eq. (109)) is additionally increased by the inter-site interactions; $K_b \neq 0, b^0 < 1$. This effect should be also included in the investigation of experimental data on the susceptibility enhancement.

### 4.2 NUMERICAL RESULTS FOR MAGNETIZATION AND CURIE TEMPERATURE

The Curie temperature, at which magnetization vanishes, is calculated from the zero of the susceptibility denominator, Eq. (93), attained with temperature

$$1 - K_U - K_b - F_{tot}^F I_T = 0 .$$

(110)

Quantity $F_{tot}^F$ calculated from this equation at nonzero temperature is larger than $F_{tot}^{cr}$, calculated from the same equation (110) at zero temperature, since $I_T$ has its maximum $I_T = \rho^0(\varepsilon_F)/b^0$ at zero temperature.

In the case of **weak Coulomb correlation** ($U = 0$) the Coulomb correlation factor, $K_U = 0$, hence the Curie temperature depends only on $K_b$ and $I_T$.

In the case of **strong Coulomb correlation** ($U >> D$) according to Eq. (110) we have to include the correlation factor $K_U$ given by Eq. (91). In this case the band is split into two sub-bands. Using the DOS given by Eqs (103) and (104) we calculate numerically the correlation factor $K_U$ from Eq. (107) where the self-energy was eliminated

$$K_U = 2 \int_{-\infty}^{+\infty} \frac{\partial \rho_\sigma(\varepsilon)}{\partial m} f(\varepsilon) d\varepsilon .$$

(111)

Alternatively, we can calculate directly the magnetization as; $m(T) = n_\sigma - n_{-\sigma}$, with $n_{\pm\sigma}$ from Eq. (36) for a given electron occupation; $n = n_\sigma + n_{-\sigma}$, and then obtain the Curie temperature by searching for the Curie point where $m(T_C) \to 0$.

The procedure for calculations is the following. We use Eq. (37) for the electron occupation number, which corresponds to a given 3d ferromagnetic element in the Table I. We adjust the value of total Stoner field, $F_{tot}^F$, to create the experimental zero temperature magnetization $m(T \to 0 K) = n_\sigma (0 K) - n_{-\sigma} (0 K)$. Having obtained $F_{tot}^F$ we calculate the on-site Stoner field, $F$, from Eq. (26) at the given assumed inter-site interactions $J, S$ and $D = 3d$ half band-width according to [63].

Next, we calculate the Curie temperature with the same constants, $F, J$ and $S$ using Eq. (38) for the magnetization and searching for the point where $m(T_C) \to 0$.

The results in **case of the weak correlation** are collected in the Table I.
TABLE I. Curie Temperatures and Values of On-site Stoner Field for Ferromagnetic Elements, Modified Stoner Model with $U = 0$

| Element | $n$  | $m$  | $D$[eV] | $T_c$[K] | $F(m)$[eV] | $T_c^{exp}$[K] |
|---------|-----|-----|---------|---------|-----------|---------------|
|         |     |     |         |         |           |               |
|          |     |     |         |         |           |               |
|          |     |     |         |         |           |               |
| Fe      | 1.4 | 0.44| 2.8     | 2050    | 3295      | 3980          |
|         |     |     |         |         |           |               |
|         |     |     |         |         |           |               |
| Co      | 1.65| 0.344| 2.65   | 1690    | 3300      | 3880          |
|         |     |     |         |         |           |               |
|         |     |     |         |         |           |               |
| Ni      | 1.87| 0.122| 2.35 | 620     | 870       | 1720          |
|         |     |     |         |         |           |               |
|         |     |     |         |         |           |               |

TABLES
It is very interesting to compare the different results for $T_c$ which are shown in this Table. Column no. 4, which is the Stoner model for semi-elliptic DOS, shows that all theoretical results of the pure Stoner model are much higher than the experimental Curie temperatures (column no. 5). This means that the Stoner model, which assumes that the on-site atomic field creates ferromagnetism, overestimates, to a large extent, the Curie temperature. The necessary on-site Stoner field is also unrealistically high. Perhaps ferromagnetism is the result of inter-site forces changing the bandwidth, since column no. 1 is closest to the experimental results. The larger the component of the on-site field (i.e. $S \to 1, J \to 0$), the more the $T_c$ results exceed the experimental values. However, one has to be careful not to overestimate these inter-site interactions since they suppose to be weak. They lower substantially the Curie temperature, but the remaining difference between theoretical and experimental values is still significant and it has to be attributed to the thermal spin fluctuations, since there is an experimental evidence of such fluctuations (see [56, 64]).

