

Hubbard model with intersite kinetic correlations

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We presented the intersite electron-electron correlation into the Hubbard III approximation. This correlation was excluded in the Hubbard III approximation and also in the equivalent coherent-potential approximation. Including it brings two spin-dependent effects: the bandwidth correction and the band shift correction, which both stimulate the ferromagnetic ground state. The band shift correction factor causes an exchange splitting between the spin-up and spin-down spectra, and its role is similar to the exchange interaction in the classic Stoner model. The spin-dependent bandwidth correction lowers the kinetic energy of electrons by decreasing the majority-spin bandwidth for some electron occupations with respect to the minority-spin bandwidth. In certain conditions it can lead to ferromagnetic alignment. A gain in the kinetic energy achieved in this way is the opposite extreme to the effect of a gain in potential energy due to exchange splitting. The band shift factor is a dominant force behind the ferromagnetism, but the presence of both factors working together is necessary to create spontaneous magnetization.

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I. INTRODUCTION

The Hubbard model¹⁻³ is extensively used to analyze strong electron correlations in the narrow energy bands. Applications of this model to itinerant magnetism, metal-insulator phase transitions, or high- T_C superconductivity are of special interest.

This model describes the dynamics of electrons in crystals. In its simple original version, it uses such quantities as the electron dispersion energy ε_k and the on-site Coulomb interaction $U = \langle i, i | 1/r | i, i \rangle$, where i is the lattice site index. The electron dispersion energy is the Fourier transform of the intersite hopping integral t_{ij} . In the systems with strong correlation, the on-site Coulomb interaction U causes a split of the spin band into two subbands: lower subband centered around the atomic level T_0 and the upper subband centered around the level $T_0 + U$.

Despite its simplicity there is no exact solution to the Hubbard Hamiltonian with the exception of the one-dimensional system;^{4,5} therefore for many years a variety of different approximations has been used for this model. The important one was the Hubbard I approximation,¹ which is rigorous in the atomic ($t_{ij}=0$) limit and in the band ($U=0$) limit. Unfortunately this approximation produces a band split into two subbands separated by an energy gap, even for arbitrarily small Coulomb repulsion. The additional odd feature of this approximation is an infinite lifetime of the pseudoparticles caused by the real value of the self-energy. These two negative features are the result of the assumption that the dominant correlation takes place only between two electrons on the same lattice site. In the Green's function language, it is implemented by assuming that the Green's function involving more than two atomic sites can be approximated by the single-site average multiplied by the two sites Green's function. Thus in Eq. (9) below the higher-order Green's function, $\langle\langle \hat{n}_{i-\sigma} c_{i\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon$ is approximated by $\langle \hat{n}_{i-\sigma} \rangle \langle \langle c_{i\sigma}; c_{j\sigma}^+ \rangle \rangle_\varepsilon$.

Further attempts to improve the solution or simply to obtain a ferromagnetic ground state included the mean-field

approximation, the so-called Hubbard III approximation³ or equivalent coherent-potential approximation (CPA),^{6,7} the slave-boson method,^{8,9} and, e.g., the dynamical mean-field theory.¹⁰ The Hubbard model was also analyzed directly by the numerical quantum Monte Carlo simulation.¹¹⁻¹³ None of these attempts brought the desired solution. Such a solution would have a ferromagnetic ground state obtained under credible approximations.

To describe realistic systems where there exist physical phenomena, such as magnetism or high-temperature superconductivity, the intersite Coulomb interactions were added to the simple Hubbard model.¹⁴⁻²⁴ In the language of purely itinerant model these are: the charge-charge interaction $V = \langle i, j | 1/r | i, j \rangle$, intersite exchange interaction $J = \langle i, j | 1/r | j, i \rangle$, the pair-hopping interaction J' , the hopping interaction $\Delta t = \langle i, i | 1/r | j, i \rangle = t - t_1$, and the exchange hopping interaction $t_{ex} = (t + t_2)/2 - t_1$. Above t , t_1 , and t_2 are the hopping constants for electron between two empty sites, two sites with one site occupied by the electron with opposite spin, and two sites which are both occupied by the opposite spin electron. There are also "hybrid" models (see Ref. 24), where the nearest-neighbor exchange interaction in the Heisenberg form $J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$ was added to the Hubbard model. For high-temperature superconducting compounds, for which there is more than one band involved in a given physical property, two-band^{19,25-28} and three-band^{23,29-35} versions of the Hubbard model were used. Some authors (see Ref. 23 and 35) have reduced the multiband, e.g., three-band model to the effective single-band model. In the models describing the copper-oxygen CuO_2 plane, the hopping integrals between different orbitals were also introduced, e.g., copper-oxygen hopping integral in the CuO_2 plane. There were also numerous studies of the one-dimensional Hubbard ring for which there is an exact solution with added interactions. In Ref. 21 the authors introduced interactions Δt , V , and J' , in Ref. 20 the authors introduced the interactions Δt and V , and in Refs. 5 and 22 they assumed $t_1=0$ and $t_2=|t|$. These studies have shown the possibility of different ordered phases.

All these additional interactions or different hopping integrals will not be considered in this paper, but we will focus

on the simple basic Hubbard model with interaction U and hopping integral t_{ij} given below by Eq. (1).

As mentioned above, Hubbard³ introduced the approximation called the Hubbard III approximation. This approximation did not produce the ferromagnetic ground state (see Refs. 36 and 37). The best way to prove it is to translate the Hubbard III result to the CPA approximation⁷ and to analyze the solution in this language.³⁶

In this paper we will describe in great detail the Hubbard III approximation with the included intersite kinetic correlation functions $\langle c_{i-\sigma}^+ c_{j-\sigma} \rangle$ and $\langle \hat{n}_{i\sigma} c_{i-\sigma}^+ c_{j-\sigma} \rangle$. These correlations were originally ignored in the Hubbard approach and in most of the subsequent papers devoted to this model. They were considered by Roth³⁸ and Nolting and co-workers^{39–43} within the framework of the two-pole approximation, which eventually led to the spectral density approach (SDA) (Refs. 39–41) and the modified alloy analogy (MAA).^{42,43} The basis of the SDA method is the Roth's two-pole approximation,³⁸ which gives the two-pole ansatz for the single-particle spectral density function. The SDA approximation brings the magnetic results in the strong-coupling limit, but it neglects the quasiparticle damping. It is the extension of the Hubbard I approximation. Such an approach perhaps can be justified for the systems with strong correlation. To correct the SDA approximation, Nolting and co-workers proposed the MAA method,^{42,43} which is a combination of the SDA and CPA methods. In the CPA method, there are two spin-independent atomic levels T_0 and $T_0 + U$, which in the MAA method are replaced by two atomic levels dependent on occupation and spin. We will analyze results of the MAA method and show that they can be obtained as a simplified version of our approach in which the intersite correlations are included directly into the Hubbard III or CPA scheme.

The paper is organized as follows. In Sec. II the general Green's function chain equations for the Hubbard model are recalled. In Sec. III the solution of this chain within the framework of the Hubbard III approximation with included intersite correlation is given. In Sec. IV the bandwidth and band shift corrections are calculated using the Hartree-Fock (H-F) approximation and the more rigorous high approximation. Based on these results the magnetic analysis of the system ground state is performed in Sec. V, showing the possibility of ferromagnetic transition at some electron occupations and highly asymmetrical density of states (DOS) under the on-site interaction U alone. Discussion and comparison with the results of SDA and MAA methods for the strongly correlated systems are presented in Sec. VI.

II. GREEN'S FUNCTION CHAIN EQUATIONS FOR THE HUBBARD MODEL

The subject of this paper is the simple Hubbard Hamiltonian in the real-space representation, which has the following form:³

$$H = - \sum_{ij\sigma} t_{ij} c_{i\sigma}^+ c_{j\sigma} + \frac{U}{2} \sum_{i\sigma} \hat{n}_{i\sigma} \hat{n}_{i-\sigma} - \sum_{i\sigma} \mu_{i\sigma} \hat{n}_{i\sigma}, \quad (1)$$

where t_{ij} is the hopping integral between i th and j th lattice sites. The operator $c_{i\sigma}^+$ ($c_{i\sigma}$) is creating (annihilating) an elec-

tron with spin $\sigma = \uparrow, \downarrow$ on the i th lattice site, $\hat{n}_{i\sigma} = c_{i\sigma}^+ c_{i\sigma}$ is the electron number operator for electrons with spin σ on the i th lattice site, and

$$\mu_{i\sigma} = \mu + F_{in} n_{i\sigma}, \quad (2)$$

with F_{in} being the on-site atomic Stoner field (exchange field) in the H-F approximation and μ is the chemical potential. In the many-body considerations below, the term with chemical potential will be absent, since it will be moved into the Fermi-Dirac statistics [see Eq. (38)].

The equation of motion for the Green's function has the following form:^{1,44}

$$\varepsilon \langle \langle A; B \rangle \rangle_{\varepsilon} = \langle [A, B]_{+} \rangle + \langle \langle [A, H]_{-}; B \rangle \rangle_{\varepsilon}, \quad (3)$$

where A and B are the single operators or their products.

Using in relation (3) the Hamiltonian (1), we obtain the following equation of motion for the Green's function $\langle \langle c_{i\sigma}; c_{j\sigma}^+ \rangle \rangle_{\varepsilon}$:

$$\varepsilon \langle \langle c_{i\sigma}; c_{j\sigma}^+ \rangle \rangle_{\varepsilon} = \delta_{ij} - \sum_l t_{il} \langle \langle c_{l\sigma}; c_{j\sigma}^+ \rangle \rangle_{\varepsilon} + U \langle \langle \hat{n}_{i-\sigma} c_{i\sigma}; c_{j\sigma}^+ \rangle \rangle_{\varepsilon}. \quad (4)$$

For the higher-order Green's function $\langle \langle \hat{n}_{i-\sigma} c_{i\sigma}; c_{j\sigma}^+ \rangle \rangle_{\varepsilon}$ appearing above on the right-hand side, the Hubbard III approximation will be used together with the Hubbard notation for the electron number operators³

$$\hat{n}_{i\sigma}^+ \equiv \hat{n}_{i\sigma}, \quad \hat{n}_{i\sigma}^- \equiv 1 - \hat{n}_{i\sigma}, \quad \sum_{\alpha=\pm} \hat{n}_{i\sigma}^{\alpha} = 1, \quad (5)$$

and for the two resonant energies

$$\varepsilon_{+} = T_0 + U, \quad \varepsilon_{-} = T_0, \quad (6)$$

where T_0 is the gravity center of the Bloch band given by

$$T_0 = \frac{1}{N} \sum_k \varepsilon_k = t_{ii}. \quad (7)$$

The same notation as in Eq. (5) will be introduced for the average electron occupations

$$n_{\sigma}^{+} = \langle \hat{n}_{i\sigma}^{+} \rangle \equiv n_{\sigma}, \quad n_{\sigma}^{-} = \langle \hat{n}_{i\sigma}^{-} \rangle \equiv 1 - n_{\sigma}. \quad (8)$$

