Hubbard III approach with hopping interaction and intersite kinetic correlations

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We analyze the Hubbard model with added hopping interaction within the full Hubbard III approximation. In the Green's-function decoupling process, the intersite kinetic correlation functions are included. This is an extension of our previous paper [G. Górski and J. Mizia, Phys. Rev. B **79**, 064414 (2009)] in which the basic Hubbard model with the intersite kinetic correlations was analyzed in the framework of the coherent potential approximation (CPA). In the CPA method, the up-spin electrons propagated in the lattice of frozen down-spin electrons. The full Hubbard III solution used now takes into account the itinerancy of down-spin electrons. The combined effect of the hopping interaction and intersite kinetic correlation leaves the position of spin bands unaffected, but it deforms the density of states (DOS) of electrons, changing in this way the average electron energy. It is the main driving force behind the ferromagnetism as opposed to the rigid shift of the entire band, which takes place in the conventional Stoner magnetism. In the numerical calculations, we have used the bands with symmetrical DOS (semielliptic or bcc-like DOS) and also with asymmetrical DOS resembling the fcc DOS. The spontaneous ferromagnetic transition was obtained under the combined action of the hopping interaction and the intersite correlation in the systems that contain even a moderately strong peak in the DOS, such as the bcc- and fcc-like DOS.

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I. INTRODUCTION

Itinerant-electron ferromagnetism is one of the basic problems in solid-state physics. The central model describing this phenomenon is the single-band Hubbard model.[1,2] Exact solution of this model is possible only for one-dimensional (1D) systems[3,4] and for infinite-dimensional systems.[5] For that reason, different approximate methods exist. Introducing the Hartree-Fock approximation, we obtain the well-known Stoner criterion for ferromagnetism, $U_C \rho(\varepsilon_F) = 1$, where U_C is the critical value of on-site repulsion and $\rho(\varepsilon_F)$ is the density of states (DOS) on the Fermi level ε_F. Hartree-Fock approximation (called also the mean-field approximation) overestimates ferromagnetic ordering and the Curie temperature. It allows for the ferromagnetic transition at relatively small U and in the broad range of concentrations, but it neglects the correlation effects that can change the shape of the DOS, even splitting it at higher U, and can change the width of the band.

Obtaining a ferromagnetic solution in a higher approximation is very elusive. Reliable solutions exist only in some specific cases. One of the earliest results was obtained by Nagaoka,[6] who invented the model of the fully polarized ferromagnetic state (Nagaoka state) in the presence of a single hole in a half-filled band at $U = \infty$. For such a model, he obtained saturate ferromagnetism for sc, bcc, fcc, and hcp lattices. Looking at the magnetic problem from a different perspective, Lieb[7] obtained the ferromagnetic ground state for asymmetric bipartite lattices with finite Coulomb interaction and different numbers of sites in each sublattice. Mielke[8] and Tasaki[9] reached the ferromagnetic ordering for the lattices with flat bands. Müller-Hartmann[10] suggested that in the 1D model with next-nearest-neighbor hopping included, one can have the ferromagnetic ground state in the system with double minima at the limit of low particle density.

The dynamical mean-field theory (DMFT)[11] has allowed for subsequent progress in solving the Hubbard model. Using the finite-temperature quantum Monte Carlo (QMC) technique within the DMFT equations, Ulmke[12] obtained ferromagnetism for the fcc-type $d = \infty$ lattice even at intermediate Coulomb interaction. Numerical calculations based on QMC[13] and the variational QMC method[14] have arrived at spontaneous ferromagnetism for the infinite-U Hubbard model.

To describe correctly the magnetic state, Vollhardt and co-workers[15] postulated (i) including the intersite interactions, (ii) including the correlation effects, and (iii) considering highly asymmetrical DOS with the peak away from the center of the band.

In addition to the on-site repulsion $U = (ii|1/r|ii)$ in real materials, the intersite interactions are also important, including the nearest-neighbor repulsion $V = (ij|1/r|ij)$, the nearest-neighbor exchange interaction $J = (ij|1/r|ji)$, the pair hopping interaction $J' = (ii|1/r|jj)$, and the correlated hopping interaction $\Delta t = (ii|1/r|ij)$, which is also called the bond-charge interaction. Although in general they are smaller than U, as postulated by Hirsch and co-workers,[16–19] they play a key role in creating ferromagnetic ordering. Among these interactions, the correlated hopping interaction Δt (Refs. 16 and 20–33) may be particularly important for creating ferromagnetism. The analysis carried out in the mean-field approximation has shown that the interaction Δt decreases critical on-site repulsion U_C for some carrier concentrations even to zero.[16,30]

One of the most accepted and frequently used approximations describing the correlation effects in the Hubbard model is the Hubbard III approximation.[2] This approximation at high enough U splits the spin band into two bands: the lower band centered around the atomic level T_0 and the upper band centered around the level $T_0 + U$. The width of these bands depends on electron concentrations with different spins. Unfortunately, this approximation did not produce the ferromagnetic ground state; see Refs. 34 and 35. The scattering correction of the Hubbard III approximation, which is equivalent with the coherent potential approximation (CPA),[36] assumes that the σ electrons move in a frozen sea of $-\sigma$ electrons, the possibility of dynamic correlations between those two groups being ignored. The intersite correlations have been also ignored; the focus instead was on the on-site correlations alone. As a result, the self-energy was obtained as independent of momentum **k** and of spin. Therefore, to correct the Hubbard III approximation for the possibility of band ferromagnetism requires introducing the intersite correlations. In our previous paper (see Ref. 37), we described in great detail the Hubbard III approximation with the intersite kinetic correlation functions included but without the intersite interactions. The Hubbard III approximation has been simplified to the CPA type of solution. The intersite kinetic correlation functions $\langle c_{i-\sigma}^{+}c_{j-\sigma}\rangle$ and $\langle \hat{n}_{i\sigma}c_{i-\sigma}^{+}c_{j-\sigma}\rangle$ were originally ignored in the Hubbard III approach and in most of the subsequent papers by other authors devoted to this model. The self-energy in this approximation has the spin-dependent, **k**-independent band-shift term and the **k**-dependent term.

Nolting and co-workers[38–40] have developed a similar model called the modified alloy analogy method approximation (MAA). It is a combination of the CPA (or alloy analogy)[36] method and the spectral density approach (SDA).[41–43] Their approximation has led to spontaneous magnetization only for some carrier concentrations and a highly asymmetric fcc type of DOS. In our paper,[37] we showed that the MAA method can be obtained as a simplified version of our approach, the approach that was based on including the intersite correlations directly into the Hubbard III or CPA scheme. Our conclusions for ferromagnetism were more restrictive than in the MAA method, since in addition to the band-shift term considered in the MAA method, we also included the bandwidth change term that was neglected in that method.

In this paper, we present an approach that includes the intersite hopping interaction Δt and the intersite correlations arising in the decoupling process. The reason for introducing the intersite hopping interaction in the full Hubbard III scheme is that this interaction has already created a bandwidth change and a band shift (see Refs. 16 and 17) in the Hartree-Fock (HF) approximation, both of which enhance ferromagnetism. In Ref. 37, we reduced both the scattering and the resonance broadening effect to the CPA-like approach, in which the $+\sigma$ electron moves in a frozen sea of $-\sigma$ electrons. In the current improved approach, the $+\sigma$ electron moves in a sea of $-\sigma$ electrons defrozen by the resonance broadening effect [see Hubbard III, Eqs. (56)–(59)]. Therefore, even the solution of the simple Hubbard model (with only repulsion U) will be improved compared to our previous paper.[37] The interaction Δt will be treated also in this full Hubbard III approach. We will show that in this model, there is a spontaneous magnetization at a broad interval of parameters. The analysis will be carried out in the Green's-function formalism using the equation-of-motion approach described by Zubarev.[44,45]

The paper is organized as follows. In Sec. II, the general Green's-function chain equations for the Hubbard model with the intersite hopping interaction are calculated. The scattering correction and the resonance broadening correction are solved together. As a result, the self-consistent set of equations for the self-energy and DOS are obtained. This shows how the hopping interaction combined with the intersite kinetic correlation deforms the DOS and produces the spin-dependent change of the average energy. In Sec. III, we derive conditions for the spontaneous transition to ferromagnetism. Discussion of the numerical results for ferromagnetic ordering is presented in Sec. IV. Finally, Sec. V is devoted to the conclusions and to summarizing the obtained results.

II. THE MODEL

We analyze the basic Hubbard model with added hopping interaction and the exchange field,

$$H = -\sum_{ij\sigma} t_{ij}c_{i\sigma}^{+}c_{j\sigma} + T_0\sum_{i\sigma}\hat{n}_{i\sigma} + \frac{U}{2}\sum_{i\sigma}\hat{n}_{i\sigma}\hat{n}_{i-\sigma} + \sum_{ij\sigma}\Delta t_{ij}(\hat{n}_{i-\sigma}+\hat{n}_{j-\sigma})c_{i\sigma}^{+}c_{j\sigma} - \sum_{i\sigma}(\mu + F_{\text{in}}n_{\sigma})\hat{n}_{i\sigma}, \tag{1}$$

where the operator $c_{i\sigma}^{+}(c_{i\sigma})$ is creating (annihilating) an electron with spin $\sigma = \uparrow,\downarrow$ on the ith lattice site, $\hat{n}_{i\sigma} = c_{i\sigma}^{+}c_{i\sigma}$ is the electron number operator for electrons with spin σ on the ith lattice site, U is the on-site Coulomb interaction, Δt_{ij} is the hopping interaction, F_{in} is the on-site atomic Stoner field (exchange field) in the HF approximation, and μ is the chemical potential. The Stoner exchange field is introduced as the test for the ferromagnetic transition, which will take place when the value of F_{in} calculated numerically drops to zero. In the many-body considerations presented later, the term $\mu + F_{\text{in}}n_{\sigma}$ will be absent, since it will be moved into the Fermi-Dirac statistics. Quantity t_{ij} is the hopping integral between the ith and jth lattice site and T_0 is the Bloch band center of gravity.[2]

To analyze Hamiltonian (1), we use the equation of motion for the Green's functions in Zubarev notation,[44]

$$\varepsilon\langle\langle A;B\rangle\rangle_{\varepsilon} = \langle [A,B]_{+}\rangle + \langle\langle [A,H]_{-};B\rangle\rangle_{\varepsilon}, \tag{2}$$

where A and B are the fermion operators.