These simple calculations would confirm the earlier attempts of understanding the itinerant ferromagnetism as the effect of ordering local moments, whose alignment disappear at the Curie temperature. However, the moments themselves exist up to the temperatures exceeding the Curie temperature by two or three times (see Mizia [65]). We could think about local moments as being created by the Stoner on-site field, but their ordering would be driven by the inter-site interactions, which is much weaker than the on-site field.

In the case of strong correlation the procedure of calculations is the same as in the case of the weak correlation. First, we adjust the on-site exchange interaction $F$ (at given inter-site parameters $J, S$) to the magnetic moment at zero temperature. We use the DOS given by Eqs (103) and (104). The correlation factor is calculated from Eq. (111). Finally, we calculate the Curie temperature from Eq. (110), or from the condition of vanishing magnetization, with the same interactions $F, J$ and $S$.

Table II shows the results of Curie temperatures obtained for the strong on-site correlation from the Stoner model ($S = 1, J = 0$), and for the cases with nonzero kinetic and exchange inter-site interactions. It can be seen that the influence of strong on-site correlation ($U = \infty$) does not lower the theoretical Curie temperature when compared to the case of no on-site correlation ($U = 0$) (see Table I), although the necessary on-site exchange field, $F$, in the case of strong on-site correlation ($U = \infty$) is lower than without it, $U = 0$ (compare Figs 5 i 6).
| Element | $n$  | $m$  | $T_c[K]$ | $F(m)$ [eV] | $T_c^{exp}[K]$ |
|---------|-----|-----|---------|-------------|---------------|
| Fe      | 1.4 | 0.44| 2420    | 4000        | 3810          | 4960          | 1043          |
|         |     |     | 0.41    | 2.45        | 1.03          | 3.06          |               |
| Co      | 1.65| 0.344| 1850    | 3270        | 3990          | 5180          | 1388          |
|         |     |     | 1.35    | 3.65        | 1.82          | 4.12          |               |
| Ni      | 1.87| 0.122| 630     | 910         | 1770          | 2020          | 627           |
|         |     |     | 1.94    | 4.2         | 2.9           | 5.16          |               |

TABLE II. Curie Temperatures and Values of On-site Stoner Field for Ferromagnetic 3d Elements, Modified Stoner Model with $U = \infty$
Now we want to focus on the temperature dependence of the magnetization $m$ which is plotted in Fig. 8. The dependence $m(T)$ was calculated for the strong correlation and without the correlation for electron occupation representing iron. In both cases we assumed; $J = 0$, $S = 1$ and $J = 0.5t$, $S = 0.6$.

One can see from this figure that the strong on-site correlation $U$ is not helping ferromagnetism at all, as the curves with $U >> D$ lay above the corresponding curves with $U = 0$.

![FIG. 8. Magnetization dependence on temperature, $m(T)$, without and with strong Coulomb correlation, $n = 1.4$, $D = 2.8$ eV for different values of parameters $J$ and $S$; $U = 0$, $J = 0$, $S = 1$- solid line, $U = \infty$, $J = 0$, $S = 1$- dashed line, $U = 0$, $J = 0.5t$, $S = 0.6$- dotted line, $U = \infty$, $J = 0.5t$, $S = 0.6$- dot-dashed line.]