Applying Eq. (3) to the higher-order Green's function $\langle \langle \hat{n}_{i-\sigma}^{\alpha} c_{i\sigma}; c_{j\sigma}^+ \rangle \rangle_{\varepsilon}$ ($\alpha = \pm$), with notation of Eqs. (5), (6), and (8), we obtain the equation³

$$\begin{aligned} & \varepsilon \langle \langle \hat{n}_{i-\sigma}^{\alpha} c_{i\sigma}; c_{j\sigma}^+ \rangle \rangle_{\varepsilon} \\ &= n_{-\sigma}^{\alpha} \left(\delta_{ij} - \sum_l t_{il} \langle \langle c_{l\sigma}; c_{j\sigma}^+ \rangle \rangle_{\varepsilon} \right) + \varepsilon_{\alpha} \langle \langle \hat{n}_{i-\sigma}^{\alpha} c_{i\sigma}; c_{j\sigma}^+ \rangle \rangle_{\varepsilon} \\ & - \sum_l t_{il} \langle \langle (\hat{n}_{i-\sigma}^{\alpha} - n_{-\sigma}^{\alpha}) c_{i\sigma}; c_{j\sigma}^+ \rangle \rangle_{\varepsilon} \\ & - \xi_{\alpha} \sum_l t_{il} \langle \langle c_{i-\sigma}^+ c_{l-\sigma} c_{i\sigma}; c_{j\sigma}^+ \rangle \rangle_{\varepsilon} - \langle \langle c_{l-\sigma}^+ c_{i-\sigma} c_{i\sigma}; c_{j\sigma}^+ \rangle \rangle_{\varepsilon}, \end{aligned} \quad (9)$$

where $\xi_{\pm} = \pm 1$.

Taking into account only the first two terms on the right-hand side of Eq. (9) gives the Hubbard I approximation.¹

Including the third term in Eq. (9), which comes from the commutator $[c_{i\sigma}, H]_-$ in the equation of motion, leads to what is known as the “scattering effect.” The last term, which comes from the commutator $[\hat{n}_{i-\sigma}, H]_-$ in the equation of motion, gives the “resonance broadening effect.”

The self-consistent solution of this equation taking into account both the “scattering effect” and the “resonance

broadening effect” was given by Hubbard³ as the following set of equations:

$$G_k^\sigma(\varepsilon) = \frac{1}{F_H^\sigma(\varepsilon) - (\varepsilon_k - T_0)}, \quad (10)$$

$$\frac{1}{F_H^\sigma(\varepsilon)} = \frac{\varepsilon - (n_{-\sigma}^+ \varepsilon_- + n_{-\sigma}^- \varepsilon_+) - \Omega_\sigma^T(\varepsilon)}{[\varepsilon - \varepsilon_- - n_{-\sigma}^+ \Omega_\sigma^T(\varepsilon)][\varepsilon - \varepsilon_+ - n_{-\sigma}^- \Omega_\sigma^T(\varepsilon)] - n_{-\sigma}^- n_{-\sigma}^+ [\Omega_\sigma^T(\varepsilon)]^2}, \quad (11)$$

$$\Omega_\sigma^T(\varepsilon) = F_H^\sigma(\varepsilon) - \frac{1}{G_{ii}^\sigma(\varepsilon)}, \quad (12)$$

$$G_{ii}^\sigma(\varepsilon) = \frac{1}{N} \sum_k G_k^\sigma(\varepsilon), \quad (13)$$

where ε_k is the electron dispersion energy.

As is now well known, the standard Hubbard III approximation is equivalent to the CPA approximation under the following change in variables between the Hubbard solution and the CPA approximation:⁷

$$F_H^\sigma(\varepsilon) \rightarrow \varepsilon - \Sigma^\sigma(\varepsilon),$$

$$G_{ii}^\sigma(\varepsilon) \rightarrow F^\sigma(\varepsilon) = \frac{1}{N} \sum_k G_k^\sigma(\varepsilon),$$

$$\Omega_\sigma^T(\varepsilon) \rightarrow \varepsilon - \Sigma^\sigma(\varepsilon) - \frac{1}{F^\sigma(\varepsilon)}, \quad (14)$$

where $F^\sigma(\varepsilon)$ is called the Slater-Koster function.

Under this change in variables, it is straightforward to demonstrate that the Hubbard's relations (10) and (11) above are identical to the CPA relations,

$$G_k^\sigma(\varepsilon) = \frac{1}{\varepsilon - (\varepsilon_k - T_0) - \Sigma^\sigma(\varepsilon)}, \quad (15)$$

and

$$\Sigma^\sigma(\varepsilon) = \varepsilon_+ n_{-\sigma}^+ + \varepsilon_- n_{-\sigma}^- + \frac{(\varepsilon_+ - \varepsilon_-)^2 n_{-\sigma}^+ n_{-\sigma}^- F^\sigma(\varepsilon)}{1 + [\Sigma^\sigma(\varepsilon) - (\varepsilon_+ n_{-\sigma}^- + \varepsilon_- n_{-\sigma}^+)] F^\sigma(\varepsilon)}. \quad (16)$$

It has been shown (see Refs. 36 and 37) that the CPA approximation [Eq. (16)] does not bring about the ferromagnetic ground state. Therefore, the above identification of CPA with Hubbard III approximation proves that the Hubbard III approximation is also not ferromagnetic.

III. HUBBARD III APPROXIMATION WITH INTERSITE KINETIC CORRELATION

In further considerations of the scattering effect and the resonance broadening effect, the new averages of the kinetic-type $\langle c_{i-\sigma}^+ c_{l-\sigma} \rangle$ and $\langle \hat{n}_{i\sigma} c_{i-\sigma}^+ c_{l-\sigma} \rangle$ will be kept. This will result in corrections to the Hubbard scattering and resonance broadening effects, which are the function of these averages.

A. Scattering effect

To consider this effect, we ignore the last term in Eq. (9) and search for the solution of function $\langle \langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) c_{l\sigma}; c_{j\sigma}^+ \rangle \rangle_\varepsilon$. The basic difference between our approach and the Hubbard III solution is that we assume the nonzero value for the intersite average $\langle \langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) \hat{n}_{l-\sigma}^\beta \rangle \rangle$. The detailed calculations are performed in Appendix A. The result is the following set of equations:

$$\begin{aligned} & (\varepsilon - \varepsilon_\alpha) \langle \langle (\hat{n}_{i-\sigma}^\alpha c_{i\sigma}; c_{j\sigma}^+) \rangle \rangle_\varepsilon + \xi_\alpha \Omega_\sigma(\varepsilon) (n_{-\sigma}^+ \langle \langle \hat{n}_{i-\sigma}^- c_{i\sigma}; c_{j\sigma}^+ \rangle \rangle_\varepsilon \\ & - n_{-\sigma}^- \langle \langle \hat{n}_{i-\sigma}^+ c_{i\sigma}; c_{j\sigma}^+ \rangle \rangle_\varepsilon) \\ & = n_{-\sigma}^\alpha \left(\delta_{ij} - \sum_l t_{il} \langle \langle c_{l\sigma}; c_{j\sigma}^+ \rangle \rangle_\varepsilon \right) \\ & + \xi_\alpha \sum_l B_{il,\sigma}^S(\varepsilon) \langle \langle c_{l\sigma}; c_{j\sigma}^+ \rangle \rangle_\varepsilon, \end{aligned} \quad (17)$$

where

$$\Omega_\sigma(\varepsilon) = \sum_{l,m} t_{il} W_{lm,i}^\sigma(\varepsilon) t_{mi}, \quad (18)$$

$$B_{il,\sigma}^S(\varepsilon) = C_-(\varepsilon) F_{H,0}^\sigma(\varepsilon) (-t_{il}) \langle \langle \hat{n}_{i-\sigma} \hat{n}_{l-\sigma} - n_{-\sigma}^2 \rangle \rangle. \quad (19)$$

All definitions are given in Appendix A and are the same as in Hubbard.³

B. Resonance broadening effect

The resonance broadening effect is described by the Green's functions $\langle \langle c_{i-\sigma}^\pm c_{i-\sigma}^\mp c_{i\sigma}; c_{j\sigma}^+ \rangle \rangle_\varepsilon$ appearing in the last term of Eq. (9). We assume the nonzero value for the intersite averages $\langle \langle \hat{n}_{l\sigma}^\alpha c_{l-\sigma}^\pm c_{i-\sigma}^\mp \rangle \rangle$ and $\langle \langle c_{l\sigma}^\alpha c_{i\sigma} c_{l-\sigma}^\pm c_{i-\sigma}^\mp \rangle \rangle$. The detailed calculations for the Green's functions $\langle \langle \hat{n}_{i-\sigma}^\alpha c_{i\sigma}; c_{j\sigma}^+ \rangle \rangle_\varepsilon$ and

$\langle\langle \hat{n}_{i-\sigma}^- c_{i\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon$ are performed in Appendix B. The result is the following set of the matrix equation:

$$\begin{aligned} & \begin{bmatrix} \varepsilon - \varepsilon_- - n_{-\sigma}^+ \Omega_{-\sigma}^B(\varepsilon) & n_{-\sigma}^- \Omega_{-\sigma}^B(\varepsilon) \\ n_{-\sigma}^+ \Omega_{-\sigma}^B(\varepsilon) & \varepsilon - \varepsilon_+ - n_{-\sigma}^- \Omega_{-\sigma}^B(\varepsilon) \end{bmatrix} \\ & \times \begin{bmatrix} \langle\langle \hat{n}_{i-\sigma}^- c_{i\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \\ \langle\langle \hat{n}_{i-\sigma}^+ c_{i\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \end{bmatrix} \\ & = \begin{bmatrix} n_{-\sigma}^- \\ n_{-\sigma}^+ \end{bmatrix} \left[\delta_{ij} - \sum_l t_{il} \langle\langle c_{l\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \right] \\ & + \begin{bmatrix} -1 \\ +1 \end{bmatrix} \left\{ \sum_l B_{il,\sigma}^B(\varepsilon) \langle\langle c_{l\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \right. \\ & \left. + S_{\sigma}^B(\varepsilon) \langle\langle c_{i\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \right\}, \end{aligned} \quad (20)$$

where

$$\begin{aligned} \Omega_{-\sigma}^B(\varepsilon) &= \sum_{lm} t_{il} t_{ml} [W_{lm,i}^\sigma(\varepsilon) - W_{lm,i}^\sigma(\varepsilon_- + \varepsilon_+ - \varepsilon)] \\ &= \Omega_{-\sigma}(\varepsilon) - \Omega_{-\sigma}(\varepsilon_- + \varepsilon_+ - \varepsilon), \end{aligned} \quad (21)$$

$$B_{il,\sigma}^B(\varepsilon) = -t_{il} F_{H,0}^\sigma(\varepsilon) C_-(\varepsilon) \langle c_{l\sigma}^+ c_{i\sigma} (c_{l-\sigma} c_{i-\sigma}^+ - c_{l-\sigma}^+ c_{i-\sigma}) \rangle, \quad (22)$$

$$S_{\sigma}^B(\varepsilon) = F_{H,0}^\sigma(\varepsilon) C_-(\varepsilon) \frac{1}{N} \sum_{li} (-t_{il}) (2 \langle \hat{n}_{l\sigma} c_{l-\sigma}^+ c_{i-\sigma} \rangle - \langle c_{l-\sigma}^+ c_{i-\sigma} \rangle). \quad (23)$$

