CORRELATION EFFECTS AND ELECTRONIC QUASIPARTICLE EXCITATIONS IN MULTIBAND TRANSITION METALS

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A self-consistent Irreducible Green Function (IGF) formalism for the description of electronic quasiparticles excitations in d-band transition metals has been developed. A generalized multiband Hubbard model with an additional interatomic interactions has been considered. The self-consistent set of equations for the Green function and self-energy was obtained. In the simplest approximation this approach gives correct results in the band limit. The possibility of extensions to obtain the results appropriate both in the band and in the atomic limit has been discussed.

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1. Introduction

In the recent years much attention has been given to the theory of correlation effects in transition metals, their compounds and disordered alloys [1]. The characteristic features of the d-electrons in transition metals may be deduced from a number of experimental facts. One of the most important conclusions obtained from analyzing the experimental data is that the d-electrons exhibit both itinerant and localized properties. Correlation phenomena are of great importance in determining the properties of these substances, especially, for describing metallic ferromagnetism of $3d$-transition metals, metal-insulator transitions, intermediate valence phenomena, etc.

There are mainly two methods for dealing with the electronic correlation problems [2]. Correlations are usually introduced in band-structure computations through a local cor-

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rection of the effective one-electron potential. The one-electron approximation of the conventional band theory has provided a basis for understanding a wide range of solid state phenomena. The adequacy of the single-particle picture is based on the density functional formalism and its extensions, the spin-density functional formalism. The first principal band structure calculations have been remarkably successful in obtaining various ground--state properties not only of nontransition but also transition metals, rare earths and actinides [3]. However, it is often not so successful in describing correctly the properties at finite temperatures.

In the second and complementary method, one therefore, starts with a model Hamiltonian for electrons and tries to calculate both the ground-state and excited-state properties [1, 4, 5]. This approach has been quite successful in calculating various ground-state properties of transition metals [1, 6–10]. Unfortunately, detailed investigations of the true nature of excited electronic states in transition metals including the damping effects and finite lifetimes began only very recently when it has been recognized that many-body effects in transition metals are very important for understanding photoemission experiments [11–14]. For transition metals with their highly localized *d*-orbitals and hence strong variation in the *d*-electron density, the effect of Coulomb correlation on energy bands has recently been investigated in paper [12] within the degenerate Hubbard model by perturbation theory (see also [11, 13]).

In this paper we present a self-consistent approach to consider the correlation effects in transition metals. The one-electron approximation is invalid in this case. Thus the use of sophisticated many-body techniques is required. For this purpose we use the Irreducible Green-Function (IGF) method developed in papers [15, 16]. The IGF method allows one to describe the quasiparticle inelastic scattering processes in a many-body system and to find quasiparticle spectra with damping in a very general way. From a technical point of view the IGF method is a special kind of the projection-operator approach in the theory of two-time Green functions [17, 18].

If one introduces irreducible parts of the Green functions (or irreducible parts of the operators from which the GF is constructed), the equation of motion for the GF can be exactly transformed into the Dyson equation. The representation of the self-energy operator in terms of high-order GF is exact, too. To perform the self-consistent calculation of the self-energy operator, we have to express it approximately in terms of low-order GF's. Recently, the IGF method has been applied to a number of solid-state problems [19–22]. A generalized Hubbard model of a *d*-band (considered in this paper) is more realistic for transition metals than the one-band Hubbard model considered previously by the IGF method in paper [16]. The complementary approach for the computation of electronic excitations in solids within the projection-operator formalism of the Mori–Zwanzig type has been developed in paper [23]. Unfortunately, explicit results have been obtained for a system with one orbital per site, which has been described only by the one-band Hubbard Hamiltonian.

The present paper is organized as follows. In the next Section we introduce the model Hamiltonian for the system with several orbitals per site. In Sect. 3 we describe the formalism associated with the irreducible Green function method and derive the exact Dyson equation

for a single-electron GF. The consideration of the generalized mean-field GF and their poles is presented in Sect. 4. The self-consistent approximative calculation of the electron self-energy operator is developed in Sect. 5. Additionally, in Appendix we contain a special kind of expansion for the self-energy.

2. *The Hamiltonian of the model*

A better understanding of the electronic correlation in solids really dates from Hubbard's introduction of the new Hamiltonian [4] that could be used to analyze major aspects of both the insulating and metallic states of solids in which electronic correlations are important. To simplify the problem, many treatments of the correlation effects are effectively restricted to a nondegenerate band. Most of them take only account of an intra--atomic integral, assuming its dominant role in magnetic properties. The model Hamiltonian which is usually referred to as the Hubbard Hamiltonian includes the intra-atomic Coulomb repulsion and the one-electron hopping energy. The Hubbard model has been investigated by many authors with various assumptions (see, e.g. [3, 4–10]). It is usually a rather difficult task to solve this model with a reasonable accuracy and correctly describe a simultaneous electron correlation in different d-states.

In this paper we want to develop a more realistic approach. An important point is to find a model which includes the different orbital states explicitly and to study the role of additional (to the Hubbard intra-atomic) terms for transition metals. Let us start with the second quantized form of the total Hamiltonian for an electron in a solid:

$$H = \sum_{ij\mu\nu\sigma} t_{ij}^{\mu\nu} a_{i\mu\sigma}^{\dagger} a_{j\nu\sigma} + \tfrac{1}{2} \sum_{ijmn\alpha\beta\gamma\delta\sigma\sigma'} \langle i\alpha, j\beta|\hat{V}|m\gamma, n\delta\rangle a_{i\alpha\sigma}^{\dagger} a_{j\beta\sigma'}^{\dagger} a_{m\gamma\sigma'} a_{n\delta\sigma}, \tag{1}$$

where

$$\langle i\alpha, j\beta|\hat{V}|m\gamma, n\delta\rangle$$

$$= \iint dr dr' \Phi_{\alpha}^{*}(r-R_i)\Phi_{\beta}^{*}(r'-R_j)V_2(|r-r'|)\Phi_{\gamma}(r'-R_m)\Phi_{\delta}(r-R_n)$$

and

$$t_{ij}^{\alpha\beta} = \int dr \Phi_{\alpha}^{*}(r-R_i)\left(-\frac{h^2}{2m}\nabla^2 + V_1(r)\right)\Phi_{\beta}(r-R_j). \tag{2}$$