Using Hamiltonian (1) in Eq. (2), we can find the following equation for the Green's function $\langle\langle c_{i\sigma};c_{j\sigma}^{+}\rangle\rangle_{\varepsilon}$:

$$\varepsilon\langle\langle c_{i\sigma};c_{j\sigma}^{+}\rangle\rangle_{\varepsilon} = \delta_{ij} + T_0\langle\langle c_{i\sigma};c_{j\sigma}^{+}\rangle\rangle_{\varepsilon} - \sum_{l} t_{il}\langle\langle c_{l\sigma};c_{j\sigma}^{+}\rangle\rangle_{\varepsilon} + U\langle\langle \hat{n}_{i-\sigma}c_{i\sigma};c_{j\sigma}^{+}\rangle\rangle_{\varepsilon} + \sum_{l}\Delta t_{il}\langle\langle(\hat{n}_{i-\sigma}+\hat{n}_{l-\sigma})c_{l\sigma};c_{j\sigma}^{+}\rangle\rangle_{\varepsilon} + \sum_{l}\Delta t_{il}\langle\langle(c_{i-\sigma}^{+}c_{l-\sigma}+c_{l-\sigma}^{+}c_{i-\sigma})c_{i\sigma};c_{j\sigma}^{+}\rangle\rangle_{\varepsilon}. \tag{3}$$

The equations of motion for functions $\langle\langle \hat{n}_{i-\sigma} c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon$ and $\langle\langle \hat{n}_{l-\sigma} c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon$ have the form

$$\begin{aligned}\varepsilon\langle\langle \hat{n}_{i-\sigma} c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon &= n_{-\sigma}\delta_{ij} + T_0\langle\langle \hat{n}_{i-\sigma} c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon + U\langle\langle \hat{n}_{i-\sigma} c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon - \sum_l t_{il}\langle\langle \hat{n}_{i-\sigma} c_{l\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon \\ &\quad - \sum_l t_{il}\langle\langle (c^+_{i-\sigma}c_{l-\sigma} - c^+_{l-\sigma}c_{i-\sigma})c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon + \sum_l \Delta t_{il}\langle\langle \hat{n}_{i-\sigma}(\hat{n}_{i-\sigma} + \hat{n}_{l-\sigma})c_{l\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon \\ &\quad + \sum_l \Delta t_{il}\langle\langle \hat{n}_{i-\sigma}(c^+_{i-\sigma}c_{l-\sigma} + c^+_{l-\sigma}c_{i-\sigma})c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon + \sum_l \Delta t_{il}\langle\langle (\hat{n}_{i\sigma} + \hat{n}_{l\sigma})(c^+_{i-\sigma}c_{l-\sigma} - c^+_{l-\sigma}c_{i-\sigma})c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon\end{aligned} \tag{4}$$

and

$$\begin{aligned}&\varepsilon\langle\langle \hat{n}_{l-\sigma} c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon \\ &\quad = n_{-\sigma}\delta_{ij} + T_0\langle\langle \hat{n}_{l-\sigma} c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon + U\langle\langle \hat{n}_{l-\sigma}\hat{n}_{i-\sigma} c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon - \sum_m t_{im}\langle\langle \hat{n}_{l-\sigma} c_{m\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon \\ &\quad - \sum_m t_{lm}\langle\langle (c^+_{l-\sigma}c_{m-\sigma} - c^+_{m-\sigma}c_{l-\sigma})c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon + \sum_m \Delta t_{im}\langle\langle \hat{n}_{l-\sigma}(\hat{n}_{i-\sigma} + \hat{n}_{m-\sigma})c_{m\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon \\ &\quad + \sum_m \Delta t_{im}\langle\langle \hat{n}_{l-\sigma}(c^+_{i-\sigma}c_{m-\sigma} + c^+_{m-\sigma}c_{i-\sigma})c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon + \sum_m \Delta t_{lm}\langle\langle (\hat{n}_{l\sigma} + \hat{n}_{m\sigma})(c^+_{l-\sigma}c_{m-\sigma} - c^+_{m-\sigma}c_{l-\sigma})c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon.\end{aligned} \tag{5}$$

The notation of $\hat{n}^\alpha_{i\sigma}$, n^α_σ, and ε_α follows the original Hubbard paper,[2] and that for the hopping interaction is the following: $\Delta t^+_{il} = \Delta t_{il}$ and $\Delta t^-_{il} = 0$.

Following Hubbard,[2] we can express the single-electron Green's function as

$$\langle\langle c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon = \sum_{\alpha=\pm} \left\langle\left\langle \hat{n}^\alpha_{i-\sigma} c_{i\sigma}; c^+_{j\sigma}\right\rangle\right\rangle_\varepsilon, \tag{6}$$

where the higher-order Green's function in the energy representation $\langle\langle \hat{n}^\alpha_{i-\sigma} c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon$ ($\alpha = \pm$) fulfills the equation

$$\begin{aligned}\varepsilon\left\langle\left\langle \hat{n}^\alpha_{i-\sigma} c_{i\sigma}; c^+_{j\sigma}\right\rangle\right\rangle_\varepsilon &= n^\alpha_{-\sigma}\left(\delta_{ij} - \sum_l t_{il}\langle\langle c_{l\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon\right) + \varepsilon_\alpha\left\langle\left\langle \hat{n}^\alpha_{i-\sigma} c_{i\sigma}; c^+_{j\sigma}\right\rangle\right\rangle_\varepsilon - \sum_l t_{il}\left\langle\left\langle \left(\hat{n}^\alpha_{i-\sigma} - n^\alpha_{-\sigma}\right)c_{l\sigma}; c^+_{j\sigma}\right\rangle\right\rangle_\varepsilon \\ &\quad - \xi_\alpha \sum_l t_{il}\langle\langle (c^+_{i-\sigma}c_{l-\sigma} - c^+_{l-\sigma}c_{i-\sigma})c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon + \sum_l\sum_{\beta=\pm}\left(\Delta t^\alpha_{il} + \Delta t^\beta_{il}\right)\left\langle\left\langle \left(\hat{n}^\alpha_{i-\sigma} - n^\alpha_{-\sigma}\right)\hat{n}^\beta_{l-\sigma} c_{l\sigma}; c^+_{j\sigma}\right\rangle\right\rangle_\varepsilon \\ &\quad + n^\alpha_{-\sigma}\sum_l\sum_{\beta=\pm}\left(\Delta t^\alpha_{il} + \Delta t^\beta_{il}\right)\left\langle\left\langle \hat{n}^\beta_{l-\sigma} c_{l\sigma}; c^+_{j\sigma}\right\rangle\right\rangle_\varepsilon + \sum_l \Delta t_{il}\left\langle\left\langle \hat{n}^\alpha_{i-\sigma}(c^+_{i-\sigma}c_{l-\sigma} + c^+_{l-\sigma}c_{i-\sigma})c_{i\sigma}; c^+_{j\sigma}\right\rangle\right\rangle_\varepsilon \\ &\quad + \xi_\alpha \sum_l \Delta t_{il}\langle\langle (\hat{n}_{i\sigma} + \hat{n}_{l\sigma})(c^+_{i-\sigma}c_{l-\sigma} - c^+_{l-\sigma}c_{i-\sigma})c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon.\end{aligned} \tag{7}$$

In a further analysis of Eq. (7), we follow the Hubbard III approach[2] and reduce Green's functions of the higher order appearing in the third, fourth, fifth, seventh, and eighth terms to Green's functions of the type $\langle\langle \hat{n}^\alpha_{i-\sigma} c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon$ and $\langle\langle c_{i\sigma}; c^+_{j\sigma}\rangle\rangle_\varepsilon$. The third and fifth terms are approximated in this way in Appendix A, and the fourth and eighth terms are approximated in Appendix B. In the course of performing these approximations, we keep the intersite averages of the type $\langle c^+_{i-\sigma} c_{j-\sigma}\rangle$ and $\langle \hat{n}_{i\sigma} c^+_{i-\sigma} c_{j-\sigma}\rangle$. This is the main difference between this paper and Hubbard's approach. For the seventh term, responsible for the hopping interaction, we use the same type of approximation, namely

$$\begin{aligned}&\sum_l \Delta t_{il}\left\langle\left\langle \hat{n}^\alpha_{i-\sigma}(c^+_{i-\sigma}c_{l-\sigma} + c^+_{l-\sigma}c_{i-\sigma})c_{i\sigma}; c^+_{j\sigma}\right\rangle\right\rangle_\varepsilon \\ &\quad \approx \sum_l \Delta t_{il}\langle c^+_{i-\sigma}c_{l-\sigma} + c^+_{l-\sigma}c_{i-\sigma}\rangle\left\langle\left\langle \hat{n}^\alpha_{i-\sigma} c_{i\sigma}; c^+_{j\sigma}\right\rangle\right\rangle_\varepsilon \\ &\quad = S^{\Delta t}_\sigma\left\langle\left\langle \hat{n}^\alpha_{i-\sigma} c_{i\sigma}; c^+_{j\sigma}\right\rangle\right\rangle_\varepsilon.\end{aligned} \tag{8}$$

The parameter $S^{\Delta t}_\sigma$ is the spin-dependent band shift created by the hopping interaction,

$$S^{\Delta t}_\sigma = \sum_l \Delta t_{il}\langle c^+_{i-\sigma}c_{l-\sigma} + c^+_{l-\sigma}c_{i-\sigma}\rangle = 2\gamma^+ I_{-\sigma}, \tag{9}$$

where $I_{-\sigma}$ is the intersite correlation parameter and $\gamma^\pm$ is the hopping interaction parameter defined as

$$I_{-\sigma} = \frac{1}{N}\sum_{il} t_{il}\langle c^+_{i-\sigma}c_{l-\sigma}\rangle, \quad \gamma^+ \equiv \gamma = \frac{\Delta t_{ij}}{t_{ij}}, \quad \gamma^- = 0. \tag{10}$$

As a result, we obtain the equation

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

$$
\begin{aligned}
&- \sum_l t_{il}\langle\langle(\hat{n}^{\alpha}_{i-\sigma} - n^{\alpha}_{-\sigma})c_{l\sigma};c^{+}_{j\sigma}\rangle\rangle_\varepsilon \\
&- \xi_\alpha \sum_l t_{il}\langle\langle(c^{+}_{i-\sigma}c_{l-\sigma} - c^{+}_{l-\sigma}c_{i-\sigma})c_{i\sigma};c^{+}_{j\sigma}\rangle\rangle_\varepsilon \\
&+ \sum_l \sum_{\beta=\pm}(\Delta t^{\alpha}_{il} + \Delta t^{\beta}_{il})\langle\langle(\hat{n}^{\alpha}_{i-\sigma} - n^{\alpha}_{-\sigma})\hat{n}^{\beta}_{l-\sigma}c_{l\sigma};c^{+}_{j\sigma}\rangle\rangle_\varepsilon \\
&+ n^{\alpha}_{-\sigma}\sum_l \sum_{\beta=\pm}(\Delta t^{\alpha}_{il} + \Delta t^{\beta}_{il})\langle\langle\hat{n}^{\beta}_{l-\sigma}c_{l\sigma};c^{+}_{j\sigma}\rangle\rangle_\varepsilon + \xi_\alpha\sum_l \Delta t_{il} \\
&\times \langle\langle(\hat{n}_{i\sigma} + \hat{n}_{l\sigma})(c^{+}_{i-\sigma}c_{l-\sigma} - c^{+}_{l-\sigma}c_{i-\sigma})c_{i\sigma};c^{+}_{j\sigma}\rangle\rangle_\varepsilon. \quad (11)
\end{aligned}
$$

In further investigations, we will use the notation $\varepsilon' = \varepsilon - S^{\Delta t}_{\sigma}$.

Analysis of this equation will proceed along the lines of the Hubbard III approximation[2] with intersite correlation included in the way developed in our previous paper.[37]

In Eq. (11), there are terms coming from the commutator $[c_{i\sigma},H]_-$. These are the second, third, fifth, and the sixth terms in Eq. (11). They lead to what is known as the "scattering correction." The fourth and last terms, which come from the commutator $[\hat{n}_{i\sigma},H]_-$, give the "resonance broadening" effect.

The difference with our previous paper[37] is the presence of additional interaction Δt_{il}. This interaction enriches the scattering correction and the resonance broadening correction terms.

The scattering correction term is expressed by the Green's functions $\langle\langle(\hat{n}^{\alpha}_{i-\sigma} - n^{\alpha}_{-\sigma})c_{l\sigma};c^{+}_{j\sigma}\rangle\rangle_\varepsilon$ and $\langle\langle(\hat{n}^{\alpha}_{i-\sigma} - n^{\alpha}_{-\sigma})\hat{n}^{\beta}_{l-\sigma}c_{l\sigma};c^{+}_{j\sigma}\rangle\rangle_\varepsilon$, which are given by Eqs. (A3) and (A6) in Appendix A.