C. Scattering and resonance broadening effects together

Finally, new forms of the scattering effect [Eq. (17)] and the resonance broadening effect [Eq. (20)] will be now combined into one equation, which can be written in the matrix form

$$\begin{aligned} & \begin{bmatrix} \varepsilon - \varepsilon_- - n_{-\sigma}^+ \Omega_{-\sigma}^T(\varepsilon) + S_{\sigma}^B(\varepsilon) & n_{-\sigma}^- \Omega_{-\sigma}^T(\varepsilon) + S_{\sigma}^B(\varepsilon) \\ n_{-\sigma}^+ \Omega_{-\sigma}^T(\varepsilon) - S_{\sigma}^B(\varepsilon) & \varepsilon - \varepsilon_+ - n_{-\sigma}^- \Omega_{-\sigma}^T(\varepsilon) - S_{\sigma}^B(\varepsilon) \end{bmatrix} \\ & \times \begin{bmatrix} \langle\langle \hat{n}_{i-\sigma}^- c_{i\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \\ \langle\langle \hat{n}_{i-\sigma}^+ c_{i\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \end{bmatrix} \\ & = \begin{bmatrix} n_{-\sigma}^- \\ n_{-\sigma}^+ \end{bmatrix} \left[\delta_{ij} - \sum_l t_{il} \langle\langle c_{l\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \right] \\ & + \begin{bmatrix} -1 \\ +1 \end{bmatrix} \sum_l \{ B_{il,\sigma}^S(\varepsilon) + B_{il,\sigma}^B(\varepsilon) \} \langle\langle c_{l\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon, \end{aligned} \quad (24)$$

where

$$\Omega_{-\sigma}^T(\varepsilon) = \Omega_{\sigma}(\varepsilon) + \Omega_{-\sigma}(\varepsilon) - \Omega_{-\sigma}(\varepsilon_- + \varepsilon_+ - \varepsilon). \quad (25)$$

Solving Eq. (24), we find the functions $\langle\langle \hat{n}_{i-\sigma}^- c_{i\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon$ and $\langle\langle \hat{n}_{i-\sigma}^+ c_{i\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon$, and after using the identity

$$\sum_{\alpha=\pm} \langle\langle \hat{n}_{i-\sigma}^\alpha c_{i\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon = \langle\langle c_{i\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon = G_{ij}^\sigma(\varepsilon), \quad (26)$$

we have

$$F_H^\sigma(\varepsilon) G_{ij}^\sigma(\varepsilon) = \delta_{ij} - \sum_l t_{il} G_{lj}^\sigma(\varepsilon) + \sum_l B_{il,\sigma}^T(\varepsilon) G_{lj}^\sigma(\varepsilon), \quad (27)$$

where

$$B_{il,\sigma}^T(\varepsilon) = \{ F_H^\sigma(\varepsilon) C_- [\varepsilon - \Omega_{\sigma}^T(\varepsilon)] \}^2 (-t_{il}) [\langle \hat{n}_{i-\sigma} \hat{n}_{l-\sigma} \rangle - n_{-\sigma}^2 + \langle c_{l\sigma}^+ c_{i\sigma} (c_{l-\sigma} c_{i-\sigma}^+ - c_{l-\sigma}^+ c_{i-\sigma}) \rangle], \quad (28)$$

$$S_{\sigma}^B(\varepsilon) = F_H^\sigma(\varepsilon) C_- [\varepsilon - \Omega_{\sigma}^T(\varepsilon)] \frac{1}{N} \sum_{li} (-t_{il}) (2 \langle \hat{n}_{l\sigma} c_{l-\sigma}^+ c_{i-\sigma} \rangle - \langle c_{l-\sigma}^+ c_{i-\sigma} \rangle), \quad (29)$$

$$\frac{1}{F_H^\sigma(\varepsilon)} = \frac{\varepsilon - (n_{-\sigma}^+ \varepsilon_- + n_{-\sigma}^- \varepsilon_+) - \Omega_{\sigma}^T(\varepsilon)}{[\varepsilon - \varepsilon_- - n_{-\sigma}^+ \Omega_{\sigma}^T(\varepsilon)] [\varepsilon - \varepsilon_+ - n_{-\sigma}^- \Omega_{\sigma}^T(\varepsilon)] - n_{-\sigma}^+ n_{-\sigma}^- [\Omega_{\sigma}^T(\varepsilon)]^2 - (\varepsilon_+ - \varepsilon_-) S_{\sigma}^B(\varepsilon)}. \quad (30)$$

In obtaining Eqs. (28) and (29), we have replaced factor $F_{H,0}^\sigma(\varepsilon) C_-(\varepsilon)$ by $F_H^\sigma(\varepsilon) C_- [\varepsilon - \Omega_{\sigma}^T(\varepsilon)]$ in Eqs. (19), (22), and (23). This was done to achieve self-consistency.

Equation (27) is solved by applying Fourier transformation to the momentum space and by using the relation

$$\sum_l B_{il,\sigma}^T(\varepsilon) G_{lj}^\sigma(\varepsilon) = \sum_k B_{k,\sigma}^T(\varepsilon) G_k^\sigma(\varepsilon) \exp[i\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)], \quad (31)$$

where

$$\begin{aligned} B_{k,\sigma}^T(\varepsilon) &= \{ F_H^\sigma(\varepsilon) C_- [\varepsilon - \Omega_{\sigma}^T(\varepsilon)] \}^2 \frac{1}{N} \sum_{il} (-t_{il}) (\langle \hat{n}_{l-\sigma} \hat{n}_{i-\sigma} \rangle - n_{-\sigma}^2 \\ & - \langle c_{l\sigma}^+ c_{i-\sigma} c_{l-\sigma} c_{i\sigma} \rangle - \langle c_{l\sigma}^+ c_{l-\sigma} c_{i-\sigma} c_{i\sigma} \rangle) \\ & \times \exp[i\mathbf{k} \cdot (\mathbf{r}_l - \mathbf{r}_i)]. \end{aligned} \quad (32)$$

As a result, we obtain from Eq. (27) the following form:

$$G_k^\sigma(\varepsilon) = \frac{1}{F_H^\sigma(\varepsilon) - (\varepsilon_k - T_0) - B_{k,\sigma}^T(\varepsilon)}. \quad (33)$$

This Green's function is the final solution of Eq. (9), which contains the scattering and resonance broadening effects with included intersite correlations. The band shift correction factor $S_{\sigma}^B(\varepsilon)$ causes exchange splitting between the spin-up and spin-down spectra, and the bandwidth correction factor $B_{k,\sigma}^T(\varepsilon)$ leads to a change in the width of the spin subbands with respect to each other. Assuming that $B_{k,\sigma}^T(\varepsilon)=0$ and $S_{\sigma}^B(\varepsilon)=0$ in Eqs. (33) and (30), we obtain the classic Hubbard III approximation.

Transforming Eqs. (33) and (30) to the CPA notation by the help of Eq. (14), we can write for the Green's function and self-energy the following relations:

$$G_k^{\sigma}(\varepsilon) = \frac{1}{\varepsilon - \Sigma^{\sigma}(\varepsilon) - (\varepsilon_k - T_0)b^{\sigma}(\varepsilon)}, \quad b^{\sigma}(\varepsilon) = 1 + \frac{B_{k,\sigma}^T(\varepsilon)}{\varepsilon_k - T_0}, \quad (34)$$

where

$$\Sigma^{\sigma}(\varepsilon) = \varepsilon_+ n_{-\sigma}^+ + \varepsilon_- n_{-\sigma}^- + \frac{(\varepsilon_+ - \varepsilon_-)[(\varepsilon_+ - \varepsilon_-)n_{-\sigma}^+ n_{-\sigma}^- - S_{\sigma}^B(\varepsilon)]F^{\sigma}(\varepsilon)}{1 + [\Sigma^{\sigma}(\varepsilon) - (\varepsilon_+ n_{-\sigma}^- + \varepsilon_- n_{-\sigma}^+)]F^{\sigma}(\varepsilon)}. \quad (35)$$

The Slater-Koster function $F^{\sigma}(\varepsilon)$ is now given by

$$F^{\sigma}(\varepsilon) = \frac{1}{N} \sum_k \frac{1}{\varepsilon - \Sigma^{\sigma}(\varepsilon) - (\varepsilon_k - T_0)b^{\sigma}(\varepsilon)}, \quad (36)$$

and the DOS for electrons with spin σ can be expressed as

$$\rho^{\sigma}(\varepsilon) = -\frac{1}{\pi} \text{Im} F^{\sigma}(\varepsilon). \quad (37)$$

The average electron occupation number with spin σ is calculated from the relation

$$n_{\sigma} = \int_{-\infty}^{\infty} \rho^{\sigma}(\varepsilon) \frac{d\varepsilon}{e^{(\varepsilon - \mu_{\sigma})/k_B T} + 1}. \quad (38)$$

The above Eqs. (29), (32), and (34)–(38) form the base for the magnetic analysis of the system ground state.

IV. CALCULATING THE BANDWIDTH AND BAND SHIFT CORRECTION

The bandwidth and band shift corrections are described by parameters $B_{k,\sigma}^T(\varepsilon)$ and $S_{\sigma}^B(\varepsilon)$ given by Eqs. (32) and (29), respectively, and they modify the Hubbard III solution.