Here, $V_1(r)$ is the effective potential composed of the ionic potentials of single atoms, and $V_2(|r-r'|)$ is the effective electron-electron interaction potential screened by s- and d-electrons. The $a_{i\alpha\sigma}^{\dagger}$ and $a_{i\alpha\sigma}$ are creation and annihilation operators, respectively, for electrons at site "i" in d-orbital $\alpha = 1, \ldots, 5$ with σ spin. As the d-functions are well localized, so using Hubbard argument we limit ourselves to the intra-atomic interactions and the Hamiltonian (1) takes form:

$$H_1 = \sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta} a_{i\alpha\sigma}^{\dagger} a_{j\beta\sigma} + \tfrac{1}{2} \sum_{i\alpha\sigma} U_{\alpha\alpha}^{(0)} n_{i\alpha\sigma} n_{i\alpha-\sigma}$$

$$+ \tfrac{1}{2} \sum_{i\alpha\beta\sigma\sigma'} (1-\delta_{\alpha\beta}) U_{\alpha\beta} n_{i\sigma\sigma} n_{i\beta\sigma'} - \tfrac{1}{2} \sum_{i\alpha\beta\sigma} (1-\delta_{\alpha\beta}) \mathscr{J}_{\alpha\beta} n_{i\alpha\sigma} n_{i\beta\sigma}$$

$$+\tfrac{1}{2}\sum_{i\alpha\beta\sigma}(1-\delta_{\alpha\beta})\mathscr{J}_{\alpha\beta}a^{\dagger}_{i\alpha\sigma}a^{\dagger}_{i\alpha-\sigma}a_{i\beta-\sigma}a_{i\beta\sigma}$$

$$-\tfrac{1}{2}\sum_{i\alpha\beta\sigma}(1-\delta_{\alpha\beta})\mathscr{J}_{\alpha\beta}a^{\dagger}_{i\alpha\sigma}a_{i\alpha-\sigma}a^{\dagger}_{i\beta-\sigma}a_{i\beta\sigma}, \tag{3}$$

where the interaction parameters are:

$$U^{(0)}_{\alpha\alpha}=\langle i\alpha, i\alpha|\hat{V}|i\alpha, i\alpha\rangle, \qquad U_{\alpha\beta}=\langle i\alpha, i\beta|\hat{V}|i\beta, i\alpha\rangle,$$

$$\mathscr{J}_{\alpha\beta}=\langle i\alpha, i\beta|\hat{V}|i\alpha, i\beta\rangle=\langle i\alpha, i\alpha|\hat{V}|i\beta, i\beta\rangle. \tag{4}$$

In the following we assume that all the d-orbitals are equivalent [8] and hence the interorbital integrals $U_{\alpha\beta}$ and $\mathscr{J}_{\alpha\beta}$ become independent of the orbital indices (also $U^{0}_{\alpha\alpha}$ does not depend on the value of α). We assume also that the interorbital hopping vanishes, i.e. $t^{\alpha\beta}_{ij}=\delta_{\alpha\beta}t^{\alpha}_{ij}$. Additionally, for our case of equivalent d-orbitals we have condition for integrals $U^{(0)}$, U and $\mathscr{J}$, namely $U^{(0)}=U+2\mathscr{J}$ [8]. The approximation of the interaction integrals by the constant values is not so bad if we remember that, for example, the anisotropy in the values of the exchange integrals for Ni is of the order of 15% [10].

In order to demonstrate how the IGF method works for a more complicated case we include in the Hamiltonian an additional term describing the direct interatomic exchange interaction ($I^{\alpha\beta}_{ij}=I_{ij}\delta_{\alpha\beta}$)

$$H_2=-\tfrac{1}{2}\sum_{ij\alpha\sigma\sigma'}I_{ij}a^{\dagger}_{i\alpha\sigma}a_{i\alpha\sigma'}a^{\dagger}_{j\alpha\sigma'}a_{j\alpha\sigma}. \tag{5}$$

We note that s-electrons are not explicitly taken into account in our model Hamiltonian $H=H_1+H_2$, so the hybridization effects are neglected. They are, however, implicitly taken into account by screening effects and effective d-band occupation.

3. The Dyson equation for the one-electron two-time Green function

For the calculation of the electronic quasiparticle spectrum of the described model with Hamiltonian $H=H_1+H_2$ let us consider the equation of motion for the one-electron two-time temperature Green Function (GF):

$$G^{\alpha\beta}_{\sigma}(i,j,t-t')=-i\theta(t-t')\langle[a_{i\alpha\sigma}(t), a^{\dagger}_{j\beta\sigma}(t')]_{+}\rangle$$

$$\equiv\langle\langle a_{i\alpha\sigma}(t); a^{\dagger}_{j\beta\sigma}(t')\rangle\rangle \tag{6}$$

with commonly used notation [24].

First performing the time t differentiation of Eq. (6) we get the equation for the Fourier transform $G^{\alpha\beta}_{\sigma}(ij;\omega)\equiv\langle\langle a_{i\alpha\sigma}|a^{+}_{j\beta\sigma}\rangle\rangle_{\omega}$

$$\sum_{n\gamma}T^{\alpha\gamma}(in)G^{\gamma\beta}_{\sigma}(nj;\omega)=\delta_{ij}\delta_{\alpha\beta}+\sum_{n\gamma}\{V^{(1)\alpha\gamma}_{in}\langle\langle a_{n\alpha\sigma}n_{n\gamma\sigma}|a^{\dagger}_{j\beta\sigma}\rangle\rangle$$

$$+V^{(2)\alpha\gamma}_{in}\langle\langle a_{n\alpha\sigma}n_{n\beta-\sigma}|a^{\dagger}_{j\beta\sigma}\rangle\rangle+2V^{(3)\alpha\beta}_{in}\langle\langle a_{n\alpha-\sigma}a^{\dagger}_{n\beta-\sigma}a_{n\beta\sigma}|a^{\dagger}_{j\beta\sigma}\rangle\rangle$$

$$+V^{(4)\alpha\beta}_{in}(\langle\langle a_{i\beta\sigma}n_{n\beta\sigma}|a^{\dagger}_{j\beta\sigma}\rangle\rangle+\langle\langle a_{i\beta-\sigma}a^{\dagger}_{i\beta-\sigma}a_{n\beta\sigma}|a^{\dagger}_{j\beta\sigma}\rangle\rangle)\}, \tag{7}$$

where

$$T^{\alpha\beta}(in) = \omega\delta_{in}\delta_{\alpha\beta} - t_{in}^{\alpha}\delta_{\alpha\beta}, \qquad V_{in}^{(1)\alpha\beta} = (U - \mathscr{J})(1 - \delta_{\alpha\beta})\delta_{in},$$

$$V_{in}^{(2)\alpha\beta} = [(U + 2\mathscr{J})\delta_{\alpha\beta} + U(1 - \delta_{\alpha\beta})]\delta_{in},$$

$$V_{in}^{(3)\alpha\beta} = -\mathscr{J}(1 - \delta_{\alpha\beta})\delta_{in},$$

$$V_{in}^{(4)\alpha\beta} = -I_{in}(1 - \delta_{in})\delta_{\alpha\beta}. \tag{8}$$

