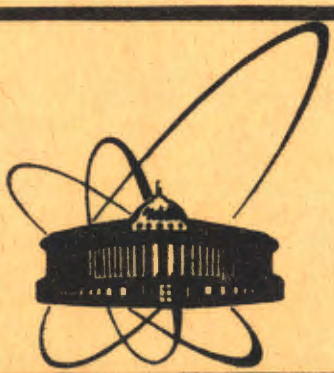

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R.Taranko, A.L.Kuzemsky

CORRELATION EFFECTS AND ELECTRONIC QUASIPARTICLE EXCITATIONS IN MULTIBAND TRANSITION METALS

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1. INTRODUCTION

In this paper we present a unified self-consistent consideration of the correlation effects in multiband transition metals. The main aim of this paper is to get more insight into the nature of electronic states in transition metals from a stand point of the quantum many-body theory. For this purpose we develope a new self-consistent formalism for the description of electronic elementary excitations in the framework of the multiband model by taking explicitly into account damping effects and finite lifetimes.

In 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 problem[2]. Correlations are usually introduced in band-structure computations through a local correction 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 extension, the spin-density functional formalism[3]. The first principle 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[4,5]. 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[1,6-8]. This approach has been quite successful in calculating various ground-state properties of transition metals[1,6-20]. Unfortunately, detailed investigations of the true nature of excited

electronic states in transition metals including the damping effects and finite lifetimes have been started only very recently when it has been recognized that many-body effects in transition metals are very important in understanding photoemission experiments [20-26]. As is pointed in paper [20], nickel, from several points of view, is the case for which many-electron correlation effects cannot be ignored. While photoemission reveals well-defined single-particle dispersion curves in nickel, they have a large energy width indicative of short quasiparticle lifetimes. Angle-resolved photoemission experiments providing direct observation of energy band dispersions in copper and nickel revealed a few problems for nickel: the presence of a satellite, narrowing of the d-band-width and other discrepancies with standard one-electron-band calculations. While explaining these features the importance of the correlation effects within the unfilled d-band has been generally recognized [20-26]. For transition metals like nickel 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 papers [27,28] within the degenerate Hubbard model by perturbation theory. A theory for the resonant 3d-band photoemission spectra in nickel has been developed in paper [29] on the basis of a hybridized s- and d -band model.

In this paper we present a new unified self-consistent approach to consider the correlation effects in transition metals like nickel The one-electron approximation is invalid in this case; thus the use of sophisticated many-body techniques is required. For this purpose we utilize the novel irreducible Green-function (IGF) method developed in papers [30,31]. The IGF method allows one completely 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 [32,33].

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 [34-41]. An important problem was to investigate the effect of the orbital degeneracy in transition metals by this method. A generalized Hubbard model of a d -band with its degeneracy fully included is more realistic

for transition metals than the one-band Hubbard model considered previously by the IGF method in paper [31]. Recently, a 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 [42]. 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. The numerical calculation is presented in Sect.6.

2. THE HAMILTONIAN OF THE MODEL

A better understanding of the electronic correlation in solids really dates [8] from Hubbard 's introduction of a new Hamiltonian [6,7] 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 of 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 intraatomic Coulomb repulsion and the one-electron hopping energy. The Hubbard model has been investigated by many authors with various assumptions (see, e.g., [1,6-19]). 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 fivefold degeneracy of d- states explicitly and to study the role of additional (to the Hubbard intra-atomic) terms for transition metaks like nickel. Let us start with the second quantized form of the total Hamiltonian for an electron in a solid. This method of describing many-particle systems is based on the choice of any complete set of orthogonal normalized wave functions. In our approach we take the set $\{\phi_\lambda(\mathbf{r}-\mathbf{R}_i)\}$ of the Wannier functions [43]. Here λ is the band index. For a degenerate d-band the second quantized form of the total Hamiltonian in

the Wannier-function representation is given by

$$H = \sum_{ij} \sum_{\mu\nu\sigma} t_{ij}^{\mu\nu} a_{i\mu\sigma}^{+} a_{j\nu\sigma} + 1/2 \sum_{ijmn} \sum_{\alpha\beta\gamma\delta\sigma\sigma'} \langle i\alpha, j\beta | \hat{v} | m\gamma, n\delta \rangle \times \quad (1)$$

$$\times a_{i\alpha\sigma}^{+} a_{j\beta\sigma'}^{+} a_{m\gamma\sigma'} a_{n\delta\sigma} ,$$

where

$$\langle i\alpha, j\beta | \hat{v} | m\gamma, n\delta \rangle = \quad (2)$$

$$= \int \phi_\alpha^*(\vec{r}-\vec{R}_i)\, \phi_\beta^*(\vec{r}\,'-\vec{R}_j)\, \hat{v}(|\vec{r}-\vec{r}\,'|)\, \phi_\gamma(\vec{r}\,'-\vec{R}_m)\, \phi_\delta(\vec{r}-\vec{R}_n)\, d^3r\, d^3r' .$$

The purpose of the present consideration is to apply the IGF method to this total many-electron Hamiltonian (1). Relevant calculations have been carried out. The obtained formulae, however, are complicated. To give a physical picture of the calculations, in this paper we restrict ourselves to the following model Hamiltonian

$$H = H_1 + H_2 + H_3 . \quad (3)$$

The one-electron energy operator of the d -band electrons is given by the expression:

$$H_1 = \sum_{ij} \sum_{\mu\nu\sigma} t_{ij}^{\mu\nu} a_{i\mu\sigma}^{+} a_{j\nu\sigma} . \quad (4)$$

The term H_2 describes one-centre Coulomb interactions of d -electrons:

$$H_2 = \frac{1}{2} \sum_{i\alpha\sigma} U_{\alpha\alpha} n_{i\alpha\sigma} n_{i\alpha-\sigma} + 1/2 \sum_{i\alpha\beta\sigma\sigma'} U'_{\alpha\beta} n_{i\alpha\sigma} n_{i\beta\sigma'} (1-\delta_{\alpha\beta}) -$$

$$- \frac{1}{2} \sum_{i\alpha\beta\sigma} I_{\alpha\beta} n_{i\alpha\sigma} n_{i\beta\sigma} (1-\delta_{\alpha\beta}) + 1/2 \sum_{i\alpha\beta\sigma} I'_{\alpha\beta} (1-\delta_{\alpha\beta}) a_{i\alpha\sigma}^{+} a_{i\alpha-\sigma}^{+} a_{i\beta-\sigma} a_{i\beta\sigma} -$$

$$- \frac{1}{2} \sum_{i\alpha\beta\sigma} I_{\alpha\beta} a_{i\alpha\sigma}^{+} a_{i\alpha-\sigma} a_{i\beta-\sigma}^{+} a_{i\beta\sigma} . \quad (5)$$

In addition to the intrasite Coulomb interaction $U_{\alpha\alpha}$ which is the only interaction present in the Hubbard model, the Hamiltonian (5) contains three more kinds of interactions. The last term H_3 describes the direct intersite exchange interaction

$$H_3 = -1/2 \sum_{ij\alpha} \sum_{\sigma\sigma'} J_{ij}^{\alpha\alpha} a_{i\alpha\sigma}^{+} a_{i\alpha\sigma'} a_{j\alpha\sigma'}^{+} a_{j\alpha\sigma} . \quad (6)$$