As mentioned earlier, the fourth and last (seventh) terms in Eq. (11), which come from the commutator $[\hat{n}_{i\sigma},H]_-$, give the "resonance broadening" effect. The functions $\langle\langle c^{\pm}_{l-\sigma}c^{\mp}_{i-\sigma}c_{i\sigma};c^{+}_{j\sigma}\rangle\rangle_\varepsilon$, $\langle\langle\hat{n}_{l\sigma}c^{\pm}_{l-\sigma}c^{\mp}_{i-\sigma}c_{i\sigma};c^{+}_{j\sigma}\rangle\rangle_\varepsilon$, and $\langle\langle\hat{n}_{i\sigma}c^{\pm}_{l-\sigma}c^{\mp}_{i-\sigma}c_{i\sigma};c^{+}_{j\sigma}\rangle\rangle_\varepsilon$, appearing in those terms, are found in Appendix B as Eqs. (B3), (B4), and (B7).

Now we insert the functions appearing in the scattering correction and resonance broadening correction from Appendixes A and B into Eq. (11). Further analysis does not include any additional approximations. Equation (11) is solved directly in the momentum space in Appendix C. From Eqs. (C7) and (C8) of Appendix C, we obtain the final relation for the Green's function $G^{\sigma}_{\mathbf{k}}(\varepsilon)$,

$$G^{\sigma}_{\mathbf{k}}(\varepsilon) = \frac{1}{\varepsilon - \Sigma^{\sigma}_{\mathrm{tot},\mathbf{k}}(\varepsilon) - (\varepsilon_{\mathbf{k}} - T_0)}, \quad (12)$$

where the self-energy $\Sigma^{\sigma}_{\mathrm{tot},\mathbf{k}}(\varepsilon)$ is the sum of the **k**-independent term $\Sigma^{\sigma}_{0}(\varepsilon)$ and the **k**-dependent term $\Sigma^{\sigma}_{1,\mathbf{k}}(\varepsilon)$,

$$\Sigma^{\sigma}_{\mathrm{tot},\mathbf{k}}(\varepsilon) = \Sigma^{\sigma}_{0}(\varepsilon) + \Sigma^{\sigma}_{1,\mathbf{k}}(\varepsilon), \quad (13)$$

which are given by

$$\Sigma^{\sigma}_{0}(\varepsilon) = n^{+}_{-\sigma}\varepsilon_{+} + n^{-}_{-\sigma}\varepsilon_{-} + S^{\Delta t}_{\sigma} + \frac{[n^{-}_{-\sigma}n^{+}_{-\sigma}(\varepsilon_{+} - \varepsilon_{-}) + S^{B}_{\sigma}(\varepsilon')][\varepsilon_{+} - \varepsilon_{-} - \Omega^{+}_{\sigma}(\varepsilon') + \Omega^{-}_{\sigma}(\varepsilon')]}{\varepsilon - S^{\Delta t}_{\sigma} - \Omega^{\mathrm{tot}}_{\sigma}(\varepsilon') - \{n^{+}_{-\sigma}[\varepsilon_{-} - \Omega^{-}_{\sigma}(\varepsilon')] + n^{-}_{-\sigma}[\varepsilon_{+} - \Omega^{+}_{\sigma}(\varepsilon')]\}} \quad (14)$$

and

$$\Sigma^{\sigma}_{1,\mathbf{k}}(\varepsilon) \equiv \gamma(\varepsilon_{\mathbf{k}} - T_0)\left\{\frac{S^{B}_{\sigma}(\varepsilon') - n^{+}_{-\sigma}n^{-}_{-\sigma}[2(\varepsilon_{+} - \varepsilon_{-}) - \Omega^{+}_{\sigma}(\varepsilon') + \Omega^{-}_{\sigma}(\varepsilon') - \gamma(\varepsilon_{\mathbf{k}} - T_0)]}{\varepsilon - S^{\Delta t}_{\sigma} - \Omega^{\mathrm{tot}}_{\sigma}(\varepsilon') - \{n^{+}_{-\sigma}[\varepsilon_{-} - \Omega^{-}_{\sigma}(\varepsilon')] + n^{-}_{-\sigma}[\varepsilon_{+} - \Omega^{+}_{\sigma}(\varepsilon')]\}} - 2n^{+}_{-\sigma}\right\}. \quad (15)$$

The **k**-dependent term $\Sigma^{\sigma}_{1,\mathbf{k}}(\varepsilon)$ is proportional to the hopping interaction and vanishes at $\Delta t \to 0$.

III. FERROMAGNETIC SOLUTION

To analyze the possibility of a ferromagnetic transition, we will use two coupled equations for electron number and magnetization,

$$n = n_{\uparrow} + n_{\downarrow}, \quad m = n_{\uparrow} - n_{\downarrow}, \quad (16)$$

where $n_{\pm\sigma}$ are given by

$$n_{\sigma} = \frac{1}{N}\sum_{\mathbf{k}}\int_{-\infty}^{\infty} S^{\sigma}_{\mathbf{k}}(\varepsilon)f_{\sigma}(\varepsilon)d\varepsilon, \quad (17)$$

where $S^{\sigma}_{\mathbf{k}}(\varepsilon)$ is the spectral density and $f_{\sigma}(\varepsilon)$ is the Fermi function with the exchange field $F_{\mathrm{in}}n_{\sigma}$ coming from the last term in the Hamiltonian (1),

$$
\begin{aligned}
S^{\sigma}_{\mathbf{k}}(\varepsilon) &= -\frac{1}{\pi}\mathrm{Im}G^{\sigma}_{\mathbf{k}}(\varepsilon), \\
f_{\sigma}(\varepsilon) &= \frac{1}{1 + \exp[(\varepsilon - \mu - F_{\mathrm{in}}n_{\sigma})/k_B T]}.
\end{aligned} \quad (18)
$$

The spectral density function depends on the intersite correlation functions I_{σ} and $\langle\hat{n}_{l\sigma}c^{+}_{l-\sigma}c_{i-\sigma}\rangle$. Parameter I_{σ} defined by Eq. (10) after transforming to momentum space can be written as

$$I_{\sigma} = -\frac{1}{N}\sum_{\mathbf{k}}(\varepsilon_{\mathbf{k}} - T_0)\int_{-\infty}^{\infty} S^{\sigma}_{\mathbf{k}}(\varepsilon)f_{\sigma}(\varepsilon)d\varepsilon. \quad (19)$$

The average $\langle\hat{n}_{l\sigma}c^{+}_{l-\sigma}c_{i-\sigma}\rangle$ is calculated using the commutator $[H,c^{+}_{l-\sigma}]_-$ (as in Ref. 42), which in the case of our Hamiltonian (1) leads to the expression

$$
\begin{aligned}
\langle\hat{n}_{l\sigma}c^{+}_{l-\sigma}c_{i-\sigma}\rangle = \frac{1}{U}\Bigg\{&\langle[H,c^{+}_{l-\sigma}]_-c_{i-\sigma}\rangle - T_0\langle c^{+}_{l-\sigma}c_{i-\sigma}\rangle + \sum_m t_{lm}\langle c^{+}_{m-\sigma}c_{i-\sigma}\rangle \\
&- \sum_m \Delta t_{lm}[\langle\hat{n}_{l\sigma}c^{+}_{m-\sigma}c_{i-\sigma}\rangle + \langle\hat{n}_{m\sigma}c^{+}_{m-\sigma}c_{i-\sigma}\rangle + \langle c^{+}_{l\sigma}c_{m\sigma}c^{+}_{l-\sigma}c_{i-\sigma}\rangle + \langle c^{+}_{m\sigma}c_{l\sigma}c^{+}_{l-\sigma}c_{i-\sigma}\rangle]\Bigg\}. \quad (20)
\end{aligned}
$$

The four operators' averages appearing in the preceding term of the hopping interaction are new with respect to Ref. 42. The importance of this interaction was pointed out in the HF approximation by Refs. 16 and 17. The averages present in the Δt interaction term are of a higher level with respect to the averages preceding them in Eq. (20); therefore, we could approximate them as follows:

$$\langle \hat{n}_{l\sigma} c^{+}_{m-\sigma} c_{i-\sigma}\rangle \approx n_{\sigma} \langle c^{+}_{m-\sigma} c_{i-\sigma}\rangle, \quad \langle \hat{n}_{m\sigma} c^{+}_{m-\sigma} c_{i-\sigma}\rangle \approx n_{\sigma} \langle c^{+}_{m-\sigma} c_{i-\sigma}\rangle,$$
$$\langle c^{+}_{l\sigma} c_{m\sigma} c^{+}_{l-\sigma} c_{i-\sigma}\rangle \approx \langle c^{+}_{l\sigma} c_{m\sigma}\rangle \langle c^{+}_{l-\sigma} c_{i-\sigma}\rangle, \quad \langle c^{+}_{m\sigma} c_{l\sigma} c^{+}_{l-\sigma} c_{i-\sigma}\rangle \approx \langle c^{+}_{m\sigma} c_{l\sigma}\rangle \langle c^{+}_{l-\sigma} c_{i-\sigma}\rangle. \tag{21}$$

Using Eqs. (21) in Eq. (20), we can write that

$$\frac{1}{N}\sum_{li}(-t_{li})\langle \hat{n}_{l\sigma} c^{+}_{l-\sigma} c_{i-\sigma}\rangle = \frac{1}{U}\left\{\frac{1}{N}\sum_{li}(-t_{li})\langle [H,c^{+}_{l-\sigma}]_{-} c_{i-\sigma}\rangle + \frac{T_0}{N}\sum_{li} t_{li}\langle c^{+}_{l-\sigma} c_{i-\sigma}\rangle - \frac{1}{N}\sum_{ilm} t_{li}(t_{lm} - \Delta t_{lm} 2n_{\sigma})\langle c^{+}_{m-\sigma} c_{i-\sigma}\rangle \right.$$
$$\left. + \frac{1}{N}\sum_{ilm} t_{li}\Delta t_{lm}(\langle c^{+}_{l\sigma} c_{m\sigma}\rangle + \langle c^{+}_{m\sigma} c_{l\sigma}\rangle)\langle c^{+}_{l-\sigma} c_{i-\sigma}\rangle \right\}. \tag{22}$$

From the Green's-function equation of motion (2) and the Zubarev relation,[44]

$$\langle [H,c^{+}_{l-\sigma}]_{-} c_{i-\sigma}\rangle = -\frac{1}{\pi}\int_{-\infty}^{\infty} \mathrm{Im}\langle\langle c_{i-\sigma};[H,c^{+}_{l-\sigma}]_{-}\rangle\rangle_{\varepsilon} f_{-\sigma}(\varepsilon) d\varepsilon, \tag{23}$$

we obtain

$$\frac{1}{N}\sum_{il}(-t_{li})\langle [H,c^{+}_{l-\sigma}]_{-} c_{i-\sigma}\rangle = \frac{1}{N}\sum_{\mathbf{k}}(\varepsilon_{\mathbf{k}} - T_0)\int_{-\infty}^{\infty} \varepsilon S^{-\sigma}_{\mathbf{k}}(\varepsilon) f_{-\sigma}(\varepsilon) d\varepsilon. \tag{24}$$

The second term in Eq. (22) has the following form:

$$\frac{T_0}{N}\sum_{li} t_{li}\langle c^{+}_{l-\sigma} c_{i-\sigma}\rangle = T_0 I_{-\sigma}. \tag{25}$$