To treat the many-body problem in a self-consistent way we follow here the IGF method [15, 16]. In the weak correlation limit (which seems to be realistic for transition metals — $U^{(0)}/W < 1$, $\mathscr{J} \approx 0.2U$ [9, 12]) we introduce, by definition, the irreducible parts of the GF in the r.h.s. of Eq. (7)

$$\ll a_{i\mu\sigma}a_{k\nu\sigma'}^{\dagger}\, a_{k\nu\sigma'}\,|a_{j\beta\sigma_1}^{\dagger}\gg = \ll (a_{i\mu\sigma}a_{k\nu\sigma'}^{\dagger}\, a_{k\nu\sigma'})^{\mathrm{ir}}|a_{j\beta\sigma_1}^{\dagger}\gg$$

$$+\langle n_{k\sigma'}\rangle \ll a_{i\mu\sigma}|a_{j\beta\sigma_1}^{\dagger}\gg + \langle a_{i\mu\sigma}a_{k\nu\sigma'}^{\dagger}\rangle \ll a_{k\nu\sigma'}|a_{j\beta\sigma_1}^{\dagger}\gg, \tag{9}$$

in which all possible mean-field contributions are removed. The choice of the IGF's is determined by the conditions

$$\langle[(a_{i\mu\sigma}n_{k\nu\sigma'})^{\mathrm{ir}},\, a_{j\beta\sigma_1}^{\dagger}]_{+}\rangle = 0. \tag{10}$$

From Eqs (9) and (10) we find

$$\langle[(a_{i\mu\sigma}n_{k\nu\sigma'})^{\mathrm{ir}},\, a_{j\beta\sigma_1}^{\dagger}]_{+}\rangle = \langle[(a_{i\mu\sigma}n_{k\nu\sigma'}$$

$$-\langle n_{k\nu\sigma'}\rangle a_{i\mu\sigma} - \langle a_{i\mu\sigma}a_{k\nu\sigma'}^{\dagger}\rangle a_{k\nu\sigma'}),\, a_{j\beta\sigma_1}^{\dagger}]_{+}\rangle \equiv 0. \tag{11}$$

So, the IGF's are defined so that they cannot be reduced to the low-order ones by any kind of decoupling. This reduction procedure is of fundamental importance in the present method because it allows us to extract all relevant (for problem under consideration) mean-field renormalizations and to put them into the "zero-order" (generalized mean-field) Green function. To demonstrate the possibilities of our method, we explicitly write the so-called "anomalous" correlation functions corresponding to spin-flip processes [25]. However, it must be stressed that because of the spin rotational invariance of our Hamiltonian we have $\langle a_{i\alpha\sigma}a_{j\beta-\sigma}^{+}\rangle = 0$. In the remaining part of this paper we do not take spin-flip terms into consideration. Thus, in the case of weak electron correlation it will be enough to define a very simple mean-field extraction. In the general case the mean-field renormalizations may have a very nontrivial structure, and a special projection procedure should be developed for higher-order GF's as it has been done for the Hubbard model in the strong correlation limit, for the theory of superconductivity in transition metals and their disordered alloys [19–20] and for the magnetic polaron problem at finite temperatures [21].

Using the definition (9) in Eq. (7) the equation of motion can be exactly transformed to the following form:

$$\sum_{l\nu}[\omega\delta_{il}\delta_{\alpha\nu} - E_{\sigma}^{\alpha\nu}(il)]G_{\sigma}^{\nu\beta}(lj;\omega) = \delta_{ij}\delta_{\alpha\beta} + \sum_{l\nu}\{V_{il}^{(1)\alpha\nu}$$

$$\times \ll (a_{l\alpha\sigma}n_{l\nu\sigma})^{\mathrm{ir}}|a_{j\beta\sigma}^{\dagger}\gg + V_{il}^{(2)\alpha\nu}\ll (a_{l\alpha\sigma}n_{l\nu-\sigma})^{\mathrm{ir}}|a_{j\beta\sigma}^{\dagger}\gg$$

$$+2V_{il}^{(3)\alpha\nu}\langle\langle(a_{l\alpha-\sigma}a_{lv-\sigma}^{\dagger}a_{lv\sigma})^{ir}|a_{j\beta\sigma}^{\dagger}\rangle\rangle+V_{il}^{(4)\alpha\nu}[\langle\langle(a_{iv\sigma}n_{lv\sigma})^{ir}|a_{j\beta\sigma}^{\dagger}\rangle\rangle$$

$$+\langle\langle(a_{iv-\sigma}a_{iv-\sigma}^{\dagger}a_{lv\sigma})^{ir}|a_{j\beta\sigma}^{\dagger}\rangle\rangle]\}, \tag{12}$$

where the renormalized energy $E_{\sigma}^{\alpha\nu}(il)$ is given by the expression

$$E_{\sigma}^{\alpha\nu}(il)=t_{il}^{\alpha}\delta_{\alpha\nu}-V_{il}^{(1)\alpha\nu}\langle a_{l\alpha\sigma}a_{lv\sigma}^{\dagger}\rangle$$

$$-\sum_{\mu}(V_{il}^{(1)\nu\mu}\delta_{\alpha\nu}\langle n_{l\mu\sigma}\rangle-\delta_{\alpha\nu}V_{il}^{(2)\nu\mu}\langle n_{l\mu-\sigma}\rangle)$$

$$-2V_{il}^{(3)\alpha\nu}\langle a_{l\alpha-\sigma}a_{lv-\sigma}^{\dagger}\rangle-V_{il}^{(4)\alpha\nu}(\langle a_{iv\sigma}a_{lv\sigma}^{+}\rangle$$

$$-\langle a_{iv-\sigma}a_{lv-\sigma}^{\dagger}\rangle)-\sum_{j}V_{il}^{(4)\alpha\nu}\langle n_{jv\sigma}\rangle\delta_{il}. \tag{13}$$