The intersite correlation functions appearing inside parameters $B_{k,\sigma}^T(\varepsilon)$ and $S_{\sigma}^B(\varepsilon)$ will be calculated either by applying the Hartree-Fock approximation or by the approximation developed by Roth³⁸ and Nolting and co-workers.⁴⁰

A. Hartree-Fock solution for $B_{k,\sigma}^T(\varepsilon)$ and $S_{\sigma}^B(\varepsilon)$

In Eqs. (32) and (29) for $B_{k,\sigma}^T(\varepsilon)$ and $S_{\sigma}^B(\varepsilon)$, we assume the following approximations for $l \neq i$:

$$\langle \hat{n}_{l-\sigma} \hat{n}_{i-\sigma} \rangle - n_{-\sigma}^2 \approx \langle c_{l-\sigma}^+ c_{l-\sigma} \rangle \langle c_{i-\sigma}^+ c_{i-\sigma} \rangle - \langle c_{l-\sigma}^+ c_{i-\sigma} \rangle \langle c_{i-\sigma}^+ c_{l-\sigma} \rangle - n_{-\sigma}^2 = -I_{-\sigma}^2,$$

$$\langle c_{l\sigma}^+ c_{i-\sigma}^+ c_{l-\sigma} c_{i\sigma} \rangle \approx \langle c_{l\sigma}^+ c_{i\sigma} \rangle \langle c_{i-\sigma}^+ c_{l-\sigma} \rangle = I_{\sigma} I_{-\sigma},$$

$$\langle c_{l\sigma}^+ c_{l-\sigma}^+ c_{i-\sigma} c_{i\sigma} \rangle \approx \langle c_{l\sigma}^+ c_{i\sigma} \rangle \langle c_{i-\sigma}^+ c_{l-\sigma} \rangle = I_{\sigma} I_{-\sigma},$$

$$\langle \hat{n}_{l\sigma} c_{l-\sigma}^+ c_{i-\sigma} \rangle \approx \langle \hat{n}_{l\sigma} \rangle \langle c_{l-\sigma}^+ c_{i-\sigma} \rangle = n_{\sigma} I_{-\sigma}, \quad (39)$$

where $I_{\sigma} = \langle c_{l\sigma}^+ c_{i\sigma} \rangle$ is the Fock parameter.

Above we modified the standard Hartree-Fock approximation by adding the intersite operator averages to the single-site operator averages. All these approximations reduce to zero when $I_{\sigma}=0$. The first expression in Eq. (39) was put explicitly to zero in the Hubbard paper.³

The parameter I_{σ} is proportional to the average kinetic energy of electrons with spin σ , $\langle K^{\sigma} \rangle = -DI_{\sigma}$, and is given by the relation,⁴⁵

$$I_{\sigma} = \langle c_{l\sigma}^+ c_{i\sigma} \rangle = \int_{-D}^D \rho^{\sigma}(\varepsilon) \left(-\frac{\varepsilon}{D} \right) \frac{d\varepsilon}{1 + e^{(\varepsilon - \mu)/k_B T}} d\varepsilon, \quad (40)$$

from which it can be directly calculated. It can also be approximated by its stochastic value, as the probability of electron hopping from the j th to i th lattice site. In the strong correlation case $U \gg D$, the stochastic interpretation brings the following result for the lower Hubbard subband.⁴⁶

$$I_{\sigma} = \frac{n_{\sigma}(1 - n_{-\sigma})}{(1 - n_{-\sigma})}. \quad (41)$$

Using this relation and assuming $\varepsilon \approx 0$ for the lower Hubbard's subband in Eqs. (30) and (A8) we can simplify the product $F_H^{\sigma}(\varepsilon) C_{-}[\varepsilon - \Omega_{\sigma}^T(\varepsilon)]$ (in the case of $U \gg D$), and we obtain

$$F_H^{\sigma}(\varepsilon) C_{-}[\varepsilon - \Omega_{\sigma}^T(\varepsilon)] \approx -\frac{1}{1 - n_{-\sigma}}. \quad (42)$$

Inserting this relation into Eqs. (32) and (29), we arrive at

$$B_{k,\sigma}^T(\varepsilon) \equiv B_{k,\sigma}^T \approx -\frac{1}{(1 - n_{-\sigma})^2} (I_{-\sigma}^2 + 2I_{\sigma} I_{-\sigma}) \varepsilon_k, \quad (43)$$

and

$$S_{\sigma}^B(\varepsilon) \equiv S_{\sigma}^B \approx -\frac{D}{(1 - n_{-\sigma})} I_{-\sigma} (1 - 2n_{\sigma}). \quad (44)$$

In the Hartree-Fock approximation, the bandwidth factor $B_{k,\sigma}^T$ and the band shift factor S_{σ}^B are real and independent on the energy ε . The bandwidth factor b^{σ} related to $B_{k,\sigma}^T$ by Eq. (34) is also real and independent on energy

$$b^{\sigma} = 1 - \frac{1}{(1 - n_{-\sigma})^2} (I_{-\sigma}^2 + 2I_{\sigma} I_{-\sigma}). \quad (45)$$

Equations (41), (44), and (45) together with the CPA relations (34)–(38) build a closed system of equations, which has to be solved self-consistently.

In Fig. 1 we show the bandwidth factor [Eq. (45)] and the band shift factor [Eq. (44)] in function of electron concentration in the paramagnetic state.

The bandwidth factor dependence on electron concentration [Fig. 1(a)] shows the contraction of the band and in-

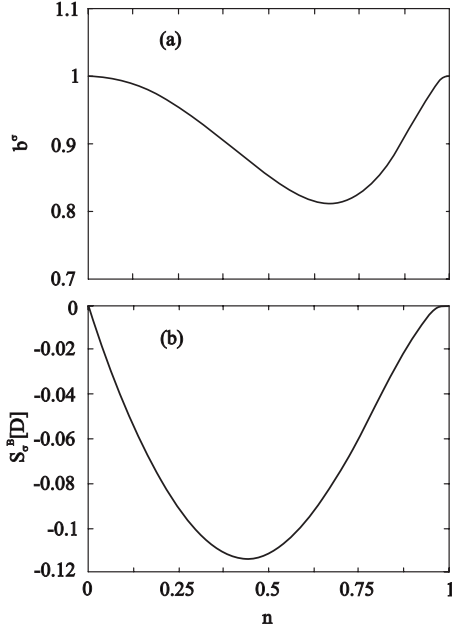


FIG. 1. (a) The bandwidth factor and (b) the band shift factor in function of electron concentration calculated in the paramagnetic state and H-F approximation. The strong correlation case is assumed.

crease in DOS under the influence of intersite correlation. The strongest reduction in the bandwidth takes place at the maximum of DOS in the lower Hubbard subband. Intersite correlation effects lead also to the shift of entire subbands. Both effects disappear at the empty ($n=0$) and full ($n=1$) lower Hubbard subband (see Fig. 1). Parameters b^σ and S_σ^B depend on magnetization m through Eqs. (41), (44), and (45) and, as will be shown in Sec. V, they can create the spontaneous magnetization (see Hirsch,¹⁷ and Górski and Mizia⁴⁵).

The results presented above obtained in the H-F approximation depict the character of intersite corrections vs electron concentration, which will be similar in the rigorous approach presented below.

B. High approximation for $B_{k,\sigma}^T(\varepsilon)$ and $S_\sigma^B(\varepsilon)$

Now, the correlation functions appearing in the bandwidth correction factor $B_{k,\sigma}^T(\varepsilon)$ and in the band shift correction factor $S_\sigma^B(\varepsilon)$ will be calculated based on the results of Nolting and Borgiel⁴⁰ and Roth.³⁸

The Fock parameter $\langle c_{l-\sigma}^+ c_{i-\sigma} \rangle$ appearing in the band shift correction factor $S_\sigma^B(\varepsilon)$ given by Eq. (29) can be written as

$$\langle c_{l-\sigma}^+ c_{i-\sigma} \rangle = \frac{1}{N} \sum_k \exp[i\mathbf{k} \cdot (\mathbf{r}_l - \mathbf{r}_i)] \int_{-\infty}^{\infty} S_{k-\sigma}(\varepsilon) \frac{d\varepsilon}{1 + e^{(\varepsilon-\mu)/k_B T}}, \quad (46)$$

where $S_{k-\sigma}(\varepsilon)$ is the single-electron spectral density

$$S_{k-\sigma}(\varepsilon) = -\frac{1}{\pi} \text{Im} G_k^{-\sigma}(\varepsilon), \quad (47)$$

with the Green's function given by Eq. (33).

The higher correlation function $\langle \hat{n}_{l\sigma} c_{l-\sigma}^+ c_{i-\sigma} \rangle$ appearing in Eq. (29) can be expressed as^{38,40}

$$\begin{aligned} \langle \hat{n}_{l\sigma} c_{l-\sigma}^+ c_{i-\sigma} \rangle &= \frac{1}{UN} \sum_k \exp[i\mathbf{k} \cdot (\mathbf{r}_l - \mathbf{r}_i)] \\ &\times \int_{-\infty}^{\infty} (\varepsilon' - \varepsilon_k) S_{k-\sigma}(\varepsilon') \\ &\times \frac{d\varepsilon'}{1 + e^{(\varepsilon' - \mu)/k_B T}}. \end{aligned} \quad (48)$$

Inserting Eqs. (46) and (48) to Eq. (29) we obtain finally

$$\begin{aligned} S_\sigma^B(\varepsilon) &= F_H^\sigma(\varepsilon) C_-[\varepsilon - \Omega_\sigma^T(\varepsilon)] \\ &\times \frac{1}{N} \sum_k \int_{-\infty}^{\infty} (\varepsilon_k - T_0) \left[\frac{2}{U} (\varepsilon' - \varepsilon_k) - 1 \right] \\ &\times S_{k-\sigma}(\varepsilon') \frac{d\varepsilon'}{1 + e^{(\varepsilon' - \mu)/k_B T}}. \end{aligned} \quad (49)$$