The third term in Eq. (22) can be written as

$$\frac{1}{N}\sum_{ilm} t_{li}(t_{lm} - \Delta t_{lm} 2n_{\sigma})\langle c^{+}_{m-\sigma} c_{i-\sigma}\rangle = (1 - 2\gamma n_{\sigma})\frac{1}{N}\sum_{\mathbf{k}}(\varepsilon_{\mathbf{k}} - T_0)^2\int_{-\infty}^{\infty} S^{-\sigma}_{\mathbf{k}}(\varepsilon) f_{-\sigma}(\varepsilon) d\varepsilon, \tag{26}$$

and the fourth term is given by

$$\frac{1}{N}\sum_{ilm} t_{li}\Delta t_{lm}(\langle c^{+}_{l\sigma} c_{m\sigma}\rangle + \langle c^{+}_{m\sigma} c_{l\sigma}\rangle)\langle c^{+}_{l-\sigma} c_{i-\sigma}\rangle = -2\gamma I_{\sigma} I_{-\sigma}. \tag{27}$$

Using the preceding results in Eq. (C5), we obtain

$$S^{B}_{\sigma}(\varepsilon') = \left\{\frac{2-\gamma}{U}\frac{1}{N}\sum_{\mathbf{k}}(\varepsilon_{\mathbf{k}} - T_0)\int_{-\infty}^{\infty}[\varepsilon - (1 - 2\gamma n_{\sigma}) \times (\varepsilon_{\mathbf{k}} - T_0)] S^{-\sigma}_{\mathbf{k}}(\varepsilon) f_{-\sigma}(\varepsilon) d\varepsilon + \left[\frac{2-\gamma}{U}(T_0 - 2\gamma I_{\sigma}) + 1\right] I_{-\sigma}\right\} F^{\sigma}_{H,0}(\varepsilon') C(\varepsilon'). \tag{28}$$

To calculate numerically the value of expressions (17), (19), and (28), we will use the relation

$$\frac{1}{N}\sum_{\mathbf{k}} f_k(\varepsilon) = \int_{-\infty}^{\infty} \rho_0(\varepsilon_0) f(\varepsilon,\varepsilon_0) d\varepsilon_0, \tag{29}$$

where $\rho_0(\varepsilon)$ is the initial DOS.

For the initial DOS, we will assume the formula

$$\rho_0(\varepsilon) = \frac{1 + \sqrt{1 - a_1^2}}{\pi D}\frac{\sqrt{D^2 - \varepsilon^2}}{D + a_1\varepsilon}, \tag{30}$$

with the asymmetry parameter a_1 varying continuously from $a_1 = 0$ corresponding to a symmetric semielliptic band (or Bethe lattice) to $a_1 \approx 1$ corresponding to the fcc lattice[15] [see Fig. 1(a)].

Another DOS that will be used has the form

$$\rho_0(\varepsilon) = \frac{C(a_2)}{D}\frac{\sqrt{D^2 - \varepsilon^2}}{D + a_2(|\varepsilon| - D)},$$
$$C(a_2) = \frac{a_2/2}{1 + \frac{(a_2-1)\pi}{2a_2} + \frac{\sqrt{2a_2-1}}{a_2}\log\frac{1-a_2}{\sqrt{2a_2-1}+a_2}}, \tag{31}$$

which for $a_2 = 0$ is again the semielliptic DOS, and for $a_2 \to 1$ has a strong singularity at the center ($\varepsilon = 0$) resembling the bcc DOS [see Fig. 1(b)].

The preceding two types of DOS are used in this paper because at $a_1,a_2 \to 1$ they represent $3d$ transition magnetic elements, which have fcc or bcc crystal structures. They both have a strong peak within the DOS, and the fcc-type DOS has, in addition, a strong asymmetry-helping ferromagnetism.[15]

IV. NUMERICAL RESULTS

We apply the formalism developed here to analyze the magnetic ordering in the electron bands with symmetrical DOS, that is, the semielliptic DOS given by Eq. (30) with $a_1 = 0$, or the bcc-like DOS given by Eq. (31) with $a_2 \neq 0$, and also in the electron bands with the asymmetric fcc-like DOS where the maximum density is shifted toward their edge [Eq. (30) with $a_1 \neq 0$]. Our main test of the ferromagnetic transition is a condition for the value of the critical on-site exchange field $F^{\mathrm{cr}}_{\mathrm{in}}$ to drop to zero. In general, it is enough

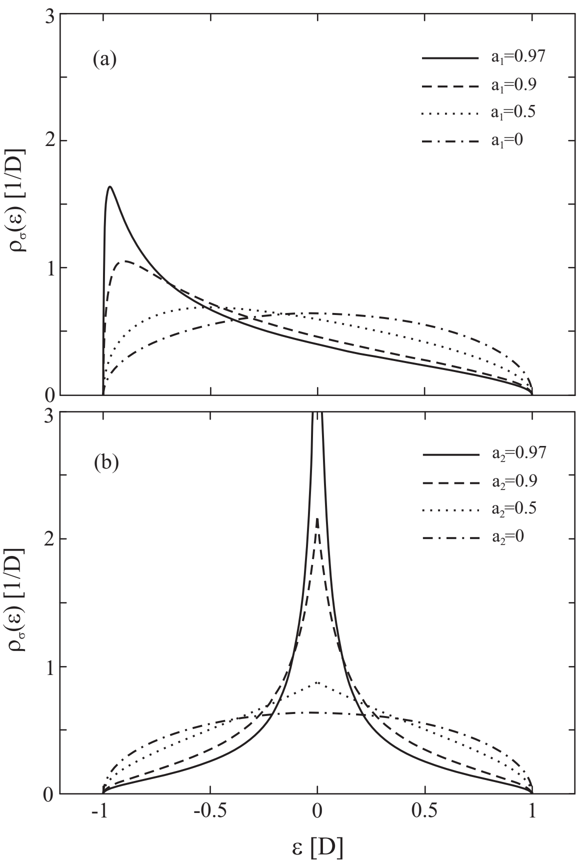

FIG. 1. Model densities of states given by Eq. (30) (a) and Eq. (31) (b) shown for different values of parameters a_1 and a_2.

for ferromagnetism to have $F_{\rm in}^{\rm cr} < F_{\rm in}$, where $F_{\rm in}$ is the constant set by the material, but in this paper we impose the rather rigorous condition for $F_{\rm in}$ to be zero. The critical $F_{\rm in}^{\rm cr}$ is calculated from equations for electron concentration and magnetization [Eqs. (16) and (17)] in the limit of $m \to 0$.

In Fig. 2, we present the dependence of $F_{\rm in}^{\rm cr}$ on electron concentration for the symmetrical semielliptic DOS ($a_1 = 0$) in the strong correlation case $U = 15D$. We compare the cases of the Hubbard III scattering effect (CPA) and the Hubbard III full approximation (HIIIF) (with the resonance broadening effect included). Both cases are calculated with and without the intersite correlation. The effect of intersite kinetic correlation is reduced to zero when the lower Hubbard band is closed, $n = 1$. In general, the curves calculated by means of the scattering effect lie lower than those for the full approximation, which involves also the resonance broadening effect allowing for the $-\sigma$ electrons to move through the lattice. Apparently, the more self-consistency we add to the solution, the farther away we are from spontaneous ferromagnetism. The curves with added intersite correlation (overlooked in the original Hubbard solution) favor ferromagnetism, but do not create spontaneous magnetization without changing the DOS or adding the hopping interaction (see later in the paper).

In Fig. 3, we present the dependence of $F_{\rm in}^{\rm cr}$ on electron concentration for the same case of the symmetrical semielliptic DOS ($a_1 = 0$) and the strong correlation case $U = 15D$ as in

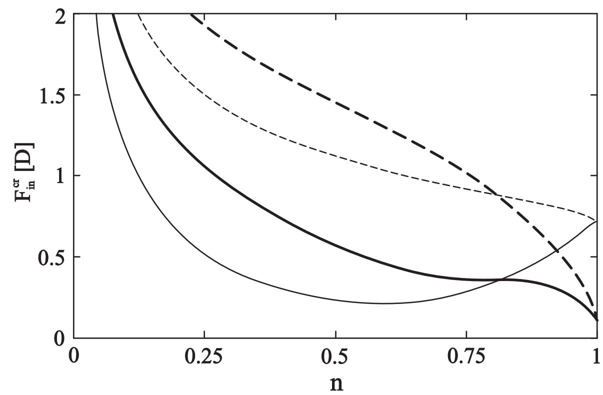

FIG. 2. Critical value of the on-site exchange interaction as a function of electron concentration calculated in the Hubbard III scattering effect approximation (CPA) with the intersite correlation (thin solid line) and without it (thin dashed line). The same curves calculated in the Hubbard III full approximation with the intersite correlation (thick solid line) and without it (thick dashed line). The semielliptic DOS is used. The Coulomb repulsion $U = 15D$, and the bandwidth $D = 1$ eV.

Fig. 2. We added the hopping interaction treated in the full Hubbard III approximation. The exchange field $F_{\rm in}^{\rm cr}$ required for ferromagnetism is strongly reduced under the influence of hopping interaction as compared to the result obtained from the same full Hubbard III approximation applied only to the on-site U interaction. The reduction of the exchange field $F_{\rm in}^{\rm cr}$ by the hopping interaction is not sufficient to drive the transition to the ferromagnetic state in this case of the semielliptic DOS, since this DOS is relatively flat and does not have strong peaks.

It has been shown within different approaches that the moderately strong peak in DOS enables ferromagnetism.[15,38–40] Therefore, in Fig. 4 we show the dependence $F_{\rm in}^{\rm cr}(n)$ for such a DOS described by Eq. (31). This symmetrical DOS has a peak in the center that grows with increasing parameter a_2 [see Fig. 1(b)] and it resembles the bcc DOS. Figure 4

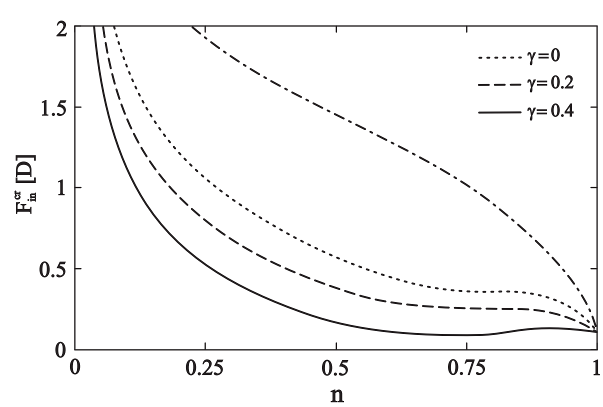

FIG. 3. Critical value of the on-site exchange interaction as a function of electron concentration calculated for the semielliptic DOS at different values of the hopping parameter γ. The Coulomb repulsion $U = 15D$ and the bandwidth $D = 1$ eV. The original Hubbard III solution (without the intersite correlation and without the hopping interaction) is shown as the dot-dashed line.

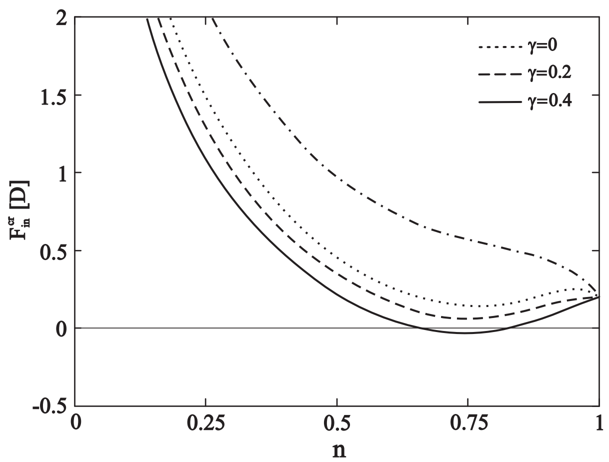

FIG. 4. Critical value of the on-site exchange interaction as a function of electron concentration calculated for the symmetrical DOS given by Eq. (31) with $a_2 = 0.9$, at different values of the hopping parameter γ. The Coulomb repulsion $U = 15D$ and the bandwidth $D = 1$ eV. The original Hubbard III solution (without the intersite correlation and without the hopping interaction) is shown for $a_2 = 0.9$ as the dot-dashed line.

shows that at $a_2 = 0.9$ and rather large $\gamma = 0.4$, we obtain spontaneous ferromagnetism. Minima of $F_{\rm in}^{\rm cr}$ correspond to electron concentrations at which the Fermi energy is localized close to the peak in the DOS.