Now we proceed to derive the Dyson equation. To calculate the IGF's $\langle\langle A(t)^{ir};B(t')\rangle\rangle$ in Eq. (12), we have to write the equation of motion after differentiation with respect to the second time variable t'. Then conditions (9) remove the inhomogeneous terms in these equations. If one introduces irreducible parts for the right-hand side operators by analogy with expression (9), the equation of motion (12) can be exactly rewritten in the following form:

$$G_{\sigma}^{\alpha\beta}(ij;\omega)=G_{\sigma}^{\alpha\beta(0)}(ij;\omega)+\sum_{nm\mu\nu}G_{\sigma}^{\alpha\mu(0)}(im;\omega)P_{\sigma}^{\mu\nu}(mn;\omega)G_{\sigma}^{\nu\beta(0)}(nj;\omega), \tag{14}$$

where the generalized mean-field Green function $G^{(0)}$ reads

$$\sum_{lv}[\omega\delta_{il}\delta_{\alpha\nu}-E_{\sigma}^{\alpha\nu}(il)]G_{\sigma}^{\nu\beta(0)}(lj;\omega)=\delta_{\alpha\beta}\delta_{ij}. \tag{15}$$

The scattering operator P is given by the expression

$$P_{\sigma}^{\alpha\beta}(ij;\omega)=\sum_{mn\mu\nu}\{V_{im}^{(1)\alpha\nu}\langle\langle(a_{m\alpha\sigma}n_{mv\sigma})^{ir}|(a_{n\beta\sigma}^{\dagger}n_{n\mu\sigma})^{ir}\rangle\rangle V_{nj}^{(1)\mu\beta}$$

$$+V_{im}^{(1)\alpha\nu}\langle\langle(a_{m\alpha\sigma}n_{mv\sigma})^{ir}|(a_{n\beta\sigma}^{\dagger}n_{n\mu-\sigma})^{ir}\rangle\rangle V_{nj}^{(2)\mu\beta}$$

$$+V_{im}^{(2)\alpha\nu}\langle\langle(a_{m\alpha\sigma}n_{mv-\sigma})^{ir}|(a_{n\beta\sigma}^{\dagger}n_{n\mu\sigma})^{ir}\rangle\rangle V_{nj}^{(1)\mu\beta}$$

$$+V_{im}^{(2)\alpha\nu}\langle\langle(a_{m\alpha\sigma}n_{n\mu-\sigma})^{ir}|(a_{n\beta\sigma}^{\dagger}n_{n\mu-\sigma})^{ir}\rangle\rangle V_{nj}^{(2)\mu\beta}\}. \tag{16}$$

Here we present for brevity the scattering operator only for a part of Hamiltonian (3), i.e. without two last terms. The full scattering operator can be written directly.

If we go further and write down the Dyson equation

$$G_{\sigma}^{\alpha\beta}(ij;\omega)=G_{\sigma}^{\alpha\beta(0)}(ij;\omega)+\sum_{nm\mu\nu}G_{\sigma}^{\alpha\mu(0)}(im;\omega)M_{\sigma}^{\mu\nu}(mn;\omega)G_{\sigma}^{\nu\beta}(nj;\omega) \tag{17}$$

we get the following equation for M:

$$P_{\sigma}^{\mu\nu}(mn;\omega)=M_{\sigma}^{\mu\nu}(mn;\omega)+\sum_{ij\alpha\beta}M_{\sigma}^{\mu\alpha}(mi;\omega)G_{\sigma}^{\alpha\beta(0)}(ij;\omega)P_{\sigma}^{\beta\nu}(jn;\omega) \tag{18}$$

from which it follows that in complete analogy to the diagrammatic technique the self-energy operator $M_\sigma^{\mu\nu}(mn;\omega)$ is defined as a proper (connected) part of the scattering operator $P_\sigma^{\mu\nu}(mn;\omega)$

$$M_\sigma^{\mu\nu}(ij;\omega) = (P_\sigma^{\mu\nu}(ij;\omega))^c. \tag{19}$$

It should be emphasized that for the retarded (and advanced) GF's the proper part has only a symbolic character. However, one may use the causal, instead of retarded, GF at any step in the calculations because the equation of motion has the same form for all three (retarded, advanced, and causal) GF's. In a certain sense there is a possibility of controlling, in the diagrammatic language, the relevant decoupling procedure in approximative self-energy calculations. Thus, in contrast to the standard equation-of-motion approach the determination of the full GF, G, has been reduced to the determination of the mean-field GF, $G^{(0)}$, and the self-energy operator M. The reason for this method of calculations is that the decoupling is only introduced into the self-energy operator, as will be clear from the next Sections.

4. Electronic states in mean-field approximation

The question now is how to describe our system in terms of the quasiparticle picture. For a translationally invariant system, to describe the low-lying excitations of the system in terms of quasiparticles, one has to choose eigenstates such that they all correspond to a definite momentum. For the degenerate band model we need the transformation relations between second quantized operators $a_{i\alpha\sigma}$ and $a_{kn\sigma}$ connecting the electron state with an orbital symmetry α centered at atomic site $\boldsymbol{R}_i$ and the Bloch state $|n\boldsymbol{k}\rangle$, where n is the band index. The exact transformation reads (see, e.g. [26]):

$$a_{kn\sigma} = N^{-1/2} \sum_{i\mu} b_{n\mu}(\boldsymbol{k}) \exp(-i\boldsymbol{k}\cdot\boldsymbol{R}_i) a_{i\mu\sigma}. \tag{20}$$

However, for the sake of simplicity we shall follow the approximative approach and use the following transformation:

$$a_{k\alpha\beta} = N^{-1/2} \sum_i \exp(-i\boldsymbol{k}\cdot\boldsymbol{R}_i) a_{i\alpha\sigma}. \tag{21}$$

The second quantized operators in Eq. (21) generate five artificial uncoupled bands for which $\alpha = 1, 2, \ldots, 5$. When coupled by $b_{n\mu}(\boldsymbol{k})$ they reproduce the realistic bands labelled by n, as given by Eq. (20). Introducing the Fourier transforms $G_\sigma^{\alpha\mu(0)}(\boldsymbol{k};\omega)$, $G_\sigma^{\alpha\mu}(k;\omega)$ and $M_\sigma^{\alpha\mu}(\boldsymbol{k};\omega)$ we can rewrite (14) in the form:

$$G_\sigma^{\alpha\beta}(\boldsymbol{k};\omega) = G_\sigma^{\alpha\beta(0)}(\boldsymbol{k};\omega) + \sum_{\mu\nu} G_\sigma^{\alpha\mu(0)}(\boldsymbol{k};\omega) M_\sigma^{\mu\nu}(\boldsymbol{k};\omega) G_\sigma^{\nu\beta}(\boldsymbol{k};\omega). \tag{22}$$