The three higher correlation functions $\langle \hat{n}_{l-\sigma} \hat{n}_{i-\sigma} \rangle$, $\langle c_{l\sigma}^+ c_{i-\sigma}^+ c_{l-\sigma} c_{i\sigma} \rangle$, and $\langle c_{l\sigma}^+ c_{l-\sigma}^+ c_{i-\sigma} c_{i\sigma} \rangle$, appearing in the bandwidth correction factor $B_{k,\sigma}^T(\varepsilon)$ given by Eq. (32), were expressed by functions: $\langle c_{l-\sigma}^+ c_{i-\sigma} \rangle$ and $\langle \hat{n}_{l\sigma} c_{l-\sigma}^+ c_{i-\sigma} \rangle$ (Refs. 38 and 41). Inserting all these functions to Eq. (32) we obtain the bandwidth correction factor $B_{k,\sigma}^T(\varepsilon)$ as

$$\begin{aligned} B_{k,\sigma}^T(\varepsilon) &= \{F_H^\sigma(\varepsilon) C_-[\varepsilon - \Omega_\sigma^T(\varepsilon)]\}^2 \frac{1}{N} \sum_{li} (-t_{li}) \left[- \left(\frac{\eta_{-\sigma}}{1 + \nu_{0\sigma} \nu_{0-\sigma}} \right. \right. \\ &+ \left. \frac{\eta_{\sigma} + \nu_{\sigma}}{1 - \nu_{0\sigma}} + \frac{\eta_{\sigma}}{1 + \nu_{0\sigma}} \right) \langle c_{l-\sigma}^+ c_{i-\sigma} \rangle - \left(\frac{\nu_{-\sigma}}{1 + \nu_{0\sigma} \nu_{0-\sigma}} \right. \\ &- \left. \frac{\nu_{\sigma}}{1 - \nu_{0\sigma}} + \frac{\nu_{\sigma}}{1 + \nu_{0\sigma}} \right) \langle \hat{n}_{l\sigma} c_{l-\sigma}^+ c_{i-\sigma} \rangle \Big] \\ &\times \exp[i\mathbf{k} \cdot (\mathbf{r}_l - \mathbf{r}_i)], \end{aligned} \quad (50)$$

where the following abbreviations were introduced:

$$\eta_{\sigma} = \frac{1}{1 - n_{-\sigma}} (\langle c_{l-\sigma}^+ c_{i-\sigma} \rangle - \langle \hat{n}_{l-\sigma} c_{l\sigma}^+ c_{i\sigma} \rangle), \quad (51)$$

$$\nu_{\sigma} = \frac{1}{n_{-\sigma}(1 - n_{-\sigma})} (\langle \hat{n}_{l-\sigma} c_{l\sigma}^+ c_{i\sigma} \rangle - n_{-\sigma} \langle c_{l\sigma}^+ c_{i\sigma} \rangle), \quad (52)$$

$$\nu_{0\sigma} = \frac{1}{n_{-\sigma}(1 - n_{-\sigma})} (\langle \hat{n}_{l\sigma} \hat{n}_{l-\sigma} \rangle - n_{\sigma} n_{-\sigma}). \quad (53)$$

With the help of Eqs. (30) and (A8), the function $F_H^\sigma(\varepsilon) C_-[\varepsilon - \Omega_\sigma^T(\varepsilon)]$, appearing in expressions for $S_\sigma^B(\varepsilon)$ and $B_{k,\sigma}^T(\varepsilon)$, will take on the following form:

$$F_H^\sigma(\varepsilon) C_-[\varepsilon - \Omega_\sigma^T(\varepsilon)] = \frac{\varepsilon_+ - \varepsilon_-}{\varepsilon - (\varepsilon_+ n_{-\sigma}^- + \varepsilon_- n_{-\sigma}^+) - \Omega_\sigma^T(\varepsilon)}. \quad (54)$$

The above expression has to be inserted back to formula (49) for $S_\sigma^B(\varepsilon)$ and formula (50) for $B_{k,\sigma}^T(\varepsilon)$. Next, we use the expressions (49) and (50) in Eqs. (34)–(38), from which we

calculate the self-energy $\Sigma^\sigma(\varepsilon)$, DOS, and the average electron numbers with spin $\pm\sigma$.

V. MAGNETISM WITH THE BANDWIDTH AND BAND SHIFT CORRECTION

In this section the consequences of including $B_{k,\sigma}^T(\varepsilon)$ and $S_\sigma^B(\varepsilon)$ for the appearance of the ferromagnetic ordering will be analyzed. The results will be compared here with the results of the standard CPA approach. In Sec. VI the comparison will be made with the similar results obtained for the strongly correlated systems by Nolting and co-workers, who have also arrived at the magnetic-ordered state using SDA (Refs. 39–41) and MAA theories.^{42,43}

To analyze the possibility of the transition to ferromagnetic ground state, one has to remember that the chemical potential in Eq. (38) has the form $\mu_\sigma = \mu + F_{in}n_\sigma$, which involves the probing constant of the exchange interaction F_{in} .

In further analysis we will use two coupled equations for electron number and magnetization

$$n = n_\uparrow + n_\downarrow, \quad m = n_\uparrow - n_\downarrow, \quad (55)$$

where $n_{\pm\sigma}$ is given by Eq. (38).

On the basis of these equations, the critical on-site exchange interaction will be calculated in the limit of $m \rightarrow 0$. The cases of strong correlation ($U \gg D$) and intermediate correlation will be analyzed. We will investigate the existence of ferromagnetism for some specific densities of states, which are relevant for different types of crystal lattices. One type of DOS, which will be analyzed, is the two-dimensional tight-binding DOS. To simplify the numerical procedure, this DOS is well represented by the analytical formula

$$\rho(\varepsilon) = \frac{1}{D} \left(e + b \log \frac{|\varepsilon|}{D} \right), \quad (56)$$

with constants e and b fitted to the numerical two-dimensional tight-binding DOS.

Another example will be the DOS with the asymmetry parameter a

$$\rho_0(\varepsilon) = \frac{1 + \sqrt{1 - a^2} \sqrt{D_0^2 - \varepsilon^2}}{\pi D_0} \frac{1}{D_0 + a\varepsilon}, \quad (57)$$

with a varying continuously from $a=0$ corresponding to a symmetric semielliptic band (or Bethe lattice) to $a \approx 1$ corresponding to a fcc lattice.⁴⁷

Density of states obtained for the unperturbed semielliptic DOS ($a=0$) and for asymmetric DOS ($a=0.7$) is shown in Fig. 2. Under the influence of intersite correlation one can see the shift of both subbands toward higher energies, reduction in the bandwidth, and increase in DOS. For the symmetric DOS with $a=0$ we have only the paramagnetic state; for the asymmetrical DOS with $a=0.7$ we have a weak ferromagnetic state.

In Fig. 3 we show the critical value of the exchange interaction calculated for the two-dimensional DOS given by Eq. (56) and for the semielliptic DOS given by Eq. (57) with $a=0$, which is close to the case of simple cubic (sc) lattice in three dimensions. We added into the same figure the CPA

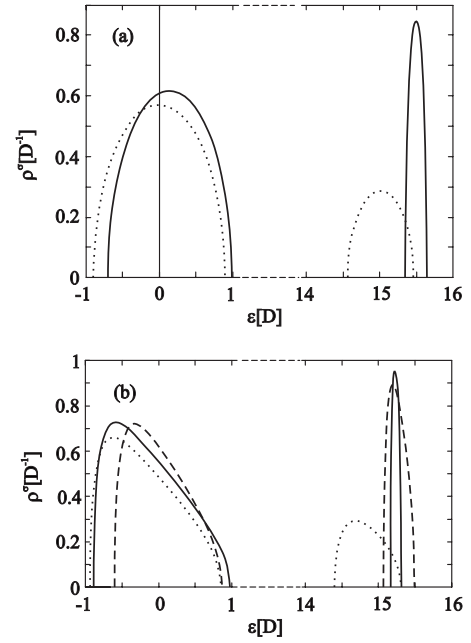


FIG. 2. Density of states calculated in the CPA approximation and with the intersite correlation treated in our high approximation. CPA approximation—dotted line in both (a) and (b). (a) Calculations in our approximation for the paramagnetic state: $a=0$ and $m=0$ —solid line. (b) Calculations in our approximation for the ferromagnetic state $a=0.7$ and $m=0.185$, solid and dashed lines are for the majority and minority-spin electrons, respectively. Other parameters are $n=0.4$, $D=1$ eV, and $U=15D$.

results for both these densities. One can see that for both DOS we have the ferromagnetic enhancement, but there is no transition to the ferromagnetic ground state. Including the intersite correlation in the CPA solution decreases significantly the exchange field necessary for ferromagnetism, but even the strong on-site Coulomb repulsion does not create ferromagnetism without exchange interaction.

We also calculated the critical value of the on-site exchange interaction for the general DOS represented by Eq. (57) with different a . It can be seen from Fig. 4 that the

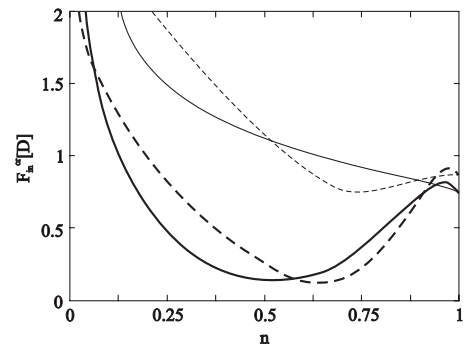


FIG. 3. Critical value of the on-site exchange interaction as function of electron concentration calculated for the semielliptic DOS and two-dimensional simple-cubic DOS. Thick solid line—our approximation, and thin solid line—CPA approximation for the semielliptic DOS. Thick dashed line—our approximation, and thin dashed line—CPA approximation for two-dimensional simple-cubic DOS. Parameters are $D=1$ eV and $U=15D$.

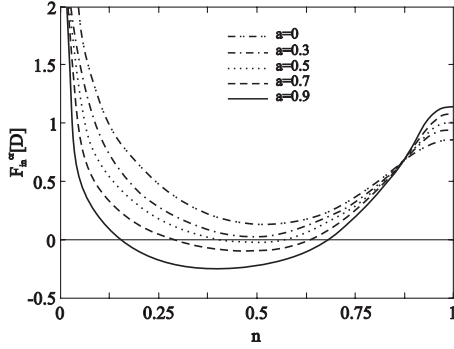


FIG. 4. Critical value of the on-site exchange interaction as function of electron concentration for the bands with the different asymmetry parameter a . Other parameters are $D=1$ eV and $U=15D$.

ferromagnetic enhancement increases as the asymmetry parameter increases. Under the influence of strong U alone, we have a ferromagnetic alignment at some electron concentrations starting from the parameter $a=0.42$. At high a (close to unity) the band looks like a fcc tight-binding DOS and then the ferromagnetic alignment, which takes place when the critical on-site exchange field is negative, covers large interval of electron occupations.

In Fig. 5 we illustrate the role of the bandwidth factor $B_{k,\sigma}^T(\varepsilon)$ and the band shift factor $S_{\sigma}^B(\varepsilon)$ in creating the ferromagnetic ground state. The numerical results of the exchange interaction are calculated for the band with the asymmetry parameter $a=0.7$. The main conclusion from this figure is that even for a highly asymmetrical band we obtain ferromagnetism at some electron concentrations, only when both the bandwidth and band shift corrections are included together. The bandwidth factor $B_{k,\sigma}^T(\varepsilon)$ and the band shift factor $S_{\sigma}^B(\varepsilon)$ work both in the same direction of decreasing the on-site exchange interaction necessary for ferromagnetism. Maximum ferromagnetic enhancement takes place roughly in the middle of the lower Hubbard subband. The band shift factor $S_{\sigma}^B(\varepsilon)$ is a dominant force behind the ferromagnetism

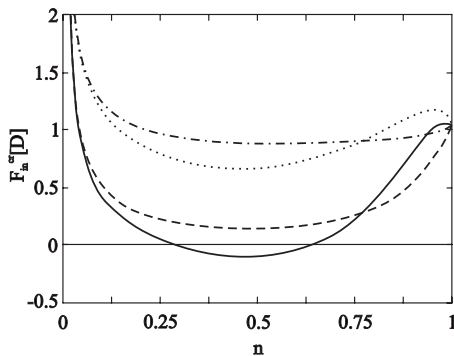


FIG. 5. Critical value of the on-site exchange interaction as function of electron concentration for the band with the asymmetry parameter $a=0.7$. Dot-dashed line is the CPA solution. Dotted line—our approximation with the bandwidth correction, dashed line—our approximation with the band shift correction, and solid line—our approximation with the bandwidth and band shift corrections. Other parameters are $D=1$ eV and $U=15D$.