Vollhardt and co-workers[15] postulated that the aforementioned peak in the DOS is particularly supportive for ferromagnetism when it is located away from the center of the band. Therefore, we performed numerical calculations for the asymmetric DOS of Eq. (30) resembling the fcc DOS, with $a_1 = 0.7$ and 0.9 [see Fig. 1(a)]. In Fig. 5, we present the dependence $F_{\rm in}^{\rm cr}(n)$ for this DOS. For the DOS with $a_1 = 0.7$, we obtain spontaneous ferromagnetism at rather high values of the hopping parameter $\gamma \sim 0.4$ and electron concentrations around $n \approx 0.6$. The ferromagnetism exists in a much broader range of electron concentrations in the case of larger asymmetry ($a_1 = 0.9$). The symmetrical DOS with the strong peak did not bring the ferromagnetism in such a broad range of electron concentrations (see Fig. 4).

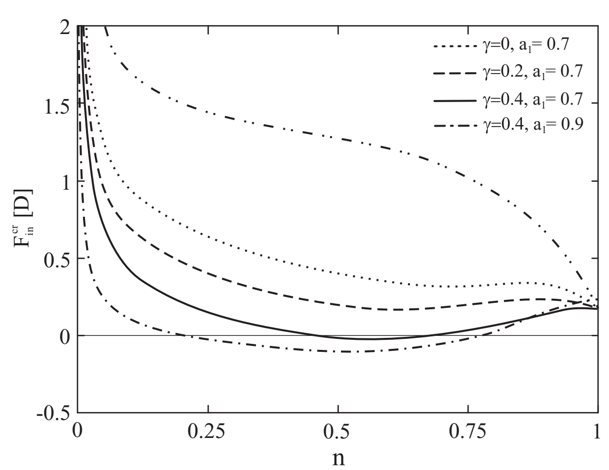

FIG. 5. Critical value of the on-site exchange interaction as a function of electron concentration calculated for the asymmetric DOS given by Eq. (30) with $a_1 = 0.7$ or 0.9, and for different values of the hopping parameter γ. The Coulomb repulsion $U = 15D$ and the bandwidth $D = 1$ eV. The original Hubbard III solution (without the intersite correlation and without the hopping interaction) is shown for $a_1 = 0.7$as the double dot-dashed line.

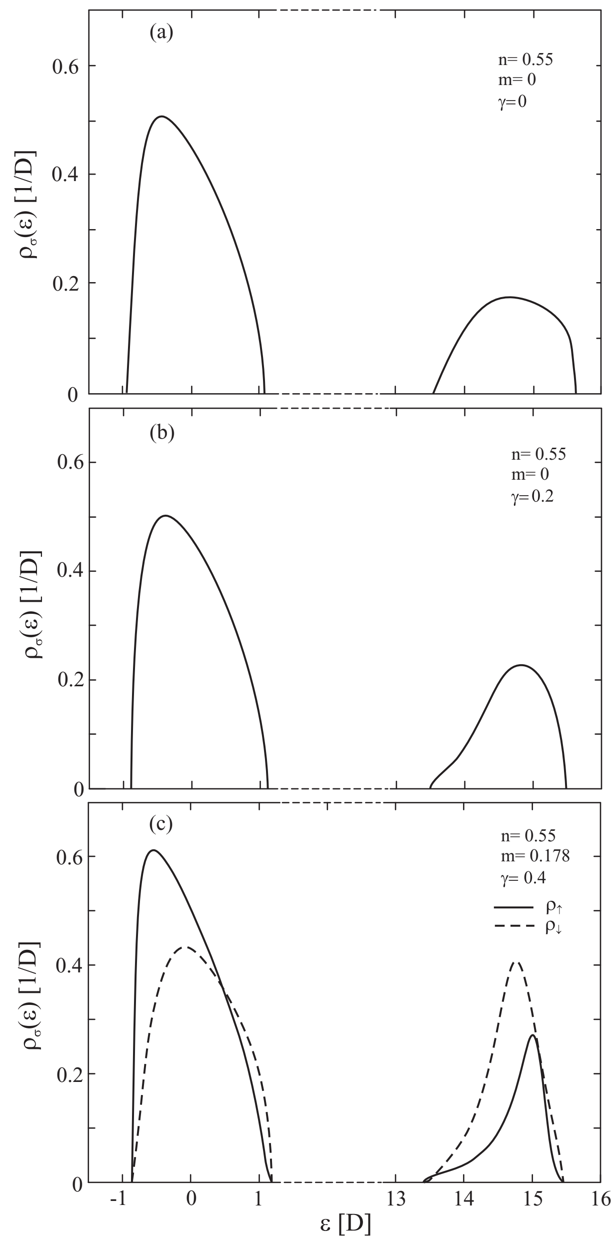

FIG. 6. Quasiparticle density of states as a function of energy for different values of the hopping parameter γ. In the calculations, we have used the asymmetric DOS with $a_1 = 0.7$. Other parameters are $U = 15D$ and $D = 1$ eV. Part (c) shows the magnetic solution.

In Fig. 6, we show the quasiparticle DOS as a function of energy for different values of the hopping parameter γ. The results show that after taking into account both the scattering and the resonance broadening corrections, the bandwidths of the lower and upper bands are equal to each other at any U. At $U \gg D$, we obtain two quasiparticle bands, with widths only slightly reduced with respect to the initial bandwidth of $2D$. This is in contradiction to the well-known result of the scattering correction or the CPA, where the bandwidth of the lower σ band was $2D(1-n_{-\sigma})^{1/2}$ and that of the upper band was $2Dn_{-\sigma}^{1/2}$. The capacities of the lower and upper σ band are still $1-n_{-\sigma}$ and $n_{-\sigma}$, as in the CPA theory. In the case of ferromagnetic ordering, the effective bandwidth is the same for spins $\uparrow$ and $\downarrow$ [Fig. 6(a)]. It is also distinct to the case of scattering correction, where for $m \neq 0$, bands with different spins had unequal widths given by the previous expressions.

In our model, the width of the spin bands does not depend on the strength of the hopping interaction. This interaction changes the shape of the upper band. The shape of the lower band does not depend on the value of the hopping interaction, but rather on the carrier concentration. This behavior is characteristic of the full Hubbard III approximation. In this approximation, the resonance broadening effect causes the dependence of Σ^{σ} self-energy on the itinerancy of $-\sigma$ electrons through the self-energy $\Sigma^{-\sigma}$. Such a result goes against the intuitive but crude HF approximation,[33] in which it is clear that the intersite hopping interaction brings both the bandwidth change and the spin-dependent band shift.

In our approach, the most essential factor for obtaining ferromagnetism is the shift of the average energy of the spin bands while their position remains unchanged. This shift is described by the factors $S_{\sigma}^{B}(\varepsilon')$ (depending on U) and $S_{\sigma}^{\Delta t}$ (depending on Δt) created by intersite correlation in the presence of the interactions mentioned earlier. In Fig. 7, we show the center of gravity of the bands for different spins for the lower and upper bands. They are defined as

$$T_{i\sigma} = \int_{\varepsilon_{\min,i}}^{\varepsilon_{\max,i}} \varepsilon \rho_{\sigma}^{i}(\varepsilon) d\varepsilon, \qquad (32)$$

where $i = 1,2$ stands for the lower and upper bands, respectively. Quantity $\rho_{\sigma}^{i}(\varepsilon)$ is the density of states in the ith band and $\varepsilon_{\min,i}$ ($\varepsilon_{\max,i}$) denotes the lower and upper boundary of the ith band.

In the lower band, both factors $S_{\sigma}^{B}(\varepsilon')$ and $S_{\sigma}^{\Delta t}$ shift the center of gravity toward higher energies. In the upper band, the effective shift of the mean energy is the result of competition between $S_{\sigma}^{B}(\varepsilon')$ and $S_{\sigma}^{\Delta t}$, and it is toward lower energy. At the transition to ferromagnetism ($m \neq 0$), the boundaries of the spin bands remain unchanged. The shift of the average

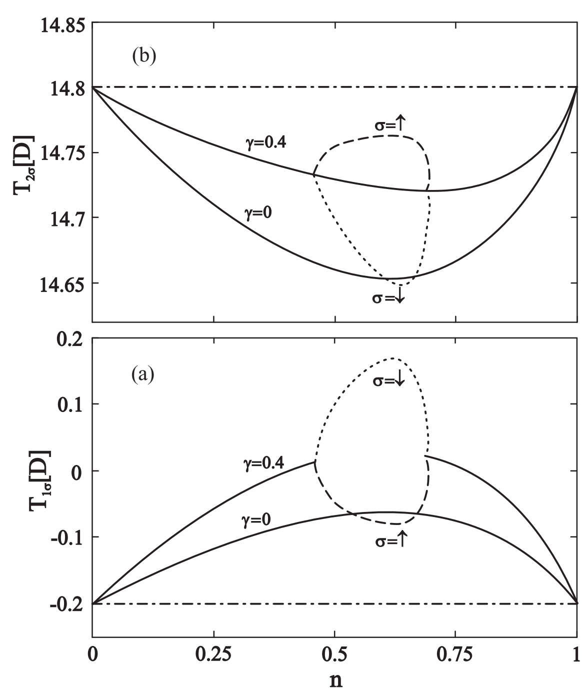

FIG. 7. Spin band center of gravity for different values of the hopping parameter γ. (a) The lower Hubbard band, (b) the upper Hubbard band. In calculations, the asymmetric DOS with $a_1 = 0.7$ was used. Other parameters are $U = 15D$ and $D = 1$ eV. The center for the original Hubbard III solution (without the intersite correlation) is shown as the dot-dashed line. In the magnetic state ($\gamma = 0.4$), the center of gravity is different for different spin directions (dotted and dashed lines).

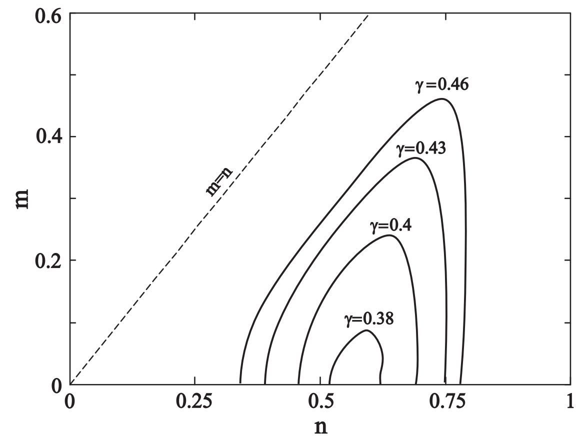

FIG. 8. Magnetization m as a function of band occupation n calculated for different values of the hopping parameter and for the asymmetric DOS [Eq. (30)] with $a_1 = 0.7$. Other parameters are $U = 15D$ and $D = 1$ eV. The dashed line is the line of the saturated ferromagnetism.