From the symbolic solution of the Eq. (22) it is seen that the problem of calculating the single-particle GF $G_\sigma^{\alpha\beta}(\boldsymbol{k};\omega)$ is reduced to the one of calculating the generalized mean-field $G_\sigma^{\alpha\beta(0)}(\boldsymbol{k};\omega)$ and the self-energy $M_\sigma^{\alpha\beta}(\boldsymbol{k};\omega)$. For example, for the Hubbard model we have

(see Eq. (15))

$$E_\sigma^{\alpha\nu}(\boldsymbol{k}) = (\varepsilon_\alpha(\boldsymbol{k}) + U^{(0)} N^{-1} \sum_q \langle n_{q\alpha-\sigma}\rangle)\delta_{\alpha\nu}, \tag{23}$$

where

$$t_{ij}^\alpha = N^{-1} \sum_{\boldsymbol{k}} \varepsilon_\alpha(\boldsymbol{k}) \exp(-i\boldsymbol{k}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)). \tag{24}$$

The spectrum of electronic low-lying excitations without damping follows immediately from the poles of the single-particle mean-field Green function $\bar{G}^{(0)}$ ($\bar{G}^{(0)}$ denotes a matrix in the space of band indices) — $\det|\omega\bar{1} - \bar{E}_\sigma| = 0$. For the most important (diagonal in the band indices) case we obtain

$$\begin{aligned} E_\sigma^\alpha(\boldsymbol{k}) = \varepsilon_\alpha(\boldsymbol{k}) + (U - \mathscr{J}) \sum_\mu (1+\delta_{\alpha\nu}) N_{\mu\sigma} + \sum_\mu [(U+2\mathscr{J})\delta_{\alpha\mu} \\ + U(1-\delta_{\alpha\mu})] N_{\mu-\sigma} + \sum_{\sigma'} N^{-1} \sum_q I(\boldsymbol{k}-\boldsymbol{q})(1 - \langle n_{q\alpha\sigma'}\rangle) \\ + I(\boldsymbol{0}) N^{-1} \sum_q \langle a_{\boldsymbol{k}+q\alpha\sigma}^\dagger a_{q\alpha\sigma}\rangle, \end{aligned} \tag{25}$$

where $N_{\mu\sigma} = N^{-1} \sum_q \langle n_{q\mu-\sigma}\rangle$.

It follows from Eq. (25) that in a complete analogy with the one-band case one can define the band splitting Δ^α in the following form:

$$\begin{aligned} \Delta^\alpha = E_\uparrow^\alpha(\boldsymbol{k}) - E_\downarrow^\alpha(\boldsymbol{k}) = U^{(0)}(N_{\alpha\uparrow} - N_{\alpha\downarrow}) + \mathscr{J} \sum_\mu (1-\delta_{\alpha\mu})(N_{\mu\uparrow} - N_{\mu\downarrow}) \\ + I(\boldsymbol{0}) N^{-1} \sum_q (\langle a_{\boldsymbol{k}+q\alpha\uparrow}^\dagger a_{q\alpha\uparrow}\rangle - \langle a_{\boldsymbol{k}+q\alpha\downarrow}^\dagger a_{q\alpha\downarrow}\rangle). \end{aligned} \tag{26}$$

The last expression generalizes the standard Hartree–Fock band splitting expression.

5. Electronic quasi-particle and their damping

Now let us take into consideration the damping effects and finite lifetimes. Hence, our next task consists in obtaining self-consistent approximate expression of the electron self-energy operator. In the general case, to find the damping of the electronic states, one needs the following expression for the single-particle Green function:

$$G_\sigma^{\alpha\nu}(\boldsymbol{k};\omega) = \{[G_\sigma^{\alpha\nu(0)}(\boldsymbol{k};\omega)]^{-1} - \Sigma_\sigma^{\alpha\nu}(\boldsymbol{k};\omega)\}^{-1}. \tag{27}$$

Here $\Sigma_\sigma^{\alpha\nu}(\boldsymbol{k};\omega)$ is a functional of $M_\sigma^{\alpha\nu}(\boldsymbol{k};\omega)$

$$\Sigma_\sigma^{\alpha\nu}(\boldsymbol{k};\omega) = F[M_\sigma^{\alpha\nu}(\boldsymbol{k};\omega)]. \tag{28}$$

If we confine ourselves to the most important diagonal case, we find that the renormalized electron energies are self-consistent solutions of the equation

$$\tilde{\varepsilon}_\sigma^\alpha(\boldsymbol{k}) - E_\sigma^\alpha(\boldsymbol{k}) - \mathrm{Re}\,\Sigma_\sigma^\alpha(\boldsymbol{k};\tilde{\varepsilon}_\sigma^\alpha(\boldsymbol{k})) = 0. \tag{29}$$

Hence, if $\boldsymbol{k}$ labels a quasiparticle electronic state, the spectral functions

$$g_\sigma^\alpha(\boldsymbol{k};\omega) \sim \operatorname{Im} G_\sigma^\alpha(\boldsymbol{k};\omega) \tag{30}$$

will have strong maxima at energies of the quasiparticle state.

Thus, now we have to find the matrix elements of self-energy M to complete our solution of the problem.