5 ANTIferromagnetism

5.1 ONSET OF ANTIferromagnetism

We can find the critical value of the total field creating AF from Eq. (89) using for $K_x$ the expression (88)

$$K_x = \int_{-\infty}^{\infty} \frac{\partial \rho^\alpha_\sigma(\varepsilon)}{\partial \varepsilon} f(\varepsilon) d\varepsilon = \int_{-\infty}^{\infty} \frac{\partial \rho^\alpha_\sigma(\varepsilon)}{\partial \Delta} f(\varepsilon) d\varepsilon = \frac{1}{N} \sum_k \int_{-\infty}^{\infty} f(\varepsilon) \left( -\frac{1}{\pi} \right) Im \left[ \frac{\partial G^{\alpha_\sigma}_{\varepsilon,k}(\varepsilon,k)}{\partial \Delta} \right]_{\Delta \to 0} d\varepsilon. \quad (112)$$

Differentiating Eq. (64) we can show that

$$\frac{\partial G^{\alpha}_{\varepsilon,k}(\varepsilon,k)}{\partial \Delta} \bigg|_{\Delta \to 0} = \left( \frac{1}{\varepsilon + \varepsilon_k} - \frac{1}{\varepsilon - \varepsilon_k} \right) \frac{1}{2\varepsilon_k}. \quad (113)$$
Using this expression in Eq. (112) we obtain the following formula

\[ K_x = -\frac{1}{N} \sum_k \left[ \frac{f(\varepsilon_k) - f(-\varepsilon_k)}{2\varepsilon_k} \right] = \frac{1}{N} \sum_k \frac{1}{4\varepsilon_k} \left[ \tanh \frac{\beta}{2} (\varepsilon_k - \mu) - \tanh \frac{\beta}{2} (-\varepsilon_k - \mu) \right] . \]  

We can calculate now \( F_{\text{tot}}^{cr} (n) \) from the relation; \( F_{\text{tot}}^{cr} = 1/K_x \). The above equation although similar to the condition for superconductivity is different in two respects (see [66]). First, the summation runs from \( k \) minimum in the band to maximum \( k \), giving a positive \( K_x \) and positive \( F_{\text{tot}}^{cr} (n) \). Second, in the denominator we have the dispersion relation \( \varepsilon_k \), which is centered on the average energy of the band not around the chemical potential, like in the case of superconductivity (see [67]).

From the expression for the electron numbers \( n^{\pm}_{\alpha} (\gamma = \alpha, \beta) \) (Eq. (70)) we obtain in the mean-field approximation that the antiferromagnetic moment per atom (in Bohr’s magnetons) is given by the following expression

\[ m = n^{\alpha}_{\sigma} - n^{\alpha}_{-\sigma} = \frac{1}{2N} \sum_k \left( P_{k}^{+\sigma} - P_{k}^{-\sigma} \right) [f(E_k) - f(-E_k)] . \]  

The chemical potential \( \mu \) is determined from the carrier concentration \( n \) on the basis of the equation, which also comes from Eq. (70)

\[ n = n^{\alpha}_{\sigma} + n^{\alpha}_{-\sigma} = \frac{1}{2N} \sum_k \left( P_{k}^{+\sigma} + P_{k}^{-\sigma} \right) [f(E_k) + f(-E_k)] . \]  

Inserting Eq. (72) into Eq. (115) and using the relation (74) we obtain

\[ 1 = -F_{\text{tot}}^{AF} \frac{1}{N} \sum_k \frac{1}{2E_k} [f(E_k) - f(-E_k)] . \]  

At the transition from AF to normal state; \( \Delta \to 0 \), and the condition (117) takes on the form

\[ 1 = -F_{\text{tot}}^{cr} \frac{1}{N} \sum_k \frac{f(\varepsilon_k) - f(-\varepsilon_k)}{2\varepsilon_k} = F_{\text{tot}}^{cr} \frac{1}{N} \sum_k \frac{1}{4\varepsilon_k} \left[ \tanh \frac{\beta}{2} (\varepsilon_k - \mu) + \tanh \frac{\beta}{2} (-\varepsilon_k - \mu) \right] \]  

where \( \varepsilon_k = \varepsilon^0_k b^{AF} \), which is the same as the result (114) coming from the static magnetic susceptibility.