Here, we take only interactions H_3 diagonal in orbital index. Thus, our Hamiltonian (3) includes only a one-centre and two-centre integrals of various kinds. In eqs. (4)-(6) these various integrals are defined as follows:

$$t_{ij}^{\mu\nu} = \langle i\mu | \hat{h} | j\nu \rangle ; \quad U_{\alpha\alpha} = \langle i\alpha, i\alpha | \hat{v} | i\alpha, i\alpha \rangle$$

$$U'_{\alpha\beta} = \langle i\alpha, i\beta | \hat{v} | i\beta, i\alpha \rangle ; \quad I_{\alpha\beta} = \langle i\alpha, i\beta | \hat{v} | i\alpha, i\beta \rangle , \quad \alpha \neq \beta \quad (7)$$

$$I'_{\alpha\beta} = \langle i\alpha, i\alpha | \hat{v} | i\beta, i\beta \rangle ; \quad J_{ij}^{\alpha\alpha} = \langle i\alpha, j\alpha | \hat{v} | i\alpha, j\alpha \rangle ; \quad i \neq j.$$

In the above equations $\hat{v}$ is assumed to represent an effective interaction screened by s- and d -electrons. It is reasonable to assume that:

$$U_{\alpha\alpha} = U ; \quad U'_{\alpha\beta} = U' ; \quad I_{\alpha\beta} = I , \quad I'_{\alpha\beta} = I' ; \quad J_{ij}^{\alpha\alpha} = J_{ij} . \quad (8)$$

Thus, the Hamiltonian (3) is specified by six parameters: the band width W and five integrals U , U' , I , I' , J. We note that s -electrons are not explicitly taken into account in our model Hamiltonian (3), 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 (3) let us consider the equation of motion for the one-electron double-time temperature Green function [44];

$$G_{\sigma\sigma'}^{\alpha\beta}(ij, t-t') = -i\Theta(t-t') \langle [a_{i\alpha\sigma}(t), a_{j\beta\sigma'}^{+}(t')]_+ \rangle = \quad (9)$$

$$= \langle\langle a_{i\alpha\sigma}(t) , a_{j\beta\sigma'}^{+}(t') \rangle\rangle .$$

First performing the time t differentiation of (9) we get the equation for the Fourier transform $G_{\sigma\sigma'}^{\alpha\beta}(ij;\omega)$

$$\sum_{\ell\nu} T^{\alpha\nu}(i\ell) G_{\sigma\sigma'}^{\nu\beta}(\ell j;\omega) = \delta_{ij} \delta_{\alpha\beta} \delta_{\sigma\sigma'} + \sum_{\ell\nu} \{ V_1^{\alpha\nu}(i\ell) \langle\langle a_{\ell\alpha\sigma} n_{\ell\nu\sigma} | a_{j\beta\sigma'}^{+} \rangle\rangle_\omega +$$

$$+ V_2^{\alpha\nu}(i\ell) \langle\langle a_{\ell\alpha\sigma} n_{\ell\nu-\sigma} | a_{j\beta\sigma'}^{+} \rangle\rangle_\omega +$$

$$+ (V_3^{a\nu}(i\ell) + V_4^{a\nu}(i\ell)) \ll a_{\ell\alpha-\sigma} a^+_{\ell\nu-\sigma} a_{\ell\nu\sigma} \mid a^+_{j\beta\sigma'} \gg_\omega +$$

$$+ V_5^{a\nu}(i\ell)(\ll a_{i\nu\sigma} n_{\ell\nu\sigma} \mid a^+_{j\beta\sigma'} \gg_\omega + \ll a_{i\nu-\sigma} a^+_{i\nu-\sigma} a_{\ell\nu\sigma} \mid a^+_{j\beta\sigma'} \gg_\omega)\}, \tag{10}$$

where

$$T^{a\nu}(i\ell) = \omega \delta_{\ell_i} \delta_{a\nu} - t^{a\nu}_{i\ell} \; ; \; V_1^{a\nu}(i\ell) = (U' - I)(1 - \delta_{a\nu}) \delta_{i\ell}$$

$$V_2^{a\nu}(i\ell) = [U \delta_{a\nu} + U'(1 - \delta_{a\nu})] \delta_{i\ell} \; ; \; V_3^{a\nu}(i\ell) = -I(1 - \delta_{a\nu}) \delta_{i\ell} \tag{11}$$

$$V_4^{a\nu}(i\ell) = -I'(1 - \delta_{a\nu}) \delta_{i\ell} \; ; \; V_5^{a\nu}(i\ell) = -J_{i\ell}(1 - \delta_{i\ell}) \delta_{a\nu} \; .$$

The aim of the present investigation is to thoroughly study the correlation effects in transition metals. Therefore, the adequate approximation is the weak correlation limit: U/W, U'/W, I/W, I'/W, $J/W < 1$.

To treat the many-body problem in a self-consistent way, we follow here the IGF method [31]. In the weak correlation limit we introduce by definition the irreducible parts of the CF in the r.h.s. of eq.(10)

$$\ll a_{i\mu\sigma} a^+_{\ell\nu\sigma'} a_{\ell\nu\sigma'} \mid a^+_{j\beta\sigma_1} \gg_\omega = \overset{ir}{\ll} a_{i\mu\sigma} a^+_{\ell\nu\sigma} a_{\ell\nu\sigma'} \mid a^+_{j\beta\sigma_1} \gg_\omega +$$

$$+ \langle n_{\ell\nu\sigma'} \rangle \ll a_{i\mu\sigma} \mid a^+_{j\beta\sigma_1} \gg_\omega + \langle a_{i\mu\sigma} a^+_{\ell\nu\sigma'} \rangle \ll a_{\ell\nu\sigma'} \mid a^+_{j\beta\sigma_1} \gg_\omega \tag{12}$$

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

$$\langle [(a_{i\mu\sigma} n_{\ell\nu\sigma'})^{ir}, a^+_{j\beta\sigma_1}]_+ \rangle = 0. \tag{13}$$

From eqs.(12) and (13) we find:

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

$$= \langle [(a_{i\mu\sigma} n_{\ell\nu\sigma'} - \langle n_{\ell\nu\sigma'} \rangle a_{i\mu\sigma} - \langle a_{i\mu\sigma} a^+_{\ell\nu\sigma} \rangle a_{\ell\nu\sigma'}), a^+_{j\beta\sigma_1}]_+ \rangle =$$

$$= \langle [a_{i\mu\sigma} n_{\ell\nu\sigma'}, a^+_{j\beta\sigma_1}]_+ \rangle - \langle n_{\ell\nu\sigma'} \rangle \delta_{ij} \delta_{\mu\beta} \delta_{\sigma\sigma_1} -$$

$$- \langle a_{i\mu\sigma} a^+_{\ell\nu\sigma} \rangle \delta_{\ell j} \delta_{\nu\beta} \delta_{\sigma'\sigma_1} \equiv 0. \tag{14}$$

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 the 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" [45]. However, it must be stressed that because of the spin rotational invariance of Hamiltonian (3) we have $\langle a_{i\alpha\sigma} a^+_{j\beta-\sigma} \rangle = 0$. The spin-flip anomalous terms must be included only for a rather special case of the system magnetized in the x direction instead of the conventional z axis. 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, i.e., $\langle n_{i\mu\sigma} \rangle$. 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 [35-38] and for the magnetic polaron problem at finite temperatures [41].