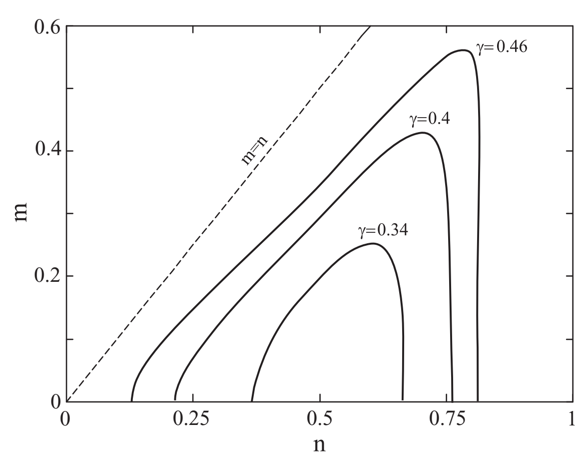

FIG. 9. Magnetization m as a function of band occupation n calculated for different values of the hopping parameter and for the asymmetric DOS [Eq. (30)] with $a_1 = 0.9$. Other parameters are $U = 15D$ and $D = 1$ eV. The dashed line is the line of the saturated ferromagnetism.

energy is caused by deformation of the density of states, unlike in the case of the conventional Stoner magnetism. Without this average energy shift, caused by the intersite correlations combined with the hopping interaction [see Eq. (9)], the ferromagnetic transition in this full Hubbard III approximation would be impossible.

In Fig. 8, we show the magnetic moment m as a function of band filling for the asymmetric DOS with $a_1 = 0.7$ and different values of the hopping parameter. It can be seen that the value of the magnetic moment is relatively low with respect to the saturation moment, $m_{\text{sat}} = n$. For concentrations higher than concentration corresponding to $m_{\max}$ [$n > n(m_{\max})$], we have two solutions for m at one concentration. This is the evidence of a first-order phase transition. For $n < n(m_{\max})$, there is only one solution and the transition is of second order. The same relation $m(n)$ is shown in Fig. 9 for the more asymmetric DOS with $a_1 = 0.9$. The spontaneous magnetization exists in a broader interval of electron occupations and for smaller values of the hopping interactions.

V. CONCLUSIONS

In this work, we have extended the classic Hubbard III approximation to include the intersite correlations and the hopping interaction. We have also changed the approximation from the CPA-like solution to the full Hubbard III scheme, taking into account the resonance broadening effect and allowing for the itinerancy of $-\sigma$ electrons. These changes have led to two noteworthy effects:

(i) Spin-dependent average band energy shift described by the parameters $S_\sigma^B(\varepsilon')$ and $S_\sigma^{\Delta t}$. This band shift is really a distortion of band shape, which leads to the change in the band center of gravity. It is expressed by the parameters $S_\sigma^B(\varepsilon')$ and $S_\sigma^{\Delta t}$, and is different for both spin bands in the ferromagnetic case. At the same time, despite the shift in the center of gravity, the bands' boundaries remain unchanged.

(ii) The wave-vector dependence of the self-energy $\Sigma_{1,\mathbf{k}}^\sigma(\varepsilon)$ created by the hopping interaction. This dependence causes shape distortion of both Hubbard bands. The DOS shape distortion for the lower band is smaller than that for the upper band. The hopping interaction, which changes the shape of the Hubbard bands, influences their widths only to a small degree.

In effect, the bandwidths in the full Hubbard III approximation remain almost constant. This result is in sharp contrast to the result of the scattering correction or the equivalent CPA approximation, where in the case of strong correlation, the on-site Coulomb interaction U alone changes the widths of the lower and upper Hubbard band to $2D(1 - n_{-\sigma})^{1/2}$ and $2Dn_{-\sigma}^{1/2}$, respectively.

We applied our model to the analysis of magnetic ordering in the system of interacting electrons. The numerical analysis has shown that including the intersite correlations and the hopping interaction reduces greatly the exchange field necessary for ferromagnetic ordering. In the systems with flat DOS such as the semielliptic DOS, the exchange field is not reduced to zero. In effect, the system does not undergo a spontaneous transition to ferromagnetism. The systems that contain even a moderately strong peak in the DOS may have this transition at some electron concentrations and at relatively high values of the hopping interaction. The main driving force for the magnetic transition is the shift in the centers of gravity of majority and minority spin bands produced by their distortion and described by the parameters $S_\sigma^B(\varepsilon')$ and $S_\sigma^{\Delta t}$. At the same time, the positions and widths of spin bands remain roughly unchanged. The wave-vector-dependent self-energy $\Sigma_{1,\mathbf{k}}^\sigma(\varepsilon)$ also does not change band boundaries. It causes band deformation different from the parameters $S_\sigma^B(\varepsilon')$ and $S_\sigma^{\Delta t}$. It raises the maximum of DOS, narrows it (especially the upper band), and at the same time leaves the band boundaries roughly unchanged. Such changes to the DOS help the ferromagnetic ordering, but the $\Sigma_{1,\mathbf{k}}^\sigma(\varepsilon)$ influence is not a key factor for ferromagnetic alignment. We have shown in our previous paper[37] that $\Sigma_{1,\mathbf{k}}^\sigma(\varepsilon)$, without the band shift caused by $S_\sigma^B(\varepsilon')$, does not cause the ferromagnetism for the fcc-type DOS. Herrmann and Nolting,[46] using the SDA approach in 3D, reached a similar conclusion. They showed that for the simple-cubic lattice, the full self-energy with the **k**-dependent part favors ferromagnetism more strongly than the local self-energy, but for the bcc and fcc lattices, the contribution of the **k**-dependent part of the self-energy to ferromagnetism is very small. Therefore, they recognized that with the increasing number of nearest neighbors, the importance of the **k**-dependent part of the self-energy decreases rapidly.

Momentum-dependent self-energy was also obtained in the cluster dynamical mean-field theory (CDMFT)[47] and the dynamical cluster approximation (DCA).[48,49] The DCA and CDMFT are two generalizations of the DMFT method to finite clusters that take into account short-range spatial correlations by adding the **k**-dependent term to the self-energy. These two methods were applied to the antiferromagnetic ordering and the d-wave pairing superconductivity (see, e.g., Ref. 50 and references therein) since this superconductivity shows a strong momentum dependence of the self-energy as inferred from photoemission experiments.[51] In the case of ferromagnetic ordering, the role of the k-dependent part of the self-energy within the DMFT method is still not clear. Using the LDA + DMFT model, Chioncel *et al.*[52] pointed out that the k-dependent part of the self-energy may not be the decisive factor for ferromagnetic alignment. This conclusion is in agreement with our present calculations, in which we have obtained the k-dependent part of the self-energy directly from the full Hubbard III solution, which included the intersite kinetic correlations.

In our previous paper,[37] we overestimated the ferromagnetic effect by using the set of CPA-like equations, although the intersite correlations were added in the Green's-function decoupling process. In this paper, we have used in analytical and numerical calculations the full Hubbard III solution, which includes the scattering and the resonance broadening effect. This is an improved approach, in which the $+\sigma$ electron moves in a sea of $-\sigma$ electrons defrozen by the resonance broadening effect [see Hubbard III, Eqs. (56)–(59)]. That sea of $-\sigma$ electrons was frozen in the CPA-like approach equivalent to the Hubbard III scattering correction [see his Eqs. (37)–(40)] used in our previous paper.[37]

This improved approach has weakened the ferromagnetic effect. The effect was brought back by the presence of the hopping interaction. The use of the hopping interaction Δt for ferromagnetism has a potential of removing a magnetic paradox that has persisted for a long time. It was shown within the mean-field approximation (Ref. 32) that the magnetic moment adjusted to the experimental value at low temperature by fitting the intersite interaction, Δt, will decrease with the temperature much faster than the moment adjusted by fitting the Stoner field. Therefore, the Curie temperature in the model with interaction Δt will be lower in comparison to the Stoner type of estimates and closer to the experimental value.[32] This decrease of T_C, together with the decrease by another intersite effect, namely the spin waves, will bring this temperature into agreement with the experimental value.

The metal-insulator transition could be analyzed along the lines of similar models,[53,54] but one should use the relatively small U comparable with half-bandwidth D. The importance of adding the hopping interaction for the metal-insulator phase transition was already stressed by Schiller,[55] who obtained the hopping interaction and the k-dependent single-particle self-energy in the simple Hubbard-like two-band model and used it for the metal-insulator transition.

In summary, this approach, which includes intersite correlations, enables ferromagnetism after taking into consideration the hopping interaction. This model, in which we have the k-dependent self-energy, may be used to analyze the other interesting phenomena existing in the strongly correlated electron systems (e.g., the metal-insulator transition in transition-metal compounds, superconductivity in high-temperature superconductors, the half-metallic ferromagnets, and heavy fermion substances).

APPENDIX A: SCATTERING EFFECT

The scattering effect is expressed by the functions $\langle\langle(\hat{n}^{\alpha}_{i-\sigma} - n^{\alpha}_{-\sigma})c_{l\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon}$ and $\langle\langle(\hat{n}^{\alpha}_{i-\sigma} - n^{\alpha}_{-\sigma})\hat{n}^{\beta}_{l-\sigma}c_{l\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon}$. To derive an equation of motion for these functions, we neglect the Green's-function terms coming from the commutator $[\hat{n}_{i\sigma},H]_{-}$ that are responsible for the "resonance broadening" correction in the higher-order equations, and we obtain

$$(\varepsilon' - \varepsilon_{\beta})\langle\langle(\hat{n}^{\alpha}_{i-\sigma} - n^{\alpha}_{-\sigma})\hat{n}^{\beta}_{l-\sigma}c_{l\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon} = (\langle\hat{n}^{\alpha}_{i-\sigma}\hat{n}^{\beta}_{l-\sigma}\rangle - n^{\alpha}_{-\sigma}n^{\beta}_{-\sigma})\delta_{lj} - \sum_{m} t_{lm}\langle\langle(\hat{n}^{\alpha}_{i-\sigma} - n^{\alpha}_{-\sigma})\hat{n}^{\beta}_{m-\sigma}c_{m\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon} + \sum_{m}\Delta t_{lm}\langle\langle(\hat{n}^{\alpha}_{i-\sigma} - n^{\alpha}_{-\sigma})\hat{n}^{\beta}_{l-\sigma}(\hat{n}_{l-\sigma} + \hat{n}_{m-\sigma})c_{m\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon}. \quad \text{(A1)}$$

Approximating the last two functions in Eq. (A1) and summing over $\beta = \pm$, we arrive at

$$\langle\langle(\hat{n}^{\alpha}_{i-\sigma} - n^{\alpha}_{-\sigma})c_{l\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon} = -\frac{1}{F^{\sigma}_{H,0}(\varepsilon')}\sum_{m} t^{\text{eff}}_{lm,\sigma}\langle\langle(\hat{n}^{\alpha}_{i-\sigma} - n^{\alpha}_{-\sigma})c_{m\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon}, \quad \text{(A2)}$$

where $t^{\text{eff}}_{lm,\sigma} = t_{lm} - 2n_{-\sigma}\Delta t_{lm}$ is the effective hopping integral. Equation (A2) is of the same type as Eq. (25) in Ref. 2. Therefore, its solution is assumed to be the following:

$$\langle\langle(\hat{n}^{\alpha}_{i-\sigma} - n^{\alpha}_{-\sigma})c_{l\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon} = -\sum_{m} W^{\sigma}_{lm,i}(\varepsilon')t^{\text{eff}}_{mi,\sigma}\langle\langle(\hat{n}^{\alpha}_{i-\sigma} - n^{\alpha}_{-\sigma})c_{i\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon} \quad \text{(A3)}$$

where

$$W^{\sigma}_{lm,i}(\varepsilon) = g^{\sigma}_{lm}(\varepsilon) - \frac{g^{\sigma}_{li}(\varepsilon)g^{\sigma}_{im}(\varepsilon)}{g^{\sigma}_{ii}(\varepsilon)}, \quad \text{(A4)}$$

$$g^{\sigma}_{lm}(\varepsilon) = \frac{1}{N}\sum_{\mathbf{k}}\frac{\exp[i\mathbf{k}\cdot(\mathbf{R}_l - \mathbf{R}_m)]}{F^{\sigma}_{H,0}(\varepsilon) - (\varepsilon^{\text{eff}}_{\mathbf{k},\sigma} - T_0)}, \quad \text{(A5)}$$

and $\varepsilon^{\text{eff}}_{\mathbf{k},\sigma}$ is the effective dispersion relation.