For the numerical analysis we will use the \( \Delta \to 0 \) limit of Eq. (116) and of Eq. (118) in their integral form,

\[ n = 2 \int_{-D_{\text{eff}}}^{D_{\text{eff}}} \rho (\varepsilon) \ f(\varepsilon) d\varepsilon \ . \]
\[ 1 = -F_{\text{tot}}^c r_{\text{eff}} \rho(\varepsilon) \frac{f(\varepsilon) - f(-\varepsilon)}{2\varepsilon} d\varepsilon = F_{\text{tot}}^c r_{\text{eff}} \rho(\varepsilon) \frac{1}{4\varepsilon} \left[ \tanh \left( \frac{\varepsilon - \mu}{\beta} \right) - \tanh \left( \frac{-\varepsilon - \mu}{\beta} \right) \right] d\varepsilon, \quad \text{with} \quad \varepsilon = \varepsilon^0 b^{AF}, \quad (120) \]

and the semi-elliptic DOS given by Eq. (101) in the case of the weak Coulomb correlation \( U \). For the strong Coulomb correlation \( U \) we will use split densities given by Eqs (103) and (104). The results will show how the critical on-site exchange field depends on the electron concentration. Figs 9 and 10 show the dependence of this interaction, \( F_{\text{cr}}^c \), on the electron concentration for different values of the inter-site and kinetic interactions, described by the parameters; \( J, S \), in the case of weak and strong Coulomb correlation \( U \). Analyzing these curves one can see that the inter-site exchange interaction \( J \) increases values of on-site exchange interaction, \( F_{\text{cr}}^c \), required for AF. The decrease in \( F_{\text{cr}}^c \) can be achieved when \( J < 0 \). This effect is opposite to the case of ferromagnetism, where stabilization of ordering was obtained for \( J > 0 \). Those two different effects of inter-site exchange interaction on magnetism can be roughly understood when one compares the expressions for total field in the case of ferromagnetism; \( F_{\text{tot}}^F = F + z [J + t_{\text{ex}} n^2 - m^2 + 2\Delta t(1 - n)] \), and antiferromagnetism \( F_{\text{tot}}^{AF} = F - z (J + 2t_{\text{ex}} I_{AF}) \). We use the word 'roughly' since in calculating the critical fields there is included also the factor of the band-width change, which does not appear in the effective fields. The result of this simplified approach with respect to the inter-site exchange energy, \( J \), is in agreement with the Heisenberg term for the interaction energy of localized spins; \( -J \sum_{i,j} S_i \cdot S_j \), which points towards ferromagnetism when \( J > 0 \), and towards antiferromagnetism when \( J < 0 \). Analyzing the influence of inter-site interaction \( J \) on long range ordering one has to remember that the negative value of this interaction stimulates the d-wave superconductivity (see e.g. [68]). As a result it will cause the coexistence of SC and AF ordering. This is why the t-J model was successful in describing coexistence of the singlet SC and antiferromagnetism. Although one has to remember that this model has a contradiction in its very origin. This contradiction lies in considering electrons as itinerant (the kinetic \( t \)-term) and localized (the potential \( J \)-term) at the same time. Including in our model the kinetic interactions; \( \Delta t \) and \( t_{\text{ex}} \), has decreased the minimum on-site exchange interaction necessary for AF. The hopping interaction \( \Delta t \) decreases \( F_{\text{cr}}^c \) by decreasing the band-width (see [69]). Positive exchange-hopping interaction \( t_{\text{ex}} \) also decreases the band-width but at the same time it decreases the effective field (see above or Eq. (62)). In effect the influence of this interaction on AF is very small.
FIG. 9. The dependence of the critical on-site exchange, $F^{cr}$, on the electron occupation. The case of the weak correlation $U$. The curves for different values of $S$ and $J$ are; $S = 1$ and $J = 0$–dot-dashed line, $S = 0.6$ and $J = 0.5t$ – solid line, $S = 1$ and $J = 0.5t$ – dashed line, $S = 0.6$ and $J = 0$ – dotted line.