Using the definition (12) in eq.(10) the equation of motion (10) can be *exactly* transformed to the following form:

$$\sum_{\ell\nu} E^{a\nu}_\sigma(i\ell) G^{\nu\beta}_\sigma(\ell j;\omega) = \delta_{ij} \delta_{a\beta} + \sum_{\ell\nu} \{V_1^{a\nu}(i\ell) \overset{ir}{\ll} a_{\ell a\sigma} n_{\ell\nu\sigma} \mid a^+_{j\beta\sigma} \gg_\omega +$$

$$+ V_2^{a\nu}(i\ell) \overset{ir}{\ll} a_{\ell a\sigma} n_{\ell\nu-\sigma} \mid a^+_{j\beta\sigma} \gg_\omega +$$

$$+ (V_3^{a\nu}(i\ell) + V_4^{a\nu}(i\ell)) \overset{ir}{\ll} a_{\ell\alpha-\sigma} a^+_{\ell\nu-\sigma} a_{\ell\nu\sigma} \mid a^+_{j\beta\sigma} \gg_\omega + \tag{15}$$

$$+ V_5^{a\nu}(i\ell)(\overset{ir}{\ll} a_{i\nu\sigma} n_{\ell\nu\sigma} \mid a^+_{j\beta\sigma} \gg_\omega + \overset{ir}{\ll} a_{i\nu-\sigma} a^+_{i\nu-\sigma} a_{\ell\nu\sigma} \mid a^+_{j\beta\sigma} \gg_\omega)\}.$$

The renormalized energy $E^{a\nu}_\sigma(i\ell)$ is given by the expression

$$E^{a\nu}_\sigma(i\ell) = T^{a\nu}(i\ell) - V_1^{a\nu}(i\ell) \langle a_{\ell a\sigma} a^+_{\ell\nu\sigma} \rangle -$$

$$- \sum_\mu (V_1^{\nu\mu}(i\ell) \delta_{a\nu} \langle n_{\ell\mu\sigma} \rangle - V_2^{\nu\mu}(i\ell) \delta_{a\nu} \langle n_{\ell\mu-\sigma} \rangle) -$$

$$- V_3^{a\nu}(i\ell) \langle a_{\ell\alpha-\sigma} a^+_{\ell\nu-\sigma} \rangle - V_4^{a\nu}(i\ell) \langle a_{\ell\nu-\sigma} a^+_{\ell\alpha-\sigma} \rangle - \tag{16}$$

$$- V_5^{a\nu}(i\ell)(\langle a_{i\nu\sigma} a^+_{\ell\nu\sigma} \rangle - \langle a_{i\nu-\sigma} a^+_{\ell\nu-\sigma} \rangle) - \sum_j V_5^{a\nu}(ij) \delta_{i\ell} \langle n_{j\nu\sigma} \rangle .$$

Now we proceed to derive the Dyson equation. To calculate the IGF's $\overset{ir}{\ll} A(t) B(t') \gg$ in eq. (15), we have to write the equa-

tions of motion after differentiation with respect to the second time variable t'. Then conditions (13) remove the inhomogeneous terms in these equations. If one introduces irreducible parts for the right-hand-side operators by analogy with expression (12), the equation of motion (15) can be *exactly* rewritten in the following form

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

where the generalized mean-field Green function G_0 reads

$$\sum_{\ell\nu} E_{\sigma}^{\alpha\nu}(i\ell)G_{0\sigma}^{\nu\beta}(\ell j;\omega)=\delta_{\alpha\beta}\delta_{ij} \ . \tag{18}$$

The scattering operator P is given by the expression

$$\begin{aligned} P_{\sigma}^{\alpha\beta}(ij;\omega)=\sum_{mn}\sum_{\mu\nu}\{ & V_1^{\alpha\nu}(im)V_1^{\mu\beta}(nj)\overset{ir}{\ll} a_{m\alpha\sigma}n_{m\nu\sigma}|a_{n\beta\sigma}^{+}n_{n\mu\sigma}\overset{ir}{\gg}_{\omega}+ \\ + & V_1^{\alpha\nu}(im)V_2^{\mu\beta}(nj)\overset{ir}{\ll} a_{m\alpha\sigma}n_{m\nu\sigma}|a_{n\beta\sigma}^{+}n_{n\mu-\sigma}\overset{ir}{\gg}_{\omega}+ \\ + & V_2^{\alpha\nu}(im)V_1^{\mu\beta}(nj)\overset{ir}{\ll} a_{m\alpha\sigma}n_{m\nu-\sigma}|a_{n\beta\sigma}^{+}n_{n\mu\sigma}\overset{ir}{\gg}_{\omega}+ \\ + & V_2^{\alpha\nu}(im)V_2^{\mu\beta}(nj)\overset{ir}{\ll} a_{m\alpha\sigma}n_{n\mu-\sigma}|a_{n\beta\sigma}^{+}n_{n\mu-\sigma}\overset{ir}{\gg}_{\omega}\}. \end{aligned} \tag{19}$$

Here we present for brevity the scattering operator only for a part of Hamiltonian (3), i.e., $H=H_1+H_2$ without two last terms in H_2. The full scattering operator can be written directly.

If we go further and write down the Dyson equation

$$G_{\sigma}^{\alpha\beta}(ij;\omega)=G_{0\sigma}^{\alpha\beta}(ij;\omega)+\sum_{mn}\sum_{\mu\nu} G_{0\sigma}^{\alpha\mu}(im;\omega)M_{\sigma}^{\mu\nu}(mn;\omega)G_{\sigma}^{\nu\beta}(nj;\omega) \tag{20}$$

we get the following equation for M

$$P_{\sigma}^{\mu\nu}(mn;\omega)=M_{\sigma}^{\mu\nu}(mn;\omega)+\sum_{ij}\sum_{\alpha\beta} M_{\sigma}^{\mu\alpha}(mi;\omega)G_0^{\alpha\beta}(ij;\omega)P_{\sigma}^{\beta\nu}(jn;\omega) \tag{21}$$

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

$$M_{\sigma}^{\mu\nu}(mn;\omega)=(P_{\sigma}^{\mu\nu}(mn;\omega))^{c}. \tag{22}$$

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 future 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 $a_{\vec{k}\alpha\sigma}$ connecting the electron state with an orbital symmetry α centered at atomic site $\vec{R}_i$ and the Bloch state $|\vec{k}\rangle$ of the same symmetry. The exact transformation reads[43,46,47]

$$a_{\vec{k}\lambda\sigma}=N^{-1/2}\sum_{j\beta}\exp[-i\vec{k}\vec{R}_j]U_{\lambda\beta}^{+}(\vec{k})a_{j\beta\sigma} \ ; \quad U^{+}=U^{-1}. \tag{23}$$

However, for the sake of simplicity, we shall follow the approximative approach of papers[13,28] where the following transformation

$$a_{\vec{k}\alpha\sigma}=N^{-1/2}\sum_{i}\exp[-i\vec{k}\vec{R}_i]a_{i\alpha\sigma} \tag{24}$$

has been used instead of the exact one, as given by eq. (23). The second quantized operators in eq.(24) generate five artificial uncoupled bands for which $\alpha = 1,2,\ldots 5$. When coupled by $U_{\lambda\beta}(\vec{k})$ they reproduce the realistic bands labelled by λ, as given by eq.(23). This is, of course, a simplification of the problem. We discuss this approximation more thoroughly in Appendix A. The adoption of the approximative expression (24) is equivalent to the following definitions of the Fourier transform

$$G_{\sigma}^{\alpha\beta}(ij;\omega)=N^{-1}\sum_{\vec{k}}\exp[i\vec{k}(\vec{R}_i-\vec{R}_j)]G^{\alpha\beta}(\vec{k},\omega) \tag{25}$$

$$M^{\alpha\beta}(ij;\omega)=N^{-1}\sum_{k}\exp[i\vec{k}(\vec{R}_i-\vec{R}_j)]M^{\alpha\beta}(\vec{k},\omega) \tag{26}$$

$$t_{ij}^{\alpha\alpha} = N^{-1} \sum_{\vec{k}} \epsilon_\alpha(\vec{k}) \exp[i\vec{k}(\vec{R}_i - \vec{R}_j)]. \quad (27)$$

Using the definitions (25)-(27) in eq.(20) we find

$$G_\sigma^{\alpha\beta}(\vec{k},\omega) = G_{0\sigma}^{\alpha\beta}(\vec{k},\omega) + \sum_{\mu\nu} G_{0\sigma}^{\alpha\mu}(\vec{k},\omega) M_\sigma^{\mu\nu}(\vec{k},\omega) G_\sigma^{\nu\beta}(\vec{k},\omega). \quad (28)$$

From the symbolic solution of the Dyson equation (28)

$$G(\vec{k},\omega) = [(G_0(\vec{k},\omega))^{-1} - M(\vec{k},\omega)]^{-1} \quad (29)$$

it is now seen how to change the problem of calculating the single-particle GF G to the one of calculating the generalized mean-field GF G_0 and the self-energy M.