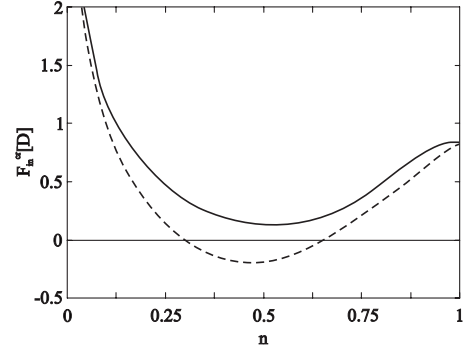


FIG. 6. Critical value of the on-site exchange interaction calculated as a function of electron concentration. The band shift and bandwidth factors treated in the H-F approximation (dashed line) and in the high approximation (solid line). Calculations were performed for the band with the asymmetry parameter $a=0$. Other parameters are $D=1$ eV and $U=15D$.

and the influence of the bandwidth factor $B_{k,\sigma}^T(\varepsilon)$ is weaker, but both these factors working together are necessary to obtain spontaneous magnetization.

Figure 6 shows the exchange field for the band shift and bandwidth factors treated in the H-F approximation and in the high approximation. One can see that the more rigorous solution eliminates ferromagnetism, over the entire interval of electron occupations for the semielliptic DOS. Ferromagnetism for this DOS is present only in the H-F approximation.

In Fig. 7 we show the magnetic moment m as a function of band filling for $U=15D$, $D=1$ eV, and different asymmetry parameters. It can be seen that the value of magnetic moment is relatively low with respect to the saturation moment $m_{\max}=n$. Calculated by us, Curie temperature dependence on band filling is very similar to $m(n)$ shown in Fig. 7.

In Fig. 8 we present the critical on-site exchange field for different values of the Coulomb interaction U calculated for asymmetrical DOS of Eq. (57) with the asymmetry parameter $a=0.7$. Both the bandwidth and band shift factors are included in the high approximation. One can see that the range of ferromagnetism is shrinking with decreasing U . It is also shifting toward higher concentrations. At the half-filled point all these curves match the corresponding CPA results,⁴⁸

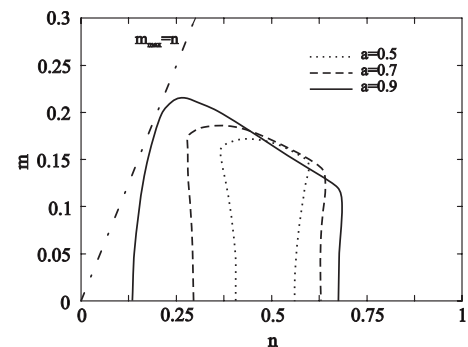


FIG. 7. Magnetization m as a function of the band occupation n for different asymmetry parameters. Other parameters are $U=15D$ and $D=1$ eV.

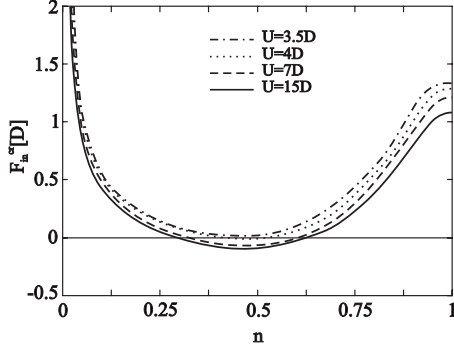


FIG. 8. Critical on-site exchange interaction calculated for asymmetrical DOS of Eq. (57) with the asymmetry parameter $a=0.7$ and different values of the Coulomb interaction U . Both the bandwidth and band shift factors are included in the high approximation.

as both correlation factors tend to zero in the limit of full subband. It has to be remembered that all values of U used in our calculations cause the band split, since they fulfill the relation $U > U_{cr} \approx D$. For the split-band case the lower subband becomes filled at $n=1$.

VI. DISCUSSION AND CONCLUSIONS

Including the intersite kinetic correlation into the basic calculations of the Hubbard model³ gives the solution, which at some values of electron occupation and Coulomb repulsion U brings the ferromagnetic ground state for the asymmetrical DOS. However, the way we calculate the intersite correlations appearing in Eqs. (29) and (32) is perhaps not yet fully self-consistent, and it is possible that the strong enforcement of the self-consistency in this calculation will eliminate the ferromagnetism, similarly as in the case of the CPA analysis.

Our results for $B_{k,\sigma}^T(\varepsilon)$ and $S_{\sigma}^B(\varepsilon)$ should be compared with similar results obtained for the strongly correlated systems by Nolting and co-workers,³⁹⁻⁴³ who have also arrived at the magnetic-ordered state using SDA and MAA theories. In the SDA method,³⁹ the higher correlation function has been defined, which can be split as follows into \mathbf{k} -dependent and \mathbf{k} -independent terms

$$n_{-\sigma} B_{D;k}^{-\sigma} + n_{-\sigma} B_S^{-\sigma}. \quad (58)$$

The function $B_{D;k}^{-\sigma}$ called as the bandwidth correction by the authors depends on the wave vector \mathbf{k} and is given by

$$B_{D;k}^{-\sigma} = \frac{1}{n_{-\sigma}(1-n_{-\sigma})} \frac{1}{N} \sum_{ij} (-t_{ij}) e^{-i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)} (\langle \hat{n}_{i-\sigma} \hat{n}_{j-\sigma} \rangle - n_{-\sigma}^2 - \langle c_{j\sigma}^+ c_{j-\sigma}^+ c_{i-\sigma} c_{i\sigma} \rangle - \langle c_{j\sigma}^+ c_{i-\sigma}^+ c_{j-\sigma} c_{i\sigma} \rangle), \quad (59)$$

where the three parts were interpreted as density correlation, double hopping, and spin exchange. The \mathbf{k} -independent term $B_S^{-\sigma}$ is the band shift correction and is given by

$$B_S^{-\sigma} = \frac{1}{n_{-\sigma}(1-n_{-\sigma})} \frac{1}{N} \sum_{ij} (-t_{ij}) \langle c_{i-\sigma}^+ c_{j-\sigma} (2\hat{n}_{i\sigma} - 1) \rangle. \quad (60)$$

In the MAA method the authors⁴³ used the CPA equations [Eq. (16) above] with two centers of gravity ε_{α} and probabilities $n_{-\sigma}^{\alpha}$ modified by the band shift $B_S^{-\sigma}$ parameter. Contrary to the normal CPA results, the MAA method in the $U \gg D$ limit in the case of a bcc lattice created a self-consistent ferromagnetic solution in the middle of the lower Hubbard subband (for electron occupations $0.65 < n < 0.75$). This range of existence of spontaneous magnetization obtained at the strong Coulomb interaction was larger than the ranges obtained at smaller U .⁴³

Different densities of states used in SDA and MAA approaches have also an influence on the range of ferromagnetism and its existence. Ferromagnetism calculated⁴³ by those methods for the case of tight-binding bcc lattice was a weak ferromagnetism. Using the tight-binding fcc DOS, the same group⁴² has obtained (in the MAA method) a strong ferromagnetism within the whole range of electron occupations $0 < n \leq 1$.

The semielliptic DOS used by us is not peaked as strongly at the half-filled point as the tight-binding bcc DOS. We did not obtain a ferromagnetism for this DOS and also not for the two-dimensional tight-binding sc DOS. Perhaps the reason for the lack of ferromagnetism for the symmetric DOS is that our approach is more self-consistent. We obtained ferromagnetism for the asymmetrical DOS of Eq. (57) for the asymmetry parameter $a > 0.42$. It did not cover the whole interval of electron occupation in the lower subband. The range of ferromagnetism was growing with growing parameter a and it was also at the maximum for $U \gg D$. For smaller U , we have obtained a smaller range of ferromagnetism (see Fig. 8).

In their numerical MAA calculations, Nolting and co-workers^{42,43} neglected the bandwidth correction. As opposed to this, the bandwidth correction was included in our numerical calculations (see, e.g., Fig. 5).

The MAA correlation function given by Eq. (58) corresponds in our approach and in our notation to the function

$$B_{k,\sigma}^T(\varepsilon) + S_{\sigma}^B(\varepsilon), \quad (61)$$

which was derived above rigorously in the Hubbard III approximation with added intersite correlation.

Our formula for the band shift [Eq. (29)] in the H-F approximation and for $U \gg D$ gives

$$F_H^{\sigma}(\varepsilon) C_{-}[\varepsilon - \Omega_{\sigma}^T(\varepsilon)] = \frac{(\varepsilon_{+} - \varepsilon_{-})}{\varepsilon - (\varepsilon_{+} n_{-\sigma}^{-} + \varepsilon_{-} n_{-\sigma}^{+}) - \Omega_{\sigma}^T(\varepsilon)} \approx -\frac{1}{(1-n_{-\sigma})}. \quad (62)$$

It has the same form as Nolting's formula [Eq. (60) above] but it has different coefficient in front of the summation. This coefficient in Eq. (62) has the opposite sign than in the Nolting expression for $n_{-\sigma} B_S^{-\sigma} : + \frac{1}{(1-n_{-\sigma})}$. Nevertheless both these coefficients shift the DOS into the same direction of higher energies due to different placement of the band shift term in those two approaches.

Our formula for the bandwidth [Eq. (32)] also has the same form as Nolting's Eq. (59), with the different coefficient in front of the summation. In the H-F and $U \gg D$, this coefficient is equal to

$$\{F_H^\sigma(\varepsilon)C_-[\varepsilon - \Omega_\sigma^T(\varepsilon)]\}^2 \approx \frac{1}{(1 - n_{-\sigma})^2}, \quad (63)$$

which is different from Nolting's coefficient in his expression for $n_{-\sigma}B_{D;k}^\sigma: \frac{1}{(1-n_{-\sigma})}$.

Summarizing the comparison with existing approximations: the MAA formulas have manifested as a simplified version of the formulas derived analytically in this paper within the pure Hubbard III scheme which included the intersite correlations $\langle c_{i-\sigma}^+ c_{j-\sigma} \rangle$ and $\langle \hat{n}_{i\sigma} c_{i-\sigma}^+ c_{j-\sigma} \rangle$.

The range of ferromagnetism is smaller in our approach than in the MAA method. It completely disappears for the two-dimensional tight-binding DOS and the semielliptic DOS. Perhaps the reason for weakening the ferromagnetic solution in our approach is the more self-consistent approximation [see Eq. (24)].