Here and in the following we present, for brevity, the results obtained only for a part of our Hamiltonian, namely for Hamiltonian without its three last terms. The results for full Hamiltonian can be written directly. In the quasimomentum representation we obtain:

$$\begin{aligned} M_\sigma^{\alpha\beta}(\boldsymbol{k};\omega) = N^{-2}\sum_{\mu\nu}\sum_{\boldsymbol{pqrs}} \{ & V^{(1)\alpha\nu}\langle\langle (a_{\boldsymbol{k}+\boldsymbol{p}\alpha\sigma}a^+_{\boldsymbol{p}+\boldsymbol{q}\nu\sigma}a_{\boldsymbol{q}\nu\sigma})^{\mathrm{ir}}| \\ & \times (a^\dagger_{\boldsymbol{k}+\boldsymbol{r}\beta\sigma}a^\dagger_{\boldsymbol{r}\mu\sigma}a_{\boldsymbol{r}+\boldsymbol{s}\mu\sigma})^{\mathrm{ir}}\rangle\rangle^{\mathrm{c}} V^{(1)\mu\beta} \\ & + V^{(1)\alpha\nu}\langle\langle (a_{\boldsymbol{k}+\boldsymbol{p}\alpha\sigma}a^\dagger_{\boldsymbol{p}+\boldsymbol{q}\nu\sigma}a_{\boldsymbol{q}\nu\sigma})^{\mathrm{ir}}|\, (a^\dagger_{\boldsymbol{k}+\boldsymbol{s}\beta\sigma}a^\dagger_{\boldsymbol{r}\mu-\sigma}a_{\boldsymbol{r}+\boldsymbol{s}\mu-\sigma})^{\mathrm{ir}}\rangle\rangle^{\mathrm{c}} V^{(2)\mu\beta} \\ & + V^{(2)\alpha\nu}\langle\langle (a_{\boldsymbol{k}+\boldsymbol{p}\alpha\sigma}a^\dagger_{\boldsymbol{p}+\boldsymbol{q}\nu-\sigma}a_{\boldsymbol{q}\nu-\sigma})^{\mathrm{ir}}|\, (a^\dagger_{\boldsymbol{k}+\boldsymbol{s}\beta\sigma}a^\dagger_{\boldsymbol{r}\mu\sigma}a_{\boldsymbol{r}+\boldsymbol{s}\mu\sigma})^{\mathrm{ir}}\rangle\rangle^{\mathrm{c}} V^{(1)\mu\beta} \\ & + V^{(2)\alpha\nu}\langle\langle (a_{\boldsymbol{k}+\boldsymbol{p}\alpha\sigma}a^\dagger_{\boldsymbol{p}+\boldsymbol{q}\nu-\sigma}a_{\boldsymbol{q}\nu-\sigma})^{\mathrm{ir}}|\, (a^\dagger_{\boldsymbol{k}+\boldsymbol{s}\beta\sigma}a^\dagger_{\boldsymbol{r}\mu-\sigma}a_{\boldsymbol{r}+\boldsymbol{s}\mu-\sigma})^{\mathrm{ir}}\rangle\rangle^{\mathrm{c}} V^{(2)\mu\beta}\}, \end{aligned} \tag{31}$$

where functions $V^{(i)\alpha\beta}$ are equivalent to these defined in Eq. (8) but without δ_{ij} factors.

It is convenient to write down $\langle\langle A|A^+\rangle\rangle$ in terms of the correlation functions in the form

$$\begin{aligned} \langle\langle a_{\boldsymbol{k}+\boldsymbol{p}\alpha\sigma}a^\dagger_{\boldsymbol{p}+\boldsymbol{q}\nu\sigma}a_{\boldsymbol{q}\nu\sigma}|a^\dagger_{\boldsymbol{k}+\boldsymbol{s}\beta\sigma}a^\dagger_{\boldsymbol{r}\mu\sigma}a_{\boldsymbol{r}+\boldsymbol{s}\mu\sigma}\rangle\rangle &= \frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{d\omega'}{\omega-\omega'}(e^{\beta\omega'}+1) \\ \times \int_{-\infty}^{+\infty} dt e^{i\omega' t}\langle a^\dagger_{\boldsymbol{k}+\boldsymbol{s}\beta\sigma}(t)a^\dagger_{\boldsymbol{r}\mu-\sigma}(t)a_{\boldsymbol{r}+\boldsymbol{s}\mu-\sigma}(t)a_{\boldsymbol{k}+\boldsymbol{p}\alpha\sigma}a^\dagger_{\boldsymbol{p}+\boldsymbol{q}\nu\sigma}a_{\boldsymbol{q}\nu\sigma}\rangle. \end{aligned} \tag{32}$$

It is reasonable to use the following pair approximation (for a low density of quasiparticles) for the correlation function in the r.h.s. of Eq. (32) in terms of single-particle correlation functions

$$\begin{aligned} & \langle a^\dagger_{\boldsymbol{k}+\boldsymbol{s}\beta\sigma}(t)a^\dagger_{\boldsymbol{r}\mu-\sigma}(t)a_{\boldsymbol{r}+\boldsymbol{s}\mu-\sigma}(t)a_{\boldsymbol{k}+\boldsymbol{p}\alpha\sigma}a^\dagger_{\boldsymbol{p}+\boldsymbol{q}\nu-\sigma}a_{\boldsymbol{q}\nu-\sigma}\rangle^{\mathrm{ir,c}} \\ & \approx \langle a^\dagger_{\boldsymbol{k}+\boldsymbol{p}\beta\sigma}(t)a_{\boldsymbol{k}+\boldsymbol{p}\alpha\sigma}\rangle\langle a^\dagger_{\boldsymbol{q}\mu-\sigma}(t)a_{\boldsymbol{q}\nu-\sigma}\rangle\langle a_{\boldsymbol{p}+\boldsymbol{q}\mu\sigma}(t)a^\dagger_{\boldsymbol{p}+\boldsymbol{q}\nu-\sigma}\rangle\delta_{\boldsymbol{k}+\boldsymbol{s},\boldsymbol{k}+\boldsymbol{p}}\delta_{\boldsymbol{r}\boldsymbol{q}}\delta_{\boldsymbol{r}+\boldsymbol{s},\boldsymbol{p}+\boldsymbol{q}}, \end{aligned} \tag{33}$$

i.e. we approximate to three-point correlation function by the product of all possible two--point correlators with different time arguments (the simultaneous averages have already been taken into account in $G^{(0)}$). Taking into account the spectral theorem we obtain from Eqs (31–33):

$$M_\sigma^{\alpha\beta}(\boldsymbol{k},\omega) = N^{-2}\sum_{\mu\nu\boldsymbol{pq}}\sum_{i=1,2} V^{(i)\alpha\nu}Q_{i\sigma}^{\alpha\mu\nu\beta}(\boldsymbol{kpq};\omega)V^{(i)\mu\beta}, \tag{34}$$

where

$$Q_{1\sigma}^{\alpha\mu\nu\beta}(\boldsymbol{kpq};\omega)=\left(-\frac{1}{\pi}\right)^3\int_{-\infty}^{+\infty}\int\int\int\frac{d\omega_1 d\omega_2 d\omega_3}{\omega+\omega_1-\omega_2-\omega_3}\{n(\omega_1)[1-n(\omega_2)-n(\omega_3)]$$