Let us first consider the mean-field GF G_0. In the momentum representation we obtain from eq.(18)

$$\sum_\nu E_\sigma^{\alpha\nu}(\vec{k}) G_0^{\nu\beta}(\vec{k},\omega) = \delta_{\alpha\beta}. \quad (30)$$

The renormalized energies $E_\sigma^{\alpha\beta}(\vec{k})$ have the form

$$E_\sigma^{\alpha\nu}(\vec{k}) = (\omega - \epsilon_\alpha(\vec{k}))\delta_{\alpha\nu} - (U'-I)(1-\delta_{\alpha\nu}) N^{-1} \sum_p \langle a_{p\alpha\sigma} a^+_{p\nu\sigma} \rangle -$$

$$- \sum_\mu ((U'-I)(1-\delta_{\alpha\mu})\delta_{\alpha\nu} N^{-1} \sum_p \langle n_{p\mu\sigma} \rangle -$$

$$- (U\delta_{\alpha\mu} + U'(1-\delta_{\alpha\mu}))\delta_{\alpha\nu} N^{-1} \sum_p \langle n_{p\mu-\sigma} \rangle + I'(1-\delta_{\alpha\nu}) N^{-1} \sum_p \langle a_{p\alpha-\sigma} a^+_{p\nu-\sigma} \rangle + \quad (31)$$

$$+ I(1-\delta_{\alpha\nu}) N^{-1} \sum_p \langle a_{p\nu-\sigma} a^+_{p\alpha-\sigma} \rangle +$$

$$+ \delta_{\alpha\nu}(J(\vec{0}) N^{-1} \sum_p \langle a^+_{k+p\nu\tau} a_{p\nu\sigma} \rangle - N^{-1} \sum_p J(\vec{k}-\vec{p}) \sum_{\sigma_1} \langle a_{p\nu\sigma_1} a^+_{p\nu\sigma_1} \rangle),$$

where

$$J(\vec{k}) = N^{-1} \sum_{ij} J_{ij} \exp[-i\vec{k}(\vec{R}_i - \vec{R}_j)]. \quad (32)$$

For the multiorbital Hubbard model ($U' = I = I' = J = 0$) we find

$$E_\sigma^{\alpha\nu}(\vec{k}) = [\omega - \epsilon_\alpha(\vec{k}) - U N^{-1} \sum_p \langle n_{p\alpha-\sigma} \rangle] \delta_{\alpha\nu}. \quad (33)$$

The spectrum of electronic low-lying excitations without damping follows immediately from the poles of the single-particle mean-field Green function G_0 (G_0 denotes a matrix in the space of band indices):

$$\det|\overline{E_\sigma}| = 0; \qquad \det|\overline{E_{-\sigma}}| = 0. \quad (34)$$

It is obvious that most important is the case diagonal in the band indices:

$$E_\sigma^{\alpha\alpha}(\vec{k}) G_{0\sigma}^{\alpha\alpha}(\vec{k},\omega) = 1 \quad (35)$$

because if a Green function is diagonal with respect to some set of single-particle functions, these functions are "natural" orbitals of the problem. Hence, we may write for the diagonal case

$$G_{0\uparrow}^{\alpha\alpha}(\vec{k},\omega) = [E_\uparrow^{\alpha\alpha}(\vec{k})]^{-1}; \qquad G_{0\downarrow}^{\alpha\alpha}(\vec{k},\omega) = [E_\downarrow^{\alpha\alpha}(\vec{k})]^{-1}, \quad (36)$$

where

$$E_\sigma^{\alpha\alpha}(\vec{k}) = \omega - \epsilon_\alpha(\vec{k}) - (U'-I) \sum_\mu (1-\delta_{\alpha\mu}) N_\sigma^\mu -$$

$$- \sum_\mu (U\delta_{\alpha\mu} + U'(1-\delta_{\alpha\mu})) N_{-\sigma}^\mu - \quad (37)$$

$$- \sum_{\sigma_1} N^{-1} \sum_p J(\vec{k}-\vec{p}) \langle a_{p\alpha\sigma_1} a^+_{p\alpha\sigma_1} \rangle + J(\vec{0}) N^{-1} \sum_p \langle a^+_{k+p\alpha\sigma} a_{p\alpha\sigma} \rangle \quad (38)$$

$$N_\sigma^\mu = N^{-1} \sum_p \langle n_{p\mu-\sigma} \rangle.$$

It follows from eq. (37) that in a complete analogy with the one-band case one can define the band splitting Δ^α in the following form

$$\Delta^\alpha = E_\uparrow^\alpha(\vec{k}) - E_\downarrow^\alpha(\vec{k}) = U(N_\uparrow^\alpha - N_\downarrow^\alpha) + I \sum_\nu (1-\delta_{\alpha\nu})(N_\uparrow^\nu - N_\downarrow^\nu) +$$

$$+ J(\vec{0}) N^{-1} \sum_p (\langle a^+_{k+p\alpha\uparrow} a_{p\alpha\uparrow} \rangle - \langle a^+_{k+p\alpha\downarrow} a_{p\alpha\downarrow} \rangle). \quad (39)$$

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

5. ELECTRONIC QUASI-PARTICLES AND THEIR DAMPING

Now let us take into consideration the damping effects and finite lifetimes. Hence, our next task consists in obtaining self-consistent approximative 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 a single-particle Green function (c.f. [40,41])

$$G_\sigma^{\alpha\nu}(\vec{k},\omega) = \{[G_{0\sigma}^{\alpha\nu}(\vec{k},\omega)]^{-1} - \Sigma_\sigma^{\alpha\nu}(\vec{k},\omega)\}^{-1}. \quad (40)$$

Here $\Sigma_\sigma^{a\nu}(\vec{k},\omega)$ is a functional of $M_\sigma^{a\nu}(\vec{k},\omega)$

$$\Sigma_\sigma^{a\nu}(\vec{k},\omega)=F[M_\sigma^{a\nu}(\vec{k},\omega)]. \tag{41}$$

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

$$\tilde{\epsilon}_\sigma^a(\vec{k})-E_\sigma^{aa}(\vec{k})-\mathrm{Re}\,\Sigma_\sigma^{aa}[\vec{k},\tilde{\epsilon}_\sigma^a(\vec{k})]=0. \tag{42}$$

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

$$g_\sigma^a(\vec{k},\omega)\propto \mathrm{Im}G_\sigma^{aa}(\vec{k},\omega) \tag{43}$$

will have a strong maxima at energies of the quasiparticle state.