FIG. 10. The dependence of the critical on-site exchange, $F^{cr}$, on the electron occupation. The case of the strong correlation $U$. The curves for different values of $S$ and $J$ are; $S = 1$ and $J = 0$–dot-dashed line, $S = 0.6$ and $J = 0.5t$ – solid line, $S = 1$ and $J = 0.5t$ – dashed line, $S = 0.6$ and $J = 0$ – dotted line. The double dotted-dashed line is for $\Delta t = t$ ($t_1 = 0$ or $S = 0$), and $t_{ex} \equiv 0$ (see Eq. (125) below).

Including into calculations the inter-site interactions; $J, J', V$, does not shift the minimum of the critical field $F^{cr}(n)$, which for the weak correlation is located at $n = 1$, and for the
strong correlation at \( n = 2/3 \). The inter-site interactions do not change the character of the critical curves, they only lower them by a factor of \( b^{AF} \) from Eq. (39) or (40). Remembering that \( \varepsilon = \varepsilon^0 b^{AF} \) this can be proved analytically

\[
K_x(n) = -\int_{-D_{eff}}^{D_{eff}} \rho(\varepsilon) \frac{f(\varepsilon) - f(-\varepsilon)}{2\varepsilon} d\varepsilon
= -\frac{1}{b^{AF}} \int_{-D}^{D} \rho^0(\varepsilon^0) \frac{f(\varepsilon^0 b^{AF}) - f(-\varepsilon^0 b^{AF})}{2\varepsilon^0} d\varepsilon^0 = \frac{1}{b^{AF}} K_x^0(n)
\]  

(121)

Since \( F_{cr}^{tot} = 1/K_x \), and \( F_0^{cr} = 1/K_x^0 \) we obtain that

\[
F_{cr}^{tot} = F_{cr}^{tot} - z(J + 2t_{ex} I_{AF}) = b^{AF} F_0^{cr}
\]

(122)

where \( F_{cr}^{tot} \) and \( F_0^{cr} \) are the critical on-site exchange fields for AF with and without the inter-site interactions, respectively.

Including the kinetic interactions, \( S < 1 \), leaves the minima of critical curves where they are as it only changes the factor \( b^{AF} \) in Eq. (122). In this chapter we assumed dependence of the hopping energy on the occupation expressed by the equation

\[
t_{ij}^\sigma = t - \Delta t(\hat{n}_{i-\sigma} + \hat{n}_{j-\sigma}) + 2t_{ex}\hat{n}_{i-\sigma}\hat{n}_{j-\sigma}
\]

(123)

This relation together with the other inter-site interactions; \( J, J', V \), expressed in the generalized Hartree-Fock approximation brought the Eq. (39) for \( b^{AF} \) with \( I_{AF} \) given by Eq. (20) or (21) in the case of \( U >> D \). The only exception from the scaling rule for critical on-site exchange interaction in the case of \( U >> D \) is the situation when \( b^{AF}(n = 1) = 0 \). This would cause the critical curve to drop at \( n = 1 \), what would make antiferromagnetism possible at this concentration. In the itinerant band model this is the situation when there is localization at half-filling. As a result we obtain at this concentration possible AF, and since the band will expand very rapidly with the occupation \( n \) departing from one there will be also a strong driving force towards SC (see [70]). In such circumstances we will have the co-existence or rather competition at \( n = 1 \) between AF and SC. Unfortunately, since \( I_{AF}(n = 1) = 0 \), the relation (39) gives \( b^{AF}(n = 1) \neq 0 \). In our previous paper (see [69]) we have the zero bandwidth at \( n = 1 \), but we have neglected the \( t_{ex} \) term in Eq. (3) or (123) above. This is equivalent to the use of Hirsch’s simplified linear approach (see [47,71])

\[
t_{ij}^\sigma = t - \Delta t(\hat{n}_{i-\sigma} + \hat{n}_{j-\sigma})
\]

(124)

instead of Eq. (123). From this relation it follows that

\[
b^{AF} = 1 - \frac{\Delta t}{t} n - \frac{2J + J' - V}{t} I_{AF}
\]

(125)

At \( \Delta t = t \) or \( t_1 = 0 \) this equation gives \( b^{AF}(n = 1) = 0 \), and we have the possibility of AF ordering, see the double dotted-dashed line in Fig. 10. AF can occur at \( n = 1 \) only when \( t_1 \equiv 0 \) what means that there is no hopping in the presence of other electrons with opposite spin, and additionally when \( t_{ex} \equiv 0 \), which leads to the strange condition that \( t_2 = -t \). Alternatively we can obtain the Eq. (124) (which leads to the AF at \( n = 1 \) from
the basic Eq. (2) in a first approximation by neglecting all the operator products of the
type; $\hat{n}_{i-\sigma} \hat{n}_{j-\sigma}$ in Eq. (2).