Using Eqs. (A1), (A2), and (A3), we can write the expression

$$\langle\langle(\hat{n}^{\alpha}_{i-\sigma} - n^{\alpha}_{-\sigma})\hat{n}^{\beta}_{l-\sigma}c_{l\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon} = -\frac{n^{\beta}_{-\sigma}F^{\sigma}_{H,0}(\varepsilon')}{\varepsilon' - \varepsilon_{\beta}}\sum_{m} W^{\sigma}_{lm,i}(\varepsilon')t^{\text{eff}}_{mi,\sigma}\langle\langle(\hat{n}^{\alpha}_{i-\sigma} - n^{\alpha}_{-\sigma})c_{i\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon}. \quad \text{(A6)}$$

APPENDIX B: RESONANCE BROADENING EFFECT

To find the functions $\langle\langle\hat{n}^{\alpha}_{l\sigma}c^{\pm}_{l-\sigma}c^{\mp}_{i-\sigma}c_{i\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon}$ appearing in the resonance broadening effect, we derive the equation of motion

$$\begin{aligned}\varepsilon\langle\langle\hat{n}^{\alpha}_{l\sigma}c^{\pm}_{l-\sigma}c^{\mp}_{i-\sigma}c_{i\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon} &= \delta_{ij}\langle\hat{n}^{\alpha}_{l\sigma}c^{\pm}_{l-\sigma}c^{\mp}_{i-\sigma}\rangle - \xi_{\alpha}\delta_{lj}\langle c^{+}_{l\sigma}c^{\pm}_{l-\sigma}c^{\mp}_{i-\sigma}c_{i\sigma}\rangle + T_0\langle\langle\hat{n}^{\alpha}_{l\sigma}c^{\pm}_{l-\sigma}c^{\mp}_{i-\sigma}c_{i\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon}\\ &- \sum_{m} t_{im}\langle\langle\hat{n}^{\alpha}_{l\sigma}c^{\pm}_{l-\sigma}c^{\mp}_{i-\sigma}c_{m\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon} \mp \sum_{m} t_{im}\langle\langle\hat{n}^{\alpha}_{l\sigma}c^{\pm}_{l-\sigma}c^{\mp}_{m-\sigma}c_{i\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon} \pm \sum_{m} t_{lm}\langle\langle\hat{n}^{\alpha}_{l\sigma}c^{\pm}_{m-\sigma}c^{\mp}_{i-\sigma}c_{i\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon}\\ &- \xi_{\alpha}\sum_{m} t_{lm}\langle\langle(c^{+}_{l\sigma}c_{m\sigma} - c^{+}_{m\sigma}c_{l\sigma})c^{\pm}_{l-\sigma}c^{\mp}_{i-\sigma}c_{i\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon} + U\langle\langle\hat{n}^{\alpha}_{l\sigma}\hat{n}^{\pm}_{l\sigma}c^{\pm}_{l-\sigma}c^{\mp}_{i-\sigma}c_{i\sigma};c^{+}_{j\sigma}\rangle\rangle_{\varepsilon}\\ &+ \sum_{m}\Delta t_{im}\langle\langle\hat{n}^{\alpha}_{l\sigma}c^{\pm}_{l-\sigma}c^{\mp}_{i-\sigma}c_{i\sigma}(c^{+}_{i-\sigma}c_{m-\sigma} + c^{+}_{m-\sigma}c_{i-\sigma});c^{+}_{j\sigma}\rangle\rangle_{\varepsilon}\end{aligned}$$

$$\pm \sum_m \Delta t_{im} \langle\langle \hat{n}^{\alpha}_{l\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma} (c^{+}_{i\sigma} c_{m\sigma} + c^{+}_{m\sigma} c_{i\sigma}); c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}$$
$$\mp \sum_m \Delta t_{lm} \langle\langle \hat{n}^{\alpha}_{l\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma} (c^{+}_{l\sigma} c_{m\sigma} + c^{+}_{m\sigma} c_{l\sigma}); c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} + \sum_m \Delta t_{im} \langle\langle \hat{n}^{\alpha}_{l\sigma} (n_{m-\sigma} + n_{i-\sigma}) c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{m\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}$$
$$\pm \sum_m \Delta t_{im} \langle\langle \hat{n}^{\alpha}_{l\sigma} (n_{m\sigma} + n_{i\sigma}) c^{\pm}_{l-\sigma} c^{\mp}_{m-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} \mp \sum_m \Delta t_{lm} \langle\langle \hat{n}^{\alpha}_{l\sigma} (n_{m\sigma} + n_{l\sigma}) c^{\pm}_{m-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}$$
$$+ \xi_{\alpha} \sum_m \Delta t_{lm} \langle\langle (n_{m-\sigma} + n_{l-\sigma}) (c^{+}_{l\sigma} c_{m\sigma} - c^{+}_{m\sigma} c_{l\sigma}) c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}. \tag{B1}$$

To truncate the infinite set of equations, we assume the following approximations in the higher-order Green's functions:

$$\begin{aligned}
&\langle\langle \hat{n}^{\alpha}_{l\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{m\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} \approx \langle \hat{n}^{\alpha}_{l\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} \rangle \langle\langle c_{m\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}, \quad \langle\langle \hat{n}^{\alpha}_{l\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{m-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} \approx \delta_{lm} n^{\alpha}_{\sigma} n^{\pm}_{-\sigma} \langle\langle c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon},\\
&\langle\langle \hat{n}^{\alpha}_{l\sigma} c^{\pm}_{m-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} \approx n^{\alpha}_{\sigma} \langle\langle c^{\pm}_{m-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}, \quad \langle\langle (c^{+}_{l\sigma} c_{m\sigma} - c^{+}_{m\sigma} c_{l\sigma}) c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} \approx 0,\\
&\langle\langle \hat{n}^{\alpha}_{l\sigma} (n_{m-\sigma} + n_{i-\sigma}) c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{m\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} \approx 2n_{-\sigma} \langle \hat{n}^{\alpha}_{l\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} \rangle \langle\langle c_{m\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon},\\
&\langle\langle \hat{n}^{\alpha}_{l\sigma} (n_{m\sigma} + n_{i\sigma}) c^{\pm}_{l-\sigma} c^{\mp}_{m-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} \approx 2n_{\sigma} \delta_{lm} n^{\alpha}_{\sigma} n^{\pm}_{-\sigma} \langle\langle c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon},\\
&\langle\langle \hat{n}^{\alpha}_{l\sigma} (n_{m\sigma} + n_{l\sigma}) c^{\pm}_{m-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} \approx 2n_{\sigma} n^{\alpha}_{\sigma} \langle\langle c^{\pm}_{m-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon},\\
&\langle\langle \hat{n}^{\alpha}_{l\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma} (c^{+}_{i-\sigma} c_{m-\sigma} + c^{+}_{m-\sigma} c_{i-\sigma}); c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} \approx \langle c^{+}_{i-\sigma} c_{m-\sigma} + c^{+}_{m-\sigma} c_{i-\sigma} \rangle \langle\langle \hat{n}^{\alpha}_{l\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon},\\
&\langle\langle \hat{n}^{\alpha}_{l\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma} (c^{+}_{i\sigma} c_{m\sigma} + c^{+}_{m\sigma} c_{i\sigma}); c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} \approx \langle c^{+}_{i\sigma} c_{m\sigma} + c^{+}_{m\sigma} c_{i\sigma} \rangle \langle\langle \hat{n}^{\alpha}_{l\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon},\\
&\langle\langle \hat{n}^{\alpha}_{l\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma} (c^{+}_{l\sigma} c_{m\sigma} + c^{+}_{m\sigma} c_{l\sigma}); c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} \approx \langle c^{+}_{l\sigma} c_{m\sigma} + c^{+}_{m\sigma} c_{l\sigma} \rangle \langle\langle \hat{n}^{\alpha}_{l\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon},\\
&\langle\langle (n_{m-\sigma} + n_{l-\sigma}) (c^{+}_{l\sigma} c_{m\sigma} - c^{+}_{m\sigma} c_{l\sigma}) c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} \approx 0.
\end{aligned} \tag{B2}$$

All the approximations without the intersite averages, $\langle c^{+}_{i-\sigma} c_{j-\sigma} \rangle$ and $\langle \hat{n}_{i\sigma} c^{+}_{i-\sigma} c_{j-\sigma} \rangle$, follow the line of Hubbard.[2] Terms with the intersite averages are the additional terms taking into account the intersite kinetic correlation.

In effect, for the function $\langle\langle c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}$, we can find the expression

$$\langle\langle c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} = -\sum_{m \neq i} W^{-\sigma}_{lm,i} (\varepsilon_{-} \pm \varepsilon_{\pm} \mp \varepsilon') t^{\mathrm{eff}}_{im,-\sigma} \langle\langle (\hat{n}^{\pm}_{i-\sigma} - n^{\pm}_{-\sigma}) c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}$$
$$+ \sum_{\alpha=\pm} \frac{\langle \hat{n}^{\alpha}_{l\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} \rangle}{\varepsilon' - (\varepsilon_{\pm} \pm \varepsilon_{-} \mp \varepsilon_{\alpha})} F^{\sigma}_{H,0}(\varepsilon) \langle\langle c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}. \tag{B3}$$

For the function $\langle\langle \hat{n}_{l\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}$, we obtain the following result:

$$\langle\langle \hat{n}_{l\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} = \frac{\langle \hat{n}_{l\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} \rangle}{\varepsilon' - (\varepsilon_{\pm} \pm \varepsilon_{-} \mp \varepsilon_{+})} F^{\sigma}_{H,0}(\varepsilon) \langle\langle c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} - \frac{n_{\sigma} F^{\sigma}_{H,0}(\varepsilon_{-} \pm \varepsilon_{\pm} \mp \varepsilon \pm 2z \Delta t I_{-\sigma})}{\varepsilon' - (\varepsilon_{\pm} \pm \varepsilon_{-} \mp \varepsilon_{+})}$$
$$\times \sum_{m \neq i} W^{-\sigma}_{lm,i} (\varepsilon_{-} \pm \varepsilon_{\pm} \mp \varepsilon') t^{\mathrm{eff}}_{im,-\sigma} \langle\langle (\hat{n}^{\pm}_{i-\sigma} - n^{\pm}_{-\sigma}) c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}. \tag{B4}$$