$$+n(\omega_2)n(\omega_3)\}\{\mathrm{Im}\,G_\sigma^{\mu\nu}(\boldsymbol{p}^+\boldsymbol{q};\omega_1)\cdot\mathrm{Im}\,G_\sigma^{\nu\mu}(\boldsymbol{q};\omega_2)\,\mathrm{Im}\,G_\sigma^{\alpha\beta}(\boldsymbol{k}+\boldsymbol{p};\omega_3)$$

$$+\mathrm{Im}\,G_{\boldsymbol{k}}^{\mu\nu}(\boldsymbol{p}+\boldsymbol{q};\omega_1)\,\mathrm{Im}\,G_\sigma^{\nu\beta}(\boldsymbol{q};\omega_2)\,\mathrm{Im}\,G_\sigma^{\alpha\mu}(\boldsymbol{k}+\boldsymbol{p};\omega_3)\},\tag{35}$$

$$Q_{2\sigma}^{\alpha\mu\nu\beta}(\boldsymbol{kpq};\omega)=\left(-\frac{1}{\pi}\right)^3\int_{-\infty}^{+\infty}\int\int\int\frac{d\omega_1 d\omega_2 d\omega_3}{\omega+\omega_1-\omega_2-\omega_3}\{n(\omega_1)[1-n(\omega_2)$$

$$-n(\omega_3)]+n(\omega_2)n(\omega_3)\}\,\mathrm{Im}\,G_\sigma^{\mu\nu}(\boldsymbol{p}+\boldsymbol{q};\omega_1)\,\mathrm{Im}\,G_\sigma^{\nu\mu}(\boldsymbol{q};\omega_2)\mathrm{Im}\,G_\sigma^{\alpha\beta}(k+\boldsymbol{p};\omega)\tag{36}$$

and $n(\omega)$ are the Fermi distribution functions.

Equations (22) and (34) form a closed self-consistent system (in our approximation) of equations for the single-particle electron GF for the generalized multiband Hubbard model described by Hamiltonian $H=H_1$ without two last terms in H_1. In principle, we may use, in the r.h.s. of Eq. (34), any relevant initial GF and find a solution by repeated integration.

For the first iteration step we choose the following simple one-pole expression (cf. Eq. (23)):

$$-\frac{1}{\pi}\,\mathrm{Im}\,G_{\boldsymbol{k}}^{\alpha\beta}(\boldsymbol{k};\omega)\approx\delta(\omega-E_{\boldsymbol{k}}^{\alpha\beta}(\boldsymbol{k}))\delta_{\alpha\beta}.\tag{37}$$

Then we obtain

$$M_\sigma^{\alpha\beta}(\boldsymbol{k};\omega)=\delta_{\alpha\beta}\left\{\frac{U^{(0)2}}{N^2}\sum_{\boldsymbol{pq}}\frac{N_\sigma^{\alpha\alpha\alpha}(\boldsymbol{kpq})}{\omega+E_{-\sigma}^{\alpha}(\boldsymbol{p}+\boldsymbol{q})-E_{-\sigma}^{\alpha}(\boldsymbol{q})-E_\sigma^{\alpha}(\boldsymbol{k}+\boldsymbol{p})}\right.$$

$$\left.+\frac{(U-\mathscr{J})^2+U^2}{N^2}\sum_{\boldsymbol{pq}}\frac{N_\sigma^{\nu\nu\alpha}(\boldsymbol{kpq})\,(1-\delta_{\alpha\nu})}{\omega+E_{-\sigma}^{\nu}(\boldsymbol{p}+\boldsymbol{q})-E_{-\sigma}^{\nu}(\boldsymbol{q})-E_\sigma^{\alpha}(\boldsymbol{k}+\boldsymbol{p})}\right\},\tag{38}$$

where

$$N_\sigma^{\alpha\beta\gamma}(\boldsymbol{kpq})=n_{\boldsymbol{p}+\boldsymbol{q}-\sigma}^{\alpha}[1-n_{\boldsymbol{k}+\boldsymbol{p}\sigma}^{\beta}-n_{\boldsymbol{q}-\sigma}^{\gamma}]+n_{\boldsymbol{k}+\boldsymbol{p}\sigma}^{\beta}n_{\boldsymbol{q}-\sigma}^{\gamma},$$

$$n_{\boldsymbol{p}\sigma}^{\alpha}=\{\exp[(E_\sigma^{\alpha}(\boldsymbol{p})-E_E)/kT]+1\}^{-1}.\tag{39}$$

As a limiting case for a simple one-band Hubbard model we directly obtain from (38) the second-order perturbation result

$$M_\sigma(\boldsymbol{k};\omega)=\frac{U^{(0)2}}{N^2}\sum_{\boldsymbol{pq}}\frac{n_{\boldsymbol{p}+\boldsymbol{q}-\sigma}(1-n_{\boldsymbol{k}+\boldsymbol{p}\sigma}-n_{\boldsymbol{q}-\sigma})+n_{\boldsymbol{k}+\boldsymbol{p}\sigma}n_{\boldsymbol{q}-\sigma}}{\omega+\varepsilon_{-\sigma}(\boldsymbol{p}+\boldsymbol{q})-\varepsilon_{-\sigma}(\boldsymbol{q})-\varepsilon_\sigma(\boldsymbol{k}+\boldsymbol{p})}.\tag{40}$$

6. Summary

We have presented in this paper the calculations of the electron Green function and self-energy for the case of the multiband transition metal described by the Hamiltonian with intra- and inter-orbital direct and exchange Coulomb interactions as well as with interatomic exchange Coulomb interaction included. We have used the irreducible Green function method in its simple formulation with a correct result in the band limit. Great advantage of this method lies in developing it to obtain the results appropriate both in the band and in the atomic limit [27]. This can be made by taking into consideration the equation of motion for the irreducible operators introduced in Eq. (9). Our resulting expressions for the Green function and the self-energy form the closed set of self-consistent equations. The self-consistency has been achieved after introducing simple decoupling of the three--point correlation function appearing in the exact expression for the self-energy. This procedure can be compared with the perturbation theory and diagram technique with the Hartree-Fock function as a bare function. In conclusion, the IFG method can be very useful in investigation of the many-body electronic effects even in very complicated systems. However, to take the vertex corrections into account one has to consider the equation of motion for the irreducible operators defined in Eq. (9) and form all possible one-particle and two-particle averages with different times in decoupling of the corresponding three--point correlation functions in the self-energy operator.