APPENDIX A

1. Scattering effect

Using Eq. (5) one can write the Green's function $\langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) c_{l\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon$ as

$$\langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) c_{l\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon = \sum_{\beta=\pm} \langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) \hat{n}_{l-\sigma}^\beta c_{l\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon. \quad (A1)$$

The equation of motion for the Green's function $\langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) \hat{n}_{l-\sigma}^\beta c_{l\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon$ has the following form:

$$\begin{aligned} & \varepsilon \langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) \hat{n}_{l-\sigma}^\beta c_{l\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \\ &= \delta_{jl} \langle\langle (\hat{n}_{i-\sigma}^\alpha - \hat{n}_{l-\sigma}^\alpha) \hat{n}_{l-\sigma}^\beta \rangle\rangle_\varepsilon + \varepsilon_\beta \langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) \hat{n}_{l-\sigma}^\beta c_{l\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \\ & - \sum_m t_{ml} \langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) \hat{n}_{l-\sigma}^\beta c_{m\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \\ & + \text{other terms.} \end{aligned} \quad (A2)$$

In the original Hubbard model,³ the first term on the right-hand side of Eq. (A2) was assumed to be zero. In our approach this average is written as

$$\langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) \hat{n}_{l-\sigma}^\beta \rangle\rangle_\varepsilon = \xi_\alpha \xi_\beta \langle\langle \hat{n}_{i-\sigma} \hat{n}_{l-\sigma} \rangle\rangle - n_{-\sigma}^2 = \xi_\alpha \xi_\beta B_{il}^\sigma. \quad (A3)$$

The factor $B_{il}^\sigma = \langle\langle \hat{n}_{i-\sigma} \hat{n}_{l-\sigma} \rangle\rangle - n_{-\sigma}^2$ is expressed in Sec. IV by the intersite averages of the type $\langle c_{i-\sigma}^+ c_{l-\sigma} \rangle$ and $\langle \hat{n}_{i\sigma} c_{i-\sigma}^+ c_{l-\sigma} \rangle$, which are assumed to be nonzero in this approach.

For the function $\langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) \hat{n}_{l-\sigma}^\beta c_{m\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon$ appearing in Eq. (A2), the following approximation is used:

$$\begin{aligned} & \langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) \hat{n}_{l-\sigma}^\beta c_{m\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \\ & \cong n_{-\sigma}^\beta \langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) c_{m\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \\ & + \langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) \hat{n}_{l-\sigma}^\beta \rangle\rangle \langle\langle c_{m\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon, \end{aligned} \quad (A4)$$

where the first term on the right-hand side is the original Hubbard III term. The additional second term is the result of assuming that $B_{il}^\sigma \neq 0$.

Inserting to Eq. (A2) the approximations (A3) and (A4), we obtain the relation

$$\begin{aligned} & (\varepsilon - \varepsilon_\beta) \langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) \hat{n}_{l-\sigma}^\beta c_{l\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \\ &= \xi_\alpha \xi_\beta B_{il}^\sigma \left(\delta_{jl} - \sum_m t_{ml} \langle\langle c_{m\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \right) \\ & - \sum_m t_{ml} n_{-\sigma}^\beta \langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) c_{m\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon. \end{aligned} \quad (A5)$$

Dividing both sides of this equation by $(\varepsilon - \varepsilon_\beta)$ and summing up over $\beta = \pm$, we have

$$\begin{aligned} & \langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) c_{l\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \\ &= \xi_\alpha C_-(\varepsilon) B_{il}^\sigma \left(\delta_{jl} - \sum_m t_{ml} \langle\langle c_{m\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \right) \\ & - \frac{1}{F_{H,0}^\sigma(\varepsilon)} t_{il} \langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) c_{i\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \\ & - \frac{1}{F_{H,0}^\sigma(\varepsilon)} \sum_{m \neq i} t_{ml} \langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) c_{m\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon, \end{aligned} \quad (A6)$$

where

$$\frac{1}{F_{H,0}^\sigma(\varepsilon)} = \frac{n_{-\sigma}^+}{\varepsilon - \varepsilon_+} + \frac{n_{-\sigma}^-}{\varepsilon - \varepsilon_-}, \quad (A7)$$

$$C_-(\varepsilon) = \frac{1}{\varepsilon - \varepsilon_+} - \frac{1}{\varepsilon - \varepsilon_-}. \quad (A8)$$

Following the Hubbard I approximation, one can write that

$$\delta_{jl} - \sum_m t_{ml} \langle\langle c_{m\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon = F_{H,0}^\sigma(\varepsilon) \langle\langle c_{l\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon. \quad (A9)$$

Inserting Eq. (A9) to Eq. (A6) we obtain the following relation:

$$\begin{aligned} & \langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) c_{l\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \\ &= \xi_\alpha C_-(\varepsilon) F_{H,0}^\sigma(\varepsilon) B_{il}^\sigma \langle\langle c_{l\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \\ & - \frac{1}{F_{H,0}^\sigma(\varepsilon)} \left[t_{il} \langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) c_{i\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \right. \\ & \left. + \sum_{m \neq i} t_{ml} \langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) c_{m\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \right]. \end{aligned} \quad (A10)$$

Equation (A10) is analogous to Eq. (25) of Hubbard,³ but it contains additionally the bandwidth correction B_{il}^σ . Solution of Eq. (A10) is the extended Hubbard solution of the following form:

$$\begin{aligned} & \langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) c_{l\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \\ &= - \sum_m W_{lm,i}^\sigma(\varepsilon) t_{mi} \langle\langle (\hat{n}_{i-\sigma}^\alpha - n_{-\sigma}^\alpha) c_{i\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon \\ & + \xi_\alpha C_-(\varepsilon) F_{H,0}^\sigma(\varepsilon) B_{il}^\sigma \langle\langle c_{l\sigma}; c_{j\sigma}^+ \rangle\rangle_\varepsilon, \end{aligned} \quad (A11)$$

where

$$W_{lm,i}^\sigma(\varepsilon) = g_{lm}^\sigma(\varepsilon) - \frac{g_{li}^\sigma(\varepsilon) g_{im}^\sigma(\varepsilon)}{g_{ii}^\sigma(\varepsilon)}, \quad (A12)$$

and

$$g_{ij}^\sigma(\varepsilon) = \sum_k \frac{\exp[i\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)]}{F_{H,0}^\sigma(\varepsilon) - (\varepsilon_k - T_0)}. \quad (\text{A13})$$

The additional second term on the right-hand side is responsible for the bandwidth correction.

Inserting the Green's function from Eq. (A11) to Eq. (9) [we are still ignoring the last term in Eq. (9), which will be dealt with in Appendix B on resonance broadening effect] we obtain the following equation for the Green's function $\langle\langle \hat{n}_{i-\sigma}^\alpha c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon$:

$$\begin{aligned} & (\varepsilon - \varepsilon_\alpha) \langle\langle \hat{n}_{i-\sigma}^\alpha c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon + \xi_\alpha \Omega_\sigma(\varepsilon) (n_{-\sigma}^+ \langle\langle \hat{n}_{i-\sigma}^- c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon \\ & - n_{-\sigma}^- \langle\langle \hat{n}_{i-\sigma}^+ c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon) \\ & = n_{-\sigma}^\alpha \left(\delta_{ij} - \sum_l t_{il} \langle\langle c_{l\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon \right) + \xi_\alpha \sum_l B_{il,\sigma}^S(\varepsilon) \langle\langle c_{l\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon, \end{aligned} \quad (\text{A14})$$

where

$$\begin{aligned} \varepsilon \langle\langle \hat{n}_{l\sigma}^\alpha c_{l-\sigma}^\pm c_{i-\sigma}^\mp c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon & = \delta_{ij} \langle\langle \hat{n}_{l\sigma}^\alpha c_{l-\sigma}^\pm c_{i-\sigma}^\mp \rangle\rangle_\varepsilon - \delta_{jl} \xi_\alpha \langle\langle c_{l\sigma}^+ c_{l-\sigma}^\pm c_{i-\sigma}^\mp c_{i\sigma} \rangle\rangle_\varepsilon - \xi_\alpha \sum_m t_{ml} \langle\langle c_{l\sigma}^+ c_{m\sigma} c_{l-\sigma}^\pm c_{i-\sigma}^\mp c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon \\ & - \langle\langle c_{m\sigma}^+ c_{l\sigma} c_{l-\sigma}^\pm c_{i-\sigma}^\mp c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon \pm \sum_m t_{ml} \langle\langle \hat{n}_{l\sigma}^\alpha c_{m-\sigma}^\pm c_{i-\sigma}^\mp c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon \\ & \mp \sum_m t_{im} \langle\langle \hat{n}_{l\sigma}^\alpha c_{l-\sigma}^\pm c_{m-\sigma}^\mp c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon - \sum_m t_{im} \langle\langle \hat{n}_{l\sigma}^\alpha c_{l-\sigma}^\pm c_{i-\sigma}^\mp c_{m\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon + (\varepsilon_\pm \pm \varepsilon_- \mp \varepsilon_\alpha) \\ & \times \langle\langle \hat{n}_{l\sigma}^\alpha c_{l-\sigma}^\pm c_{i-\sigma}^\mp c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon. \end{aligned} \quad (\text{B2})$$

For the moment we consider only the case with the upper indices above. For the Green's functions appearing in Eq. (B2), we use the approximations which neglect the three center averages and we obtain the following results:

$$\langle\langle c_{l\sigma}^+ c_{m\sigma} c_{l-\sigma}^\pm c_{i-\sigma}^\mp c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon \cong - \langle\langle c_{l\sigma}^+ c_{i\sigma} c_{l-\sigma}^\pm c_{i-\sigma}^\mp \rangle\rangle_\varepsilon \langle\langle c_{m\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon, \quad (\text{B3})$$

$$\langle\langle c_{m\sigma}^+ c_{l\sigma} c_{l-\sigma}^\pm c_{i-\sigma}^\mp c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon \cong 0, \quad (\text{B4})$$

$$\langle\langle \hat{n}_{l\sigma}^\alpha c_{m-\sigma}^\pm c_{i-\sigma}^\mp c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon \cong n_{\sigma'}^\alpha \langle\langle c_{m-\sigma}^\pm c_{i-\sigma}^\mp c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon, \quad (\text{B5})$$

$$\langle\langle \hat{n}_{l\sigma}^\alpha c_{l-\sigma}^\pm c_{m-\sigma}^\mp c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon \cong \delta_{lm} n_{\sigma'}^\alpha n_{-\sigma}^+ \langle\langle c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon, \quad (\text{B6})$$

$$\langle\langle \hat{n}_{l\sigma}^\alpha c_{l-\sigma}^\pm c_{i-\sigma}^\mp c_{m\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon \cong \langle\langle \hat{n}_{l\sigma}^\alpha c_{l-\sigma}^\pm c_{i-\sigma}^\mp \rangle\rangle_\varepsilon \langle\langle c_{m\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon. \quad (\text{B7})$$

$$\Omega_\sigma(\varepsilon) = \sum_{l,m} t_{il} W_{lm,i}^\sigma(\varepsilon) t_{mi}, \quad (\text{A15})$$

$$B_{il,\sigma}^S(\varepsilon) = C_{-\sigma}(\varepsilon) F_{H,0}^\sigma(\varepsilon) (-t_{il}) (\langle\langle \hat{n}_{i-\sigma} \hat{n}_{l-\sigma} \rangle\rangle_\varepsilon - n_{-\sigma}^2). \quad (\text{A16})$$

The only difference between Eq. (A14) and the Hubbard³ solution is the presence of the term with $B_{il,\sigma}^S(\varepsilon)$ on the right-hand side.