Thus, now we have to find the matrix elements of self-energy $\hat{M}$ to complete our solution of the problem. To find explicit expressions for $M_\sigma^{a\nu}(\vec{k},\omega)$, we have to evaluate higher-order Green functions in eq.(19). In the quasimomentum representation we obtain from eqs.(19) and (26)

$$\begin{aligned}M_\sigma^{a\beta}(\vec{k},\omega)=N^{-2}\sum_{\mu\nu}\sum_{pqrs}\{&V_1^{a\nu}V_1^{\mu\beta}\,{}^{ir}\!\ll a_{k+p\alpha\sigma}a^+_{p+q\nu\sigma}a_{q\nu\sigma}\,|\,a^+_{k+s\beta\sigma}a^+_{r\mu\sigma}a_{r+s\mu\sigma}\gg_\omega^{ir,c}+\\&+V_1^{a\nu}V_2^{\mu\beta}\,{}^{ir}\!\ll a_{k+p\alpha\sigma}\;a^+_{p+q\nu\sigma}\;a_{q\nu\sigma}\,|\,a^+_{k+s\beta\sigma}a^+_{r\mu-\sigma}a_{r+s\mu-\sigma}\gg_\omega^{ir,c}+\\&+V_2^{a\nu}V_1^{\mu\beta}\,{}^{ir}\!\ll a_{k+p\alpha\sigma}\,a^+_{p+1q\nu-\sigma}a_{q\nu-\sigma}\,|\,a^+_{k+s\beta\sigma}a^+_{r\mu\sigma}\;a_{r+s\mu\sigma}\gg_\omega^{ir,c}+\\&+V_2^{a\nu}V_2^{\mu\beta}\,{}^{ir}\!\ll a_{k+p\alpha\sigma}\,a^+_{p+q\nu-\sigma}a_{q\nu-\sigma}\,|\,a^+_{k+s\beta\sigma}a^+_{r\mu-\sigma}a_{r+s\mu-\sigma}\gg_\omega^{ir,c}\}.\end{aligned} \tag{44}$$

It is convenient to write down $\ll A\,|\,A^+\gg$ in terms of the correlation functions in the form

$$\begin{aligned}&\ll a_{k+p\alpha\sigma}\;a^+_{p+q\nu\sigma}a_{q\nu\sigma}\,|\,a^+_{k+s\beta\sigma}a^+_{r\mu\sigma}\;a_{r+s\mu\sigma}\gg_\omega=\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{d\omega'}{\omega-\omega'}(e^{\beta\omega'}+1)\times\\&\times\int_{-\infty}^{\infty}dt\,e^{i\omega' t}<a^+_{k+s\beta\sigma}(t)a^+_{r\mu-\sigma}(t)\;a_{r+s\mu-\sigma}(t)a_{k+p\alpha\sigma}a^+_{p+q\nu\sigma}a_{q\nu\sigma}>.\end{aligned} \tag{45}$$

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.(45) in terms of single-particle correlation functions

$$<a^+_{k+s\beta\sigma}(t)a^+_{r\mu-\sigma}(t)a_{r+s\mu-\sigma}(t)a_{k+p\alpha\sigma}\;a^+_{p+q\nu-\sigma}a_{q\nu-\sigma}>^{ir,c}\simeq<a^+_{k+p\beta\sigma}(t)a_{k+p\alpha\sigma}>\times$$

$$\times<a^+_{q\mu-\sigma}(t)a_{q\nu-\sigma}><a_{p+q\mu\sigma}(t)a^+_{p+q\nu-\sigma}>\times\delta_{k+s,k+p}\cdot\delta_{rq}\cdot\delta_{r+s,p+q} \tag{46}$$

Taking into account the spectral theorem we obtain from (44)–(46)

$$M_\sigma^{a\beta}(\vec{k},\omega)=N^{-2}\sum_{\mu\nu}\sum_{pq}\{V_1^{a\nu}V_1^{\mu\beta}Q_{1\sigma}^{a\mu\nu\beta}(\vec{k}\vec{p}\vec{q};\omega)+V_2^{a\nu}V_2^{\mu\beta}Q_{2\sigma}^{a\mu\nu\beta}(\vec{k}\vec{p}\vec{q};\omega)\}, \tag{47}$$

where

$$\begin{aligned}Q_{1\sigma}^{a\mu\nu\beta}(\vec{k}\vec{p}\vec{q};\omega)=(-\tfrac{1}{\pi})^3\iiint_{-\infty}^{\infty}\frac{d\omega_1 d\omega_2 d\omega_3}{\omega+\omega_1-\omega_2-\omega_3}\{n(\omega_1)[1-n(\omega_2)-n(\omega_3)]+n(\omega_2)n(\omega_3)\}\times\\\times\{\mathrm{Im}G_\sigma^{\mu\nu}(\vec{p}+\vec{q},\omega_1)\mathrm{Im}G_\sigma^{\nu\mu}(\vec{q},\omega_2)\mathrm{Im}G_\sigma^{a\beta}(\vec{k}+\vec{p},\omega_3)+\\+\mathrm{Im}G_\sigma^{\mu\nu}(\vec{p}+\vec{q},\omega_1)\mathrm{Im}G_\sigma^{\nu\beta}(\vec{q},\omega_2)\mathrm{Im}G_\sigma^{a\mu}(\vec{k}+\vec{p},\omega_3)\}\end{aligned} \tag{48}$$

$$\begin{aligned}Q_{2\sigma}^{a\mu\nu\beta}(\vec{k}\vec{p}\vec{q};\omega)=(-\tfrac{1}{\pi})^3\iiint_{-\infty}^{\infty}\frac{d\omega_1 d\omega_2 d\omega_3}{\omega+\omega_1-\omega_2-\omega_3}\{n(\omega_1)[1-n(\omega_2)-n(\omega_3)]+n(\omega_2)n(\omega_3)\}\times\\\times\mathrm{Im}G_{-\sigma}^{\mu\nu}(\vec{p}+\vec{q},\omega_1)\mathrm{Im}G_{-\sigma}^{\nu\mu}(\vec{q},\omega_2)\mathrm{Im}G_\sigma^{a\beta}(\vec{k}+\vec{p},\omega_3).\end{aligned} \tag{49}$$

Equations (29) and (47) form a closed self-consistent system of equations for the single-particle electron GF for the generalized multiband Hubbard model described by Hamiltonian (3). In principle, we may use, in the r.h.s. of eq.(47), 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.(33))

$$-\frac{1}{\pi}\mathrm{Im}G_\sigma^{a\beta}(\vec{k},\omega)\cong\delta(\omega-E_\sigma^{a\beta}(\vec{k}))\delta_{a\beta},\quad E_\sigma^{a\nu}(\vec{k})=[\omega-\epsilon_a(\vec{k})-UN_{-\sigma}^a]\delta_{a\nu}. \tag{50}$$

Then we obtain

$$\begin{aligned}M_\sigma^{a\beta}(\vec{k},\omega)=\delta_{a\beta}\{&\frac{U^2}{N^2}\sum_{pq}\frac{N_\sigma^{aaa}(\vec{k}\vec{p}\vec{q})}{\omega+E_{-\sigma}^a(\vec{p}+\vec{q})-E_{-\sigma}^a(\vec{q})-E_\sigma^a(\vec{k}+\vec{p})}+\\&+\frac{(U'-I)^2+(U')^2}{N^2}\sum_{pq\nu}\frac{N_\sigma^{\nu\nu a}(\vec{k}\vec{p}\vec{q})(1-\delta_{a\nu})}{\omega+E_{-\sigma}^\nu(\vec{p}+\vec{q})-E_{-\sigma}^\nu(\vec{q})-E_\sigma^a(\vec{k}+\vec{p})}\},\end{aligned} \tag{51}$$

where

$$N_\sigma^{\nu_1\nu_2\nu_3}(\vec{k}\vec{p}\vec{q})=n_{p+q,-\sigma}^{\nu_1}[1-n_{k+p\sigma}^{\nu_2}-n_{q-\sigma}^{\nu_3}]+n_{k+p\sigma}^{\nu_2}n_{q-\sigma}^{\nu_3} \tag{52}$$

$$n_{p\sigma}^\nu=[\exp(\beta E_\sigma^\nu(\vec{p}))+1]^{-1}. \tag{53}$$

For a simple one-band Hubbard model we directly obtain from (51) the result by Kuzemsky[31]:

$$M_\sigma(\vec{k},\omega)=\frac{U^2}{N^2}\sum_{pq}\frac{n_{p+q\sigma}[1-n_{k+p\sigma}-n_{q-\sigma}]+n_{k+p\sigma}n_{q-\sigma}}{\omega+E_{-\sigma}(\vec{p}+\vec{q})-E_{-\sigma}(\vec{q})-E_\sigma(\vec{k}+\vec{p})}. \tag{54}$$