5.2 NUMERICAL RESULTS FOR MAGNETIZATION AND NEEL’S TEMPERATURE

The analysis of Eqs (116) and (117) in their integral form will give the magnetization
dependence on the temperature for different values of the on-site and inter-site interactions.

$$n = \int_{-D}^{D} \rho(\varepsilon) [f(E) + f(-E)] d\varepsilon$$  \hspace{1cm} (126)

$$1 = -F_{AF} \int_{-D}^{D} \rho(\varepsilon) \frac{[f(E) - f(-E)]}{2E} d\varepsilon$$  \hspace{1cm} (127)

where

$$E = \sqrt{\varepsilon^2 + \Delta^2} \quad \Delta = F_{tot}^{AF} m \quad F_{tot}^{AF} = F - z (J + 2t_{ex} I_{AF}).$$  \hspace{1cm} (128)

From the above equations we find numerically the sub-lattice magnetization, and the
Neel’s temperature, which is the temperature where this magnetization drops to zero. Fig.
11 presents the dependence of Neel’s temperature, $T_N$, on electron concentration for different
values of the inter-site and kinetic interactions for the weak Coulomb correlation. All the
curves are for the same on-site exchange field. The curves with nonzero inter-site exchange
interaction $J$ have a lower Neel’s temperature, because this interaction decreases the effective
exchange interaction; $F_{tot}^{AF}$, $F_{tot}^{AF} = F - z (J + 2t_{ex} I_{AF})$. This effect is stronger than the
decrease of the bandwidth due to $J$ (see Eq. (39)), which increases $T_N$. The assisted
hopping interaction $\Delta t = t(1 - S)$, and kinetic-exchange interaction $t_{ex} = \frac{t}{2}(1 - S)^2$ increase
the Neel temperature by decreasing the bandwidth (Eq. (39)).

![Graph showing the dependence of Neel's temperature on electron concentration](image)

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FIG. 11. Dependence of the Neel’s temperature \( (T_N) \) on electron concentration for \( D = 0.5 \text{ eV}, F = 0.34 \text{ eV} \) and for different values of \( S \) and \( J \) in the case of the weak Coulomb correlation; \( S = 1 \) and \( J = 0 \) – dot-dashed line, \( S = 0.7 \) and \( J = 0.2t \) – solid line, \( S = 1 \) and \( J = 0.2t \) – dashed line, \( S = 0.7 \) and \( J = 0 \) – dotted line.

Figure 12 shows the magnetization versus temperature for electron occupation \( n = 0.95 \) and for various values of the inter-site and kinetic interactions. Again, all the curves are calculated for the same internal exchange field \( F = 0.34 \text{ eV} \). Similarly to the calculations of Neel temperature (in Fig. 11) at constant value of the on-site exchange field, the highest magnetization is obtained for parameter \( S < 1 \), which means that magnetization is enhanced when electron hopping is inhibited in the presence of other electrons.

![Graph showing magnetization versus temperature](image)

**FIG. 12.** Magnetization versus temperature for band filling \( n = 0.96, D = 0.5 \text{ eV}, F = 0.34 \text{ eV} \) and for different values of \( S \) and \( J \); \( S = 1 \) and \( J = 0 \) – dot-dashed line, \( S = 0.7 \) and \( J = 0.2t \) – solid line, \( S = 1 \) and \( J = 0.2t \) – dashed line, \( S = 0.7 \) and \( J = 0 \) – dotted line. This is the case of the weak Coulomb correlation.