APPENDIX B

Resonance broadening effect

Using Eq. (5) for the Green's functions $\langle\langle c_{l-\sigma}^\pm c_{i-\sigma}^\mp c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon$ we can write that

$$\langle\langle c_{l-\sigma}^\pm c_{i-\sigma}^\mp c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon = \sum_{\alpha=\pm} \langle\langle \hat{n}_{l\sigma}^\alpha c_{l-\sigma}^\pm c_{i-\sigma}^\mp c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon. \quad (\text{B1})$$

The functions $\langle\langle \hat{n}_{l\sigma}^\alpha c_{l-\sigma}^\pm c_{i-\sigma}^\mp c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon$ fulfill the following equation of motion:

We apply the same procedure to the case of lower indices in Eq. (B2). After inserting both these sets of equations into Eq. (B2), we arrive at the relation

$$\begin{aligned} & [\varepsilon - (\varepsilon_\pm \pm \varepsilon_- \mp \varepsilon_\alpha)] \langle\langle \hat{n}_{l\sigma}^\alpha c_{l-\sigma}^\pm c_{i-\sigma}^\mp c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon \\ & = \langle\langle \hat{n}_{l\sigma}^\alpha c_{l-\sigma}^\pm c_{i-\sigma}^\mp \rangle\rangle_\varepsilon \left(\delta_{ij} - \sum_m t_{im} \langle\langle c_{m\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon \right) \\ & - \xi_\alpha \langle\langle c_{l\sigma}^+ c_{i\sigma} c_{l-\sigma}^\pm c_{i-\sigma}^\mp \rangle\rangle_\varepsilon \left(\delta_{jl} - \sum_m t_{lm} \langle\langle c_{m\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon \right) \\ & \pm n_{\sigma'}^\alpha \sum_m t_{ml} \langle\langle c_{m-\sigma}^\pm c_{i-\sigma}^\mp c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon \\ & \mp t_{il} n_{\sigma'}^\alpha n_{-\sigma}^+ \langle\langle c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle_\varepsilon. \end{aligned} \quad (\text{B8})$$

Dividing both sides by $\varepsilon - (\varepsilon_\pm \pm \varepsilon_- \mp \varepsilon_\alpha)$, using Eq. (A9) and summing up over $\alpha = \pm$, we arrive at the relation

$$\begin{aligned} \langle\langle c_{l-\sigma}^{\pm} c_{i-\sigma}^{\mp} c_{i\sigma}^{\pm}; c_{j\sigma}^{\pm} \rangle\rangle_{\varepsilon} &= \sum_{\alpha} \frac{\langle \hat{n}_{l\sigma}^{\alpha} c_{l-\sigma}^{\pm} c_{i-\sigma}^{\mp} \rangle}{\varepsilon - (\varepsilon_{\pm} \pm \varepsilon_{-} \mp \varepsilon_{\alpha})} F_{H,0}^{\sigma}(\varepsilon) \langle\langle c_{i\sigma}; c_{j\sigma}^{\pm} \rangle\rangle_{\varepsilon} - \frac{1}{F_{H,0}^{-\sigma}(\varepsilon_{-} \pm \varepsilon_{\pm} \mp \varepsilon)} \left[\sum_m t_m \langle\langle c_{m-\sigma}^{\pm} c_{i-\sigma}^{\mp} c_{i\sigma}; c_{j\sigma}^{\pm} \rangle\rangle_{\varepsilon} \right. \\ &\quad \left. - t_{il} n_{-\sigma}^{\pm} \langle\langle c_{i\sigma}; c_{j\sigma}^{\pm} \rangle\rangle_{\varepsilon} \right] - \sum_{\alpha} \frac{\xi_{\alpha}}{\varepsilon - (\varepsilon_{\pm} \pm \varepsilon_{-} \mp \varepsilon_{\alpha})} \langle c_{l\sigma}^{\pm} c_{i\sigma} c_{l-\sigma}^{\pm} c_{i-\sigma}^{\mp} \rangle F_{H,0}^{\sigma}(\varepsilon) \langle\langle c_{l\sigma}; c_{j\sigma}^{\pm} \rangle\rangle_{\varepsilon}. \end{aligned} \quad (\text{B9})$$

The term in the square brackets above is the Hubbard solution.³ The two extra terms are the corrections for the intersite correlations. The solution to Eq. (B9) is the sum of the Hubbard solution and the intersite correction, and it takes on the following form:

$$\begin{aligned} \langle\langle c_{l-\sigma}^{\pm} c_{i-\sigma}^{\mp} c_{i\sigma}^{\pm}; c_{j\sigma}^{\pm} \rangle\rangle_{\varepsilon} &= - \sum_m W_{lm,i}^{-\sigma}(\varepsilon_{-} \pm \varepsilon_{\pm} \mp \varepsilon) t_{mi} \langle\langle (n_{i-\sigma}^{\pm} - n_{-\sigma}^{\pm}) c_{i\sigma}; c_{j\sigma}^{\pm} \rangle\rangle_{\varepsilon} + \sum_{\alpha} \frac{\langle \hat{n}_{l\sigma}^{\alpha} c_{l-\sigma}^{\pm} c_{i-\sigma}^{\mp} \rangle}{\varepsilon - (\varepsilon_{\pm} \pm \varepsilon_{-} \mp \varepsilon_{\alpha})} F_{H,0}^{\sigma}(\varepsilon) \langle\langle c_{i\sigma}; c_{j\sigma}^{\pm} \rangle\rangle_{\varepsilon} \\ &\quad - \sum_{\alpha} \frac{\xi_{\alpha} \langle c_{l\sigma}^{\pm} c_{i\sigma} c_{l-\sigma}^{\pm} c_{i-\sigma}^{\mp} \rangle}{\varepsilon - (\varepsilon_{\pm} \pm \varepsilon_{-} \mp \varepsilon_{\alpha})} F_{H,0}^{\sigma}(\varepsilon) \langle\langle c_{l\sigma}; c_{j\sigma}^{\pm} \rangle\rangle_{\varepsilon}, \end{aligned} \quad (\text{B10})$$

where the last two extra terms are responsible for the intersite averages.

Inserting to Eq. (9) the Green's function from Eq. (B10), still ignoring in Eq. (9) the terms with the Green's function $\langle\langle (\hat{n}_{i-\sigma}^{\alpha} - n_{-\sigma}^{\alpha}) c_{l\sigma}; c_{j\sigma}^{\pm} \rangle\rangle_{\varepsilon}$ describing the scattering correction, one obtains for the Green's functions $\langle\langle \hat{n}_{i-\sigma}^{\pm} c_{i\sigma}; c_{j\sigma}^{\pm} \rangle\rangle_{\varepsilon}$ and $\langle\langle \hat{n}_{i-\sigma}^{\pm} c_{i\sigma}; c_{j\sigma}^{\pm} \rangle\rangle_{\varepsilon}$, the matrix equation

$$\begin{aligned} &\begin{bmatrix} \varepsilon - \varepsilon_{-} - n_{-\sigma}^{+} \Omega_{-\sigma}^B(\varepsilon) & n_{-\sigma}^{-} \Omega_{-\sigma}^B(\varepsilon) \\ n_{-\sigma}^{+} \Omega_{-\sigma}^B(\varepsilon) & \varepsilon - \varepsilon_{+} - n_{-\sigma}^{-} \Omega_{-\sigma}^B(\varepsilon) \end{bmatrix} \\ &\times \begin{bmatrix} \langle\langle \hat{n}_{i-\sigma}^{-} c_{i\sigma}; c_{j\sigma}^{\pm} \rangle\rangle_{\varepsilon} \\ \langle\langle \hat{n}_{i-\sigma}^{+} c_{i\sigma}; c_{j\sigma}^{\pm} \rangle\rangle_{\varepsilon} \end{bmatrix} = \begin{bmatrix} n_{-\sigma}^{-} \\ n_{-\sigma}^{+} \end{bmatrix} \left[\delta_{ij} - \sum_l t_{il} \langle\langle c_{l\sigma}; c_{j\sigma}^{\pm} \rangle\rangle_{\varepsilon} \right] \\ &+ \begin{bmatrix} -1 \\ +1 \end{bmatrix} \left\{ \sum_l B_{il,\sigma}^B(\varepsilon) \langle\langle c_{l\sigma}; c_{j\sigma}^{\pm} \rangle\rangle_{\varepsilon} + S_{\sigma}^B(\varepsilon) \langle\langle c_{i\sigma}; c_{j\sigma}^{\pm} \rangle\rangle_{\varepsilon} \right\}, \end{aligned} \quad (\text{B11})$$

where

$$\begin{aligned} \Omega_{-\sigma}^B(\varepsilon) &= \sum_{lm} t_{il} t_{mi} [W_{lm,i}^{\sigma}(\varepsilon) - W_{lm,i}^{\sigma}(\varepsilon_{-} + \varepsilon_{+} - \varepsilon)] \\ &= \Omega_{-\sigma}(\varepsilon) - \Omega_{-\sigma}(\varepsilon_{-} + \varepsilon_{+} - \varepsilon), \end{aligned} \quad (\text{B12})$$

$$B_{il,\sigma}^B(\varepsilon) = -t_{il} F_{H,0}^{\sigma}(\varepsilon) C_{-}(\varepsilon) \langle c_{l\sigma}^{\pm} c_{i\sigma} (c_{l-\sigma} c_{i-\sigma}^{\pm} - c_{l-\sigma}^{\pm} c_{i-\sigma}) \rangle, \quad (\text{B13})$$

$$S_{\sigma}^B(\varepsilon) = F_{H,0}^{\sigma}(\varepsilon) C_{-}(\varepsilon) \sum_{li} (-t_{il}) (2 \langle \hat{n}_{l\sigma} c_{l-\sigma}^{\pm} c_{i-\sigma} \rangle - \langle c_{l-\sigma}^{\pm} c_{i-\sigma} \rangle). \quad (\text{B14})$$

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