In the region of the resonance between the one-particle and collective excitations another approximation is possible, instead of (46):

$$\langle a^+_{j\beta\sigma_1}(t)a^+_{j\mu\sigma_2}(t)a_{j\mu\sigma_2}(t)a_{i\alpha\sigma_3}a^+_{i\nu\sigma_4}a_{i\nu\sigma_4}\rangle \approx$$

$$\approx \langle a^+_{j\beta\sigma_1}(t)a_{i\alpha\sigma_3}\rangle\langle n_{j\mu\sigma_2}(t)n_{i\nu\sigma_4}\rangle + \langle a^+_{j\beta\sigma_1}(t)a_{i\nu\sigma_4}\rangle$$

$$\times\langle n_{j\mu\sigma_2}(t)a_{i\alpha\sigma_3}a^+_{i\nu\sigma_4}\rangle + \langle a^+_{j\mu\sigma_2}(t)a_{i\alpha\sigma_3}\rangle\langle a^+_{j\beta\sigma_1}(t)a_{j\mu\sigma_2}(t)n_{i\nu\sigma_4}\rangle + \tag{55}$$

$$+\langle a^+_{j\mu\sigma_2}(t)a_{i\nu\sigma_4}\rangle\langle a^+_{j\beta\sigma_1}(t)a_{j\mu\sigma_2}(t)a_{i\alpha\sigma_3}a^+_{i\nu\sigma_4}\rangle +$$

$$+\langle a_{j\mu\sigma_2}(t)a^+_{i\nu\sigma_4}\rangle\langle a^+_{j\beta\sigma_1}(t)a^+_{j\mu\sigma_2}(t)a_{i\alpha\sigma_3}a^+_{i\nu\sigma_4}\rangle. \tag{56}$$

For the multiband Hubbard model ($U'=I=I'=J=0$) we find

$$M^{\alpha\beta}_\sigma(\vec{k},\omega)=\frac{U^2}{\pi^2N^2}\sum_{ij}e^{i\vec{k}(\vec{R}_i-\vec{R}_j)}\int_{-\infty}^{\infty}\iint\frac{d\omega_1 d\omega_2}{\omega-\omega_1+\omega_2}\times$$

$$\times\Big\{\frac{n_F(\omega_1)n_F(\omega_2)}{n_F(\omega_1-\omega_3)}\left(\mathrm{Im}\ll a_{i\alpha\sigma}\,|\,a^+_{j\beta\sigma}\gg_{\omega_1}\cdot\mathrm{Im}\ll n_{i\alpha-\sigma}\,|\,n_{j\beta-\sigma}\gg_{\omega_2}+\right.$$

$$+\mathrm{Im}\ll a^+_{i\alpha-\sigma}\,|\,a_{j\beta-\sigma}\gg_{\omega_1}\cdot\mathrm{Im}\ll a_{i\alpha\sigma}a^+_{i\alpha-\sigma}\,|\,a^+_{j\beta\sigma}a_{j\beta-\sigma}\gg_{\omega_2}\Big)+ \tag{57}$$

$$+\frac{(1-n_F(\omega_1))n_F(\omega_2)}{n_F(\omega_2-\omega_3)}\mathrm{Im}\ll a_{j\beta-\sigma}\,|\,a^+_{i\alpha-\sigma}\gg_{\omega_1}\cdot\mathrm{Im}\ll a_{i\alpha\sigma}a_{i\alpha-\sigma}\,|\,a^+_{j\beta\sigma}a^+_{j\beta-\sigma}\gg_{\omega_2}\Big\}$$

6. NUMERICAL RESULTS

Let us apply the results of previous sections to the reasonable model calculations of the self-energy and spectral density. In the pair approximation (46) the general expression for the self-energy has the form (cf. eqs.(48), (49))

$$M_\sigma(\vec{k},\omega)=\frac{U^2}{N^2}\sum_{pq}\int_{-\infty}^{\infty}\iiint\frac{d\omega_1 d\omega_2 d\omega_3}{\omega+\omega_1-\omega_2-\omega_3}\{n(\omega_1)(1-n(\omega_2)-n(\omega_3))+n(\omega_2)n(\omega_3)\}\times$$

$$\times g_{p+q,-\sigma}(\omega_1)g_{k+p,\sigma}(\omega_2)g_{q,-\sigma}(\omega_3), \tag{58}$$

where

$$g_{k\sigma}(\omega)=-\frac{1}{\pi}\mathrm{Im}\,G_\sigma(k,\omega+i\epsilon). \tag{59}$$

For our artificial uncoupled bands (24) it is reasonable to accept the effective one-band model with a possible total number of 10 electrons per atom to proceed the numerical calculations. For this model we have calculated the self-energy $M(\vec{k},\omega)$ according to formula (58), where for the spectral density of states and dispersion law we take

$$g_k(\omega)=\delta(\omega-\epsilon(\vec{k}))$$

$$\epsilon(\vec{k})=E_0-4t\left(\cos\frac{ak_x}{2}\cos\frac{ak_y}{2}+\cos\frac{ak_x}{2}\cos\frac{ak_z}{2}+\cos\frac{ak_y}{2}\cos\frac{ak_z}{2}\right). \tag{60}$$

In general, formula (58) provides a self-consistent way for obtaining the self-energy $M(\vec{k},\omega)$ and Green function $G(\vec{k},\omega)$. However, because of a rather tedious integration method in 9-dimensional space (6-dimensional space for the $\vec{k}$-integration and 3-dimensional space for energy integration) we calculate the self-energy in first iteration step only for the model density of states of the FCC lattice.

The calculations were done with the appropriate set of metal parameters for FCC lattice. The band-width $W = 4.6$ eV for a band filling 86% and 94%. These values of parameters approximatively represent the ones for d-bands in transition metals, namely, in Co and Ni, respectively. All calculations were done for temperature $kT = 0.03$ eV.

The integrals which appear in eq. (58) were calculated by the Monte-Carlo method, and quite a bit noise showing by calculated curves is mainly due to our limit of the computer time. For each energy and $\vec{k}$-vector approximately 250000 points in 6-dimensional space of the quasi-momentum vectors $(\vec{p},\vec{q})$ were randomly generated. Of course, we first calculated the imaginary part of our self-energy and then obtained the real part by the Kramers-Kronig relation.

In Figs.1-4 we show real and imaginary parts of the self-energy $M(\vec{k},\omega)$ calculated at different points of the Brillouin zone.

In Figs.1-3 the self-energy curves have been calculated for energy bands of width 4.6 eV and the band filling equal to 86% for Γ, X and L symmetry points in the Brillouin zone, respectively.

In Fig.4 the same curves have been calculated for the band-filling equal to 96% for Γ symmetry point.