**TABLE III.** Neel’s Temperatures and Values of On-site Stoner Field for Antiferromagnetic Elements, \( U = 0 \)

| Element | \( n \) | \( m \) | \( D \) [eV] | \( T_N \) [K] | \( F^{AF}(m) \) [eV] | No. 5 |
|---------|-------|-------|-----------|--------------|----------------|------|
|         |       |       |           |              |                |      |
| No. | $S$ | $J$ | $T_{N}^{exp}[K]$ |
|-----|-----|-----|-----------------|
| 1   | 0.6 | 0.5t| 311 [72]        |
| 2   | 0.6 | 0  | 2110            |
| 3   | 1   | 0.5t| 10820           |
| 4   | 1   | 0  | 540 [56]        |

| Element | $S$ | $J$ | $T_{N}^{exp}[K]$ |
|---------|-----|-----|-----------------|
| Cr      | 1.08| 0.08| 3.5             |
|         | 2.37| 1.47|                 |
| Mn      | 1.24| 0.48| 2.8             |
|         | 2.41| 2.65|                 |

Cr: 1.08 0.08 3.5 520 2.37 1430 1530 2440 311 [72]

Mn: 1.24 0.48 2.8 2110 2.41 5840 7090 10820 540 [56]
Table III shows the Neel’s temperature calculated for the 3d antiferromagnetic elements (Cr and Mn) in the case of the weak correlation. First the on-site exchange interaction, $F$, at a given assumed inter-site interactions $J$ and $S$, was found from Eq. (43) after fitting $F_{tot}^{AF}$ to the experimental magnetic moment at $T = 0$. Next, using the same $F$ the Neel’s temperature was calculated. The results show that the inter-site, $J$, and kinetic, $S$, interactions decreased the Neel’s temperature (column no. 1). The difference between experimental and theoretical Neel’s temperature is even larger than in the case of ferromagnetism (confer Table I). The large difference has to be attributed, as in the case of $F$, to the spin waves or spin fluctuations (see [56,64,72]).

6. CONCLUSION

We will summarize now the results for ferromagnetism and antiferromagnetism obtained in this article. Our analysis of the Hubbard model was focused on the influence of the on-site and inter-site Coulomb correlation and the kinetic interactions on magnetism. We analyzed magnetic susceptibility, the values of critical exchange interaction, the transition temperature and the magnetization.

In analyzing the ferromagnetic ordering we have found three driving forces contributing to this ordering.

(i) spin dependent band shift (Stoner shift) coming from the on-site $F$ and inter-site exchange interactions $J$, $V$ and the kinetic interactions $\Delta t$, $t_{ex}$ (represented by the parameter $S$),

(ii) spin dependent change of the band width and band capacity depending on the electron concentrations due to the on-site Coulomb repulsion described by the on-site correlation factor $K_U$. Increased capacity of the majority spin sub-band drives the magnetism.

(iii) spin dependent change of the band width and band shape depending on the electron concentrations due to the inter-site interactions described by the inter-site correlation factor $K_b$. Narrowing of the majority spin sub-band drives the magnetism.

The first effect is the classic effect known since the approach of Weiss [73] and Slater [74] to magnetism. This is lowering of the potential exchange energy during the transition from the paramagnetic to ferromagnetic state. During this transition there is an increase in the kinetic energy. The balance of the sum of these two energies decides whether the actual transition takes place. This balance leads to the existence of the critical values for different interactions, above which the transition takes place. In its original form it gives us the Stoner condition for ferromagnetism; $F_{cr}^{F} \rho (\varepsilon_F) > 1$. In the new development, described in points two and three above, the increase in the kinetic energy is moderated by the on-site and inter-site correlation effects. These correlations will also change (decrease) different critical interactions coming from the total energy balance. The inter-site and on-site correlations are coming into the critical condition throughout the correlation factors, which appear in the denominator of the susceptibility (Eq. (84)) and as the coefficient of second order term in the free energy expansion over magnetization (Eq. (85)), which is proportional to the inverse of susceptibility. The inter-site and on-site correlations reduce significantly the denominator of the static magnetic susceptibility (Eq. (84)). For this reason the magnetic susceptibility is enhanced for the materials with strong electron correlation (Eq. (109)). The zeros of the
denominator give the critical values of the total interaction, which is greatly reduced with respect to the classic Stoner model.