We derive now the equation of motion for the second type of functions: $\langle\langle \hat{n}_{i\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}$, appearing in the resonance broadening effect in Eq. (11),

$$\begin{aligned}
&\varepsilon \langle\langle \hat{n}_{i\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}\\
&= T_0 \langle\langle \hat{n}_{i\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} - \sum_m t_{im} \langle\langle \hat{n}_{i\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{m\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} \mp \sum_m t_{im} \langle\langle \hat{n}_{i\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{m-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}\\
&\quad \pm \sum_m t_{lm} \langle\langle \hat{n}_{i\sigma} c^{\pm}_{m-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} - \sum_m t_{im} \langle\langle (c^{+}_{i\sigma} c_{m\sigma} - c^{+}_{m\sigma} c_{i\sigma}) c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}\\
&\quad + U \langle\langle \hat{n}_{i\sigma} \hat{n}^{\pm}_{l\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} + \sum_m \Delta t_{im} \langle\langle \hat{n}_{i\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma} (c^{+}_{i-\sigma} c_{m-\sigma} + c^{+}_{m-\sigma} c_{i-\sigma}); c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}\\
&\quad \pm \sum_m \Delta t_{im} \langle\langle \hat{n}_{i\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma} (c^{+}_{i\sigma} c_{m\sigma} + c^{+}_{m\sigma} c_{i\sigma}); c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} \mp \sum_m \Delta t_{lm} \langle\langle \hat{n}_{i\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma} (c^{+}_{l\sigma} c_{m\sigma} + c^{+}_{m\sigma} c_{l\sigma}); c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}\\
&\quad + \sum_m \Delta t_{im} \langle\langle \hat{n}_{i\sigma} (n_{m-\sigma} + n_{i-\sigma}) c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{m\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} \pm \sum_m \Delta t_{im} \langle\langle \hat{n}_{i\sigma} (n_{m\sigma} + n_{i\sigma}) c^{\pm}_{l-\sigma} c^{\mp}_{m-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}\\
&\quad \mp \sum_m \Delta t_{lm} \langle\langle \hat{n}_{i\sigma} (n_{m\sigma} + n_{l\sigma}) c^{\pm}_{m-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon} + \sum_m \Delta t_{im} \langle\langle (n_{m-\sigma} + n_{i-\sigma}) (c^{+}_{i\sigma} c_{m\sigma} - c^{+}_{m\sigma} c_{i\sigma}) c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma} \rangle\rangle_{\varepsilon}.
\end{aligned} \tag{B5}$$

Keeping in line with the previous approximations made in Eq. (B2), we assume in Eq. (B5) the following approximations:

$$\begin{aligned}
&\langle\langle \hat{n}_{i\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{m\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon \approx 0,\\
&\langle\langle \hat{n}_{i\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{m-\sigma} c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon \approx \delta_{lm} n_\sigma n^{\pm}_{-\sigma} \langle\langle c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon,\\
&\langle\langle \hat{n}_{i\sigma} c^{\pm}_{m-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon \approx n_\sigma \langle\langle c^{\pm}_{m-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon,\\
&\langle\langle (c^{+}_{i\sigma} c_{m\sigma} - c^{+}_{m\sigma} c_{i\sigma}) c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon \approx 0,\\
&\langle\langle \hat{n}_{i\sigma}(n_{m-\sigma} + n_{i-\sigma}) c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{m\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon \approx 0,\\
&\langle\langle \hat{n}_{i\sigma}(n_{m\sigma} + n_{i\sigma}) c^{\pm}_{l-\sigma} c^{\mp}_{m-\sigma} c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon\\
&\quad\approx 2n_\sigma \delta_{lm} n_\sigma n^{\pm}_{-\sigma} \langle\langle c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon,\\
&\langle\langle \hat{n}_{i\sigma}(n_{m\sigma} + n_{l\sigma}) c^{\pm}_{m-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon\\
&\quad\approx 2n_\sigma n_\sigma \langle\langle c^{\pm}_{m-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon,
\end{aligned} \tag{B6}$$

which leads to the following relation:

$$\begin{aligned}
&\langle\langle \hat{n}_{i\sigma} c^{\pm}_{l-\sigma} c^{\mp}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon\\
&\quad= -\frac{n_\sigma F^{\sigma}_{H,0}(\varepsilon_- \pm \varepsilon_\pm \mp \varepsilon')}{\varepsilon' - (T_0 + U n^{\mp}_\sigma)} \sum_{m\neq i} W^{-\sigma}_{lm,i}(\varepsilon_- \pm \varepsilon_\pm \mp \varepsilon') t^{\text{eff}}_{im,-\sigma}\\
&\qquad\times \langle\langle (\hat{n}^{\pm}_{i-\sigma} - n^{\pm}_{-\sigma}) c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon.
\end{aligned} \tag{B7}$$

APPENDIX C: SCATTERING AND RESONANCE BROADENING CORRECTIONS

Now we insert functions appearing in the scattering correction of Appendix A [Eqs. (A3) and (A6)] and the resonance broadening correction of Appendix B [Eqs. (B3), (B4), and (B7)] into Eq. (11), obtaining

$$\begin{aligned}
(\varepsilon' - \varepsilon_\alpha)\langle\langle \hat{n}^{\alpha}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon =& \, n^{\alpha}_{-\sigma}\left(\delta_{ij} - \sum_l t_{il}\langle\langle c_{l\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon\right) + n^{\alpha}_{-\sigma}\sum_{\beta=\pm}(\gamma^\alpha + \gamma^\beta)\sum_l t_{il}\langle\langle \hat{n}^{\beta}_{l-\sigma} c_{l\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon\\
&+ \left[1 - X^{\alpha}_\sigma(\varepsilon')\right]\lambda_\sigma(\varepsilon')\langle\langle (\hat{n}^{\alpha}_{i-\sigma} - n^{\alpha}_{-\sigma}) c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon - \xi_\alpha\left[1 - X^{B}_{1,-\sigma}(\varepsilon')\right]\lambda_{-\sigma}(\varepsilon')\langle\langle (\hat{n}^{-}_{i-\sigma} - n^{-}_{-\sigma}) c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon\\
&- \xi_\alpha\left[1 - X^{B}_{2,-\sigma}(\varepsilon')\right]\lambda_{-\sigma}(\varepsilon_+ + \varepsilon_- - \varepsilon')\langle\langle (\hat{n}^{+}_{i-\sigma} - n^{+}_{-\sigma}) c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon + \xi_\alpha S^{B}_\sigma(\varepsilon')\langle\langle c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon,
\end{aligned} \tag{C1}$$

where

$$\begin{aligned}
\lambda_\sigma(\varepsilon') &= \sum_{lm} t_{il} W^{\sigma}_{lm,i}(\varepsilon') t^{\text{eff}}_{mi,\sigma}, X^{\alpha}_\sigma(\varepsilon')\\
&= \sum_{\beta=\pm}(\gamma^\alpha + \gamma^\beta)\frac{n^{\beta}_{-\sigma} F^{\sigma}_{H,0}(\varepsilon')}{\varepsilon' - \varepsilon_\beta},
\end{aligned} \tag{C2}$$

$$X^{B}_{1,-\sigma}(\varepsilon') = \gamma n_\sigma F^{\sigma}_{H,0}(\varepsilon')\left[\frac{1}{\varepsilon' - (T_0 + U n^{+}_\sigma)} + \frac{1}{\varepsilon' - \varepsilon_+}\right], \tag{C3}$$

$$\begin{aligned}
&X^{B}_{2,-\sigma}(\varepsilon')\\
&\quad= \gamma n_\sigma F^{\sigma}_{H,0}(\varepsilon_+ + \varepsilon_- - \varepsilon')\left[\frac{1}{\varepsilon' - (T_0 + U n^{-}_\sigma)} + \frac{1}{\varepsilon' - \varepsilon_-}\right],
\end{aligned} \tag{C4}$$

and

$$\begin{aligned}
S^{B}_\sigma(\varepsilon') = \frac{1}{N}\sum_{il}(-t_{il})[(2-\gamma)\langle \hat{n}_{l\sigma} c^{+}_{l-\sigma} c_{i-\sigma}\rangle\\
- \langle c^{+}_{l-\sigma} c_{i-\sigma}\rangle] F^{\sigma}_{H,0}(\varepsilon') C(\varepsilon').
\end{aligned} \tag{C5}$$

To solve this equation, we will use the following Fourier transforms:

$$\begin{aligned}
\langle\langle c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon &= \frac{1}{N}\sum_{\mathbf{k}} G^{\sigma}_{\mathbf{k}}(\varepsilon)\exp[i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)],\\
\langle\langle \hat{n}^{\alpha}_{i-\sigma} c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_\varepsilon &= \frac{1}{N}\sum_{\mathbf{k}} \Gamma^{\alpha}_{\mathbf{k},\sigma}(\varepsilon)\exp[i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)],
\end{aligned} \tag{C6}$$

where the functions $\Gamma^{\alpha}_{\mathbf{k},\sigma}(\varepsilon)$ fulfill the relation

$$\Gamma^{-}_{\mathbf{k},\sigma}(\varepsilon) + \Gamma^{+}_{\mathbf{k},\sigma}(\varepsilon) = G^{\sigma}_{\mathbf{k}}(\varepsilon). \tag{C7}$$

Taking into account the preceding relations, we can write Eq. (C1) in a final form as

$$\begin{aligned}
&\begin{bmatrix} \varepsilon' - \Omega^{\text{tot}}_\sigma(\varepsilon') - \varepsilon'_+ + 2n^{+}_{-\sigma}\gamma(\varepsilon_{\mathbf{k}} - T_0) & n^{+}_{-\sigma}\gamma(\varepsilon_{\mathbf{k}} - T_0)\\ n^{-}_{-\sigma}\gamma(\varepsilon_{\mathbf{k}} - T_0) & \varepsilon' - \Omega^{\text{tot}}_\sigma(\varepsilon') - \varepsilon'_- \end{bmatrix}\begin{bmatrix}\Gamma^{+}_{\mathbf{k},\sigma}(\varepsilon)\\ \Gamma^{-}_{\mathbf{k},\sigma}(\varepsilon)\end{bmatrix}\\
&\quad= \begin{bmatrix} n^{+}_{-\sigma}\\ n^{-}_{-\sigma}\end{bmatrix}\left\{1 + (\varepsilon_{\mathbf{k}} - T_0)G^{\sigma}_{\mathbf{k}}(\varepsilon) - \Omega^{\text{tot}}_\sigma(\varepsilon')G^{\sigma}_{\mathbf{k}}(\varepsilon)\right\} - \begin{bmatrix} n^{+}_{-\sigma}\Omega^{+}_\sigma(\varepsilon')\\ n^{-}_{-\sigma}\Omega^{-}_\sigma(\varepsilon')\end{bmatrix} G^{\sigma}_{\mathbf{k}}(\varepsilon) + \begin{bmatrix} +1\\ -1\end{bmatrix} S^{B}_\sigma(\varepsilon')G^{\sigma}_{\mathbf{k}}(\varepsilon);
\end{aligned} \tag{C8}$$

where

$$\varepsilon'_\alpha = \varepsilon_\alpha - \Omega^{\alpha}_\sigma(\varepsilon'), \quad \Omega^{\alpha}_\sigma(\varepsilon') = X^{\alpha}_\sigma(\varepsilon')\lambda_\sigma(\varepsilon'), \tag{C9}$$

$$\Omega^{\text{tot}}_\sigma(\varepsilon') = \lambda_\sigma(\varepsilon') + \left[1 - X^{B}_{1,-\sigma}(\varepsilon')\right]\lambda_{-\sigma}(\varepsilon') - \left[1 - X^{B}_{2,-\sigma}(\varepsilon')\right]\lambda_{-\sigma}(\varepsilon_+ + \varepsilon_- - \varepsilon'). \tag{C10}$$

In the functions $X^{B}_{1,-\sigma}(\varepsilon')$, $X^{B}_{2,-\sigma}(\varepsilon')$, $X^{+}_\sigma(\varepsilon')$, and $X^{-}_\sigma(\varepsilon')$ we replace their argument by $\varepsilon' = \varepsilon_\pm - S^{\Delta t}_\sigma$.

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