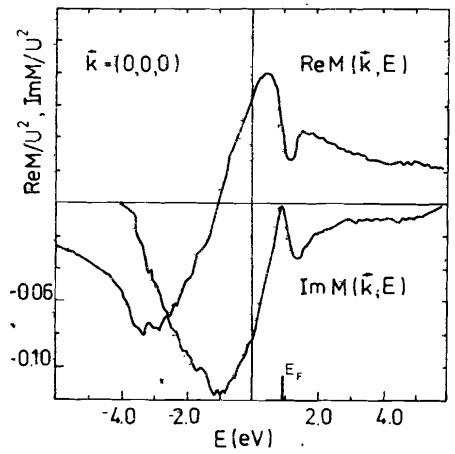


Fig.1. Real and imaginary parts of self-energy calculated for point Γ of the Brillouin zone ($\vec{k}=(0,0,0)$) and for model s-type tight-binding energy dispersion curve in fcc crystal lattice. The width of band W = 4.6 eV (from -3.45 eV to 1.15 eV), E_F = 0.95 eV, band-filling equals 86%, kT = 0.03 eV.

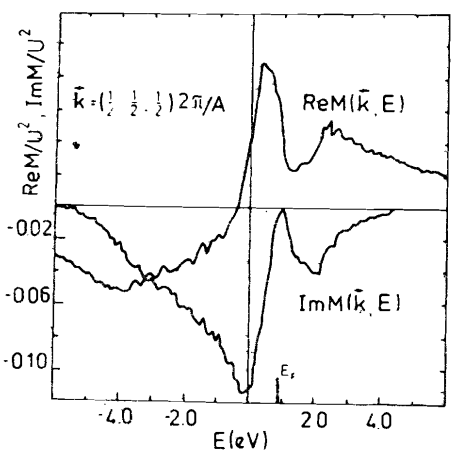


Fig.4. Real and imaginary parts of self-energy calculated for point Γ of the fcc Brillouin zone for E_F = 1.07 eV and band-filling equal 94%. Other parameters are the same as in Fig.1.

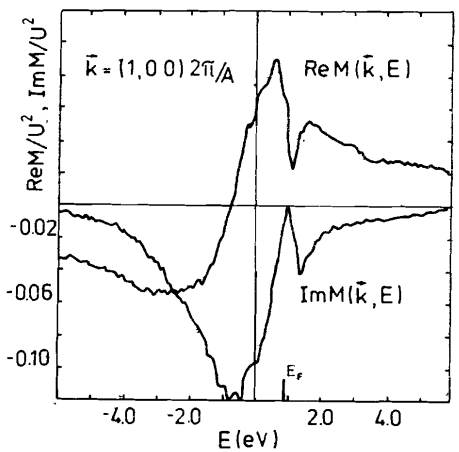


Fig.2. Real and imaginary parts of self-energy calculated for point X of the fcc Brillouine zone. Other parameters are the same as in Fig.1.

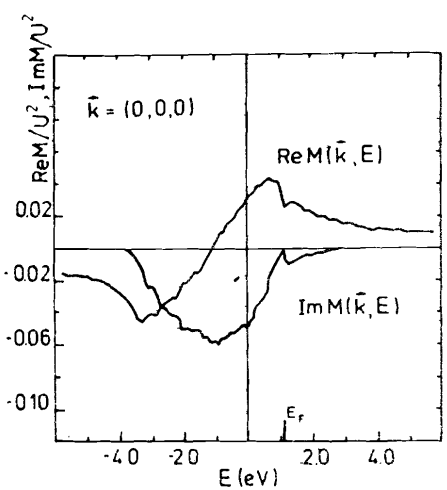


Fig.3. Real and imaginary parts of self-energy calculated for point L of the fcc Brillouin zone. Other parameters are the same as in Fig.1.

Then, we may see that the differences between self-energy curves calculated for different $\vec{k}$ -vectors are relatively substantial. For our model start-density of states (FCC lattice) the most different from other self-energy curves is the case of Γ point. In comparison with these ones for X and L points we can observe the absence of a long tail in the imaginary part and a considerable decrease of a real part for the states near the bottom of the band. These features of the imaginary part of self-energy may lead to broadening of the initial Bloch states with the $\vec{k}$ -vector lying far away from Γ point in comparison with the ones for $\vec{k}$ -vector from the vicinity of Γ point. In Fig.4 we present similar calculations for Γ point but for a different band-filling, namely, for band filling equal 94%. The main difference is only in the absolute value, and the shape and general trends are similar to the ones for smaller band fillings.

In Figs.5-7 we show the spectral densities for the same $\vec{k}$ -values along the Γ, X symmetry line. For computational convenience the spectral density curves are evaluated at complex energies, $E=\omega+0.001i$. The presence of the finite imaginary part in energy effectively causes these curves to be averaged over an energy interval of order ~0.001 eV. Because of a very small part of the energy these curves are broadened very slightly, and their peak heights are somewhat reduced from the true results which would be obtained in the limit of vanishing imaginary part.

In Figs.5-6 we present the spectral density of states for band width W = 4.6 eV (the band extends from -3.45 eV to 1.15 eV) for the band-filling equal to 85% and for two values of parameter U/W = 0.33 and 0.66, respectively. Small irregularities on the curve in Fig.6 come again from a too small number of random points used in the Monte-Carlo integration in the imaginary part of self-energy. As was expected, with increasing value of the Coulomb integral U the spectral density curve becomes broader and exhibits a much more rich structure. Roughly speaking, at Γ point we have a long tail from the upper side of a band with a great peak on the lower side of the band. Then, when we will move, for example, along the ΓX symmetry line towards X point we obtain a longer tail on a lower energy side, and at the same time we have a reconstruction of the main peak from the one side of the Fermi energy level to another side. The similar behaviour of spectral density can be seen for other parameters, i.e., for the band filling equal to 84% and for U/W = 0.33, as represented in Fig.7.

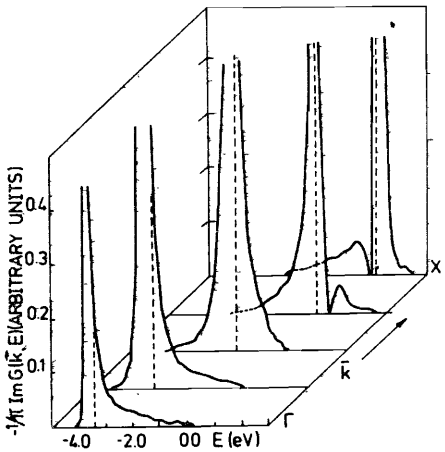
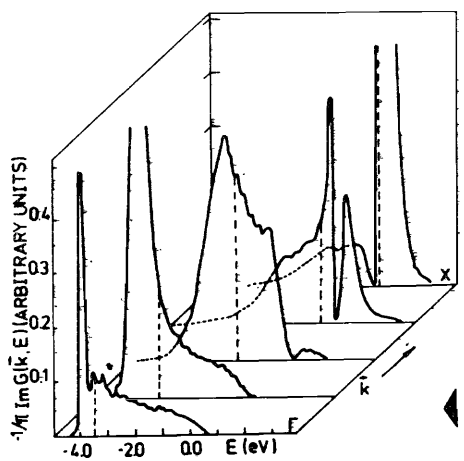


Fig.5. Spectral density of states of model s-type tight-binding energy dispersion curve with self-energy calculated from formula (58). Parameters: U/W = 0.33, W = 4.6 eV, E_F = = 0.95 eV, band-filling equals 86%. The vertical dashed line represents a one-electron eigenvalue.

Fig.6. The same as in Fig.5 but for U/W= 0.65.