Analysis of the inter-site correlation has shown the great decrease of the Curie temperature towards the experimental values (see Table I and II). First, the direct calculations within the original Stoner model (see Section 4.2) have pointed out that the Curie temperature, after fitting the Stoner shift to the experimental magnetic moment at zero temperature, is much too high (see Table I). Next, using the modified H-F approximation for the inter-site interactions, which is equivalent to introducing the inter-site correlation in the first order approximation, we arrived at much lower Curie temperatures. Considering the simplicity of the model, and the additional presence of spin waves which are out of the scope of this chapter, the results were close enough to the experimental data (see Table I). Apparently the inter-site interactions are 'softer' and decrease faster with the temperature than the on-site Stoner field used in the original Stoner model (see also [75]). Adding up the on-site strong correlation $U$ to the Stoner model do not improve the values of the theoretical Curie temperature (see Table II). This fact can be understood better after examining Fig. 6 and Fig. 7, where the critical field (initializing magnetization) has dropped down at half-filling but not at the end of the band, where the 3d elements are located.

As already established in the past the electron on-site correlation can help in creating antiferromagnetism (AF) at half-filled band, where the antiferromagnetic 3d elements (Cr, Mn) are located, by dropping the critical field for AF to zero (see Fig. 9) in the case of the weak on-site correlation. The strong $U$, which gives the correct results for the cohesion energy in the middle of the 3d row (see [63,76,77]), shifts the zeros of the critical field for AF to the maxima of the two split sub-bands, which are located at $n = 2/3$, and $n = 4/3$ (see Fig. 10). Unfortunately, this does not agree with the experimental evidence for AF, which is present around $n \approx 1$. The introduction of inter-site interactions in the modified H-F approximation does not shift these minima. It only lowers the critical curves (see Fig. 10). The inter-site interactions $(J,J',V)$ do not reduce the bandwidth at $n = 1$ (which would lower the critical curves at this concentration), in the case of the strong Coulomb correlation, since $I_{AF}(n = 1) = 0$ (see Eqs (20) and (21)).

There is one exception to this rule. We can obtain AF at half-filling at large $U$ if the bandwidth at $n = 1$ goes to zero. This can be achieved in the linear approximation, which was described in §5.1. The bandwidth was reduced to zero by assuming that the hopping integral in the presence of another electron is forbidden at concentration $n = 1$; $t_1 = 0$, and additionally that $t_{ex} \equiv 0$ (see Eq. (125)).

In conclusion the antiferromagnetism at half-filling in the high correlation case can appear when the bandwidth goes to zero at this concentration. It can go to zero either as: $1 - n \frac{\Delta U}{t_0}$, due to the presence of the assisted hopping interaction or due to some other interaction, whose strength is proportional to $n$.

This situation can describe the high temperature superconducting cuprate YBa$_2$Cu$_3$O$_6$, where at the half-filling and the strong Coulomb correlation there is, initially, the antiferromagnetic order. The superconductivity will appear upon doping only away from the half-filling at the electron concentration $n \approx 0.95 - 0.8$ (see e.g. [78]).

The temperature dependence of AF was analyzed numerically in Section 5.2. Again, as in the case of ferromagnetism the direct calculations within the original Stoner model have pointed out that the Neel’s temperature, after fitting the Stoner shift to the experimental
magnetic moment at zero temperature, is much too high (see Table III). Next, using the modified H-F approximation for the inter-site interaction, we arrived at much lower Curie temperatures. They are not as close to the experimental data as in the case of ferromagnetism. The reason for this could be the existence of non-linear modes of excitations in Chromium and Magnesium (see e.g. [72]). Nevertheless, as already mentioned above, the model is very simple, the details of the realistic DOS as well as the magnetization decrease through the spin waves excitation or moment fluctuations could be included, which would bring the theoretical results to complete agreement with the experimental data.
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