APPENDIX

The perturbation theory for self-energy

In paper [12] it was mentioned that an expansion of self-energy to higher orders in the Coulomb integral $U^{(0)}$ would improve the description of the correlation effects. Therefore, we want to describe briefly how the special kind of expansion for the self-energy can be made in a very simple workable way. Following paper [16] we may write (the diagonal case)

$$-\frac{1}{\pi}\,\mathrm{Im}\,G_\sigma^\alpha(\boldsymbol{k};\omega)=\frac{1}{\pi}\,\frac{\Gamma_\sigma^\alpha(\boldsymbol{k};\omega)}{[\omega-\tilde{E}_\sigma^\alpha(\boldsymbol{k})]^2+(\Gamma_\sigma^\alpha(\boldsymbol{k};\omega))^2}$$

$$\approx(1-\Lambda_\sigma^\alpha(\boldsymbol{k})\delta(\omega-\tilde{E}_\sigma^\alpha(\boldsymbol{k}))+\frac{1}{\pi}\,\frac{\Gamma_\sigma^\alpha(\boldsymbol{k};\omega)}{[\omega-\tilde{E}_\sigma^\alpha(\boldsymbol{k})]^2}\,, \tag{A.1}$$

where

$$\Gamma_\sigma^\alpha(\boldsymbol{k};\omega)=-\mathrm{Im}\,M_\sigma^\alpha(\boldsymbol{k};\omega), \tag{A.2}$$

$$\tilde{E}_\sigma^\alpha(\boldsymbol{k})=E_\sigma^\alpha(\boldsymbol{k})+\mathrm{Re}\,M_\sigma^\alpha(\boldsymbol{k};\tilde{E}_\sigma^\alpha(\boldsymbol{k})). \tag{A.3}$$

The unknown coefficient $(1-\Lambda_\sigma^\alpha(\boldsymbol{k}))$ in (A.1) must be determined from a normalization condition

$$-\frac{1}{\pi}\int_{-\infty}^{+\infty}\mathrm{Im}\,G_\sigma^\alpha(\boldsymbol{k};\omega)d\omega=1. \tag{A.4}$$

Then we obtain

$$\Lambda_\sigma^\alpha(\boldsymbol{k}) = \frac{U^{(0)2}}{N^2} \sum_{\boldsymbol{pq}} \frac{N_\sigma^{\alpha\alpha\alpha}(\boldsymbol{kpq})}{\Omega^{\alpha\alpha\alpha}(\boldsymbol{kpq}) - \tilde{E}_\sigma^\alpha(\boldsymbol{k})} + \frac{(U-\mathscr{J})^2 + U^2}{N^2} \sum_{\boldsymbol{pqv}} \frac{N_\sigma^{\nu\nu\alpha}(\boldsymbol{kpq})\,(1-\delta_{\alpha\nu})}{\Omega^{\nu\nu\alpha}(\boldsymbol{kpq}) - \tilde{E}_\sigma^\alpha(\boldsymbol{k})}, \quad \text{(A.5)}$$

where

$$\Omega^{\alpha\beta\gamma}(\boldsymbol{kpq}) = -\varepsilon_\alpha(\boldsymbol{p}+\boldsymbol{q}) + \varepsilon_\beta(\boldsymbol{k}+\boldsymbol{p}) + \varepsilon_\gamma(\boldsymbol{q}). \quad \text{(A.6)}$$

For the occupation numbers we obtain:

$$\begin{aligned} n_\sigma^\alpha = {} & \sum_{\boldsymbol{k}} n(\tilde{E}_\sigma^\alpha(\boldsymbol{k})) + U^{(0)2} N^{-2} \sum_{\boldsymbol{pqk}} \frac{N_\sigma^{\alpha\alpha\alpha}(\boldsymbol{kpq})}{[\Omega^{\alpha\alpha\alpha}(\boldsymbol{kpq}) - \tilde{E}_\sigma^\alpha(\boldsymbol{k})]^2} \\ & \times [n(\Omega^{\alpha\alpha\alpha}(\boldsymbol{kpq}) - n(\tilde{E}_\sigma^\alpha(\boldsymbol{k}))] \\ & + [(U-\mathscr{J})^2 + U^2] N^{-2} \sum_{\boldsymbol{kpqv}} \frac{N_\sigma^{\nu\nu\alpha}(\boldsymbol{kpq})\,(1-\delta_{\alpha\nu})}{[\Omega^{\nu\nu\alpha}(\boldsymbol{kpq}) - \tilde{E}_\sigma^\alpha(\boldsymbol{k})]^2} \\ & \times [n(\Omega^{\nu\nu\alpha}(\boldsymbol{kpq}) - n(\tilde{E}_\sigma^\alpha(\boldsymbol{k}))]. \end{aligned} \quad \text{(A.7)}$$

The first term in Eq. (A.7) describes the mean-field renormalization effect, and next two terms represent the effects of inelastic scattering. The partial density of states in this approximation is given by

$$\begin{aligned} D_\sigma^\alpha(\omega) = {} & N^{-2} \sum_{\boldsymbol{k}} (1 - \Lambda_\sigma^\alpha(\boldsymbol{k})) \delta(\omega - \tilde{E}_\sigma^\alpha(\boldsymbol{k})) \\ & + N^{-1} \sum_{\boldsymbol{k}} \{ U^{(0)2} N^{-2} \sum_{\boldsymbol{pq}} N_\sigma^{\alpha\alpha\sigma}(\boldsymbol{kpq}) \delta(\omega - \Omega^{\alpha\alpha\alpha}(\boldsymbol{kpq})) \\ & + \frac{(U-\mathscr{J})^2 + U^2}{(\omega - \tilde{E}_\sigma^\alpha(\boldsymbol{k})]^2} N^{-2} \sum_{\boldsymbol{pqv}} (1-\delta_{\alpha\nu}) N_\sigma^{\nu\nu\alpha}(\boldsymbol{kpq}) \delta(\omega - \Omega^{\nu\nu\alpha}(\boldsymbol{kpq})). \end{aligned} \quad \text{(A.8)}$$

If we use Eq. (A.8) for the calculation of the self-energy by substitution of Eq. (A.8) into the r.h.s. of Eqs (35), (36) we straightforwardly obtain a perturbation-type expansion for the self-energy up to order $U^{(0)6}$, U^6 and $\mathscr{T}^6$.

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