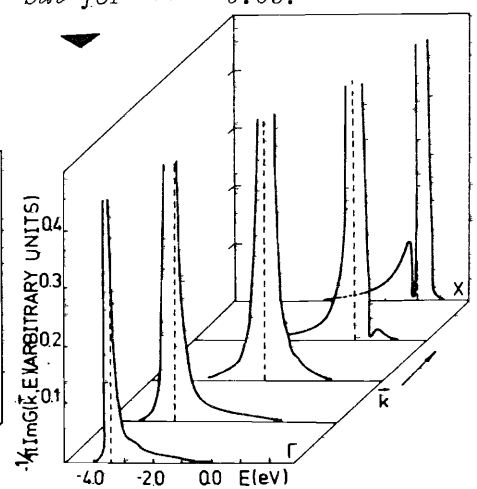


Fig.7. The same as in Fig.5 but for E_F = 1.07 and band-filling equal to 94%.

7. SUMMARY AND CONCLUSIONS

We have provided a relatively simple method that enables one to calculate electronic quasiparticle spectra including electron-electron inelastic scattering processes in a self-consistent way. The most important conclusion to be drawn from this paper is that the conventional one-electron approximation of the band theory is not always a sufficiently good approximation for transition metals, especially for metals like nickel. The adequate description of electronic quasiparticle spectra in multiband transition metals requires a much stronger role of the many-body correlation effects than believed some years ago. Our results give further information about correlation effects in transition metals as compared to that one obtained in papers[26-29,42] however, our approach is a more general one.

In conclusion, we hope to have provided some insight into the nature of electronic states within the realistic many-band model of transition metals. The approach developed here can be useful for studying photoelectron and X-ray excited Auger spectra of transition metals. To extend it for transition metal compounds, we must consider the strong correlation case and generalize the formalism used for such a case as it has been done for the one-band Hubbard model earlier[31]. Also, the approach developed here can be extended to the description of the correlation effects in the antiferromagnetic transition metals and in disordered transition metal alloys. We hope that these important problems will be considered in future works.

APPENDIX A

Wannier Functions and Tight-Binding Functions for Degenerate Bands

To compare our results with those obtained in Kleinman and Mednick calculations[26], we shall now briefly comment on the inter-relation between Wannier function and tight-binding-function representation of the electronic states for the multiband metal, e.g., for degenerate d-bands in transition metals.

In our paper we need the complete orthonormal Wannier function basis $\{\phi_\lambda(\vec{r}-\vec{R}_i)\}$ for introducing only the second quantized operators $a_{i\mu\sigma}$ and $a^+_{i\mu\sigma}$. Our main calculations, i.e., definition of the irreducible mean-field GF (18), etc., are in a very general form. However, to find the spectrum of electronic quasiparticle excitations we must introduce into our consideration the wave vector $\vec{k}$. Hence, we must accept a certain relation between Wannier and Bloch functions, or equivalently, between second-quantized operators representing Wannier localized states and Bloch extended states. Construction of Wannier functions for degenerate band is an essentially complex problem. At the present time there seems to be generally accepted the practical method developed by Kohn[43]. It is well known that such a relation for composite bands we need is of the form[43,46,47]

$$\Psi_\lambda(\vec{k},\vec{r}) = N^{-\frac{1}{2}} \sum_{i\lambda'} \phi_{\lambda'}(\vec{r}-\vec{R}_i)\, e^{i\vec{k}\vec{R}_i}\, U_{\lambda'\lambda}(\vec{k}) \tag{A.1}$$

or equivalently

$$a^+_{\vec{k}\lambda\sigma} = N^{-\frac{1}{2}} \sum_{i\lambda'} e^{i\vec{k}\vec{R}_i}\, a^+_{i\lambda'\sigma}\, U_{\lambda'\lambda}(\vec{k})$$

$$a^+_{i\lambda\sigma} = N^{-\frac{1}{2}} \sum_{\vec{k}\lambda'} e^{i\vec{k}\vec{R}_i}\, a^+_{\vec{k}\lambda'\sigma}\, U_{\lambda'\lambda}(\vec{k}) \tag{A.2}$$

$$a_{k\lambda\sigma} = N^{-1/2} \sum_{i\lambda'} e^{-i\vec{k}\vec{R}_i} a_{i\lambda'\sigma} U^{+}_{\lambda\lambda'}(\vec{k})$$

$$a_{i\lambda\sigma} = N^{-1/2} \sum_{k\lambda'} e^{i\vec{k}\vec{R}_i} a_{\vec{k}\lambda'\sigma} U_{\lambda\lambda'}(\vec{k}), \qquad (A.3)$$

where $U(\vec{k})$ is a unitary matrix. When we substitute the Bloch function (A.1) into the Schroedinger equation, we obtain for matrix $U(\vec{k})$ some eigenvalue problem

$$\sum_{\lambda'} \epsilon_{\lambda\lambda'}(\vec{k}) U_{\lambda'\lambda_1}(\vec{k}) = E U_{\lambda\lambda_1}(\vec{k})$$

$$\epsilon_{\lambda\lambda'}(\vec{k}) = \sum_i e^{i\vec{k}\vec{R}_i} \langle \phi_{\lambda'}(\vec{r}) | H | \phi_{\lambda_1}(\vec{r}-\vec{R}_i) \rangle. \qquad (A.4)$$

In the case of generalized transformations (A.2), (A.3) we must change our definition of the Fourier transition, Eqs.(25), (26) as follows:

$$G^{\alpha\beta}_{\sigma}(ij;\omega) = N^{-1} \sum_{\lambda\lambda'} e^{i\vec{k}(\vec{R}_i - \vec{R}_j)} U_{\alpha\lambda}(\vec{k}) G^{\lambda\lambda'}_{\sigma}(\vec{k},\omega) U^{+}_{\lambda'\beta}(\vec{k}) \quad .$$

$$G^{\alpha\beta}_{\sigma}(\vec{k},\omega) = N^{-1} \sum_{ij} \sum_{\lambda\lambda'} e^{-i\vec{k}(\vec{R}_i - \vec{R}_j)} U^{+}_{\alpha\lambda}(\vec{k}) G^{\lambda\lambda'}_{\sigma}(ij;\omega) U_{\lambda'\beta}(\vec{k}) \qquad (A.5)$$

and similar equations for the self-energy.

Because of a very complicated form for $E^{\alpha\nu}_{\sigma}(\vec{k})$, Eq.(31), written in terms of general transformations here we give only $E^{\alpha\nu}_{\sigma}(\vec{k})$ for Hamiltonian $H = H_1 + H_2$ without last two terms in H_2. Then we have:

$$E^{\alpha\nu}_{\sigma}(\vec{k}) = (\omega - \epsilon_{\nu}(\vec{k}))\delta_{\alpha\nu} - \frac{U'-I}{N} \sum_{p} \sum_{\lambda_1\lambda_2\lambda_3\lambda_4} (1-\delta_{\lambda_1\lambda_2}) \times$$

$$(U^{+}_{\alpha\lambda_1}(\vec{k}) U_{\lambda_2\nu}(\vec{k}) U_{\lambda_1\lambda_3}(\vec{p}) U^{+}_{\lambda_4\lambda_2}(\vec{p}) + U^{+}_{\alpha\lambda_1}(\vec{k}) U_{\lambda_1\nu}(\vec{k}) U_{\lambda_2\lambda_3}(\vec{p}) U^{+}_{\lambda_4\lambda_2}(\vec{p})) \times$$

$$\times \langle a_{p\lambda_3\sigma} a^{+}_{p\lambda_4\sigma} \rangle -$$

$$- \frac{U}{N} \sum_{p} \sum_{\lambda_1\lambda_2\lambda_3} U^{+}_{\alpha\lambda_1}(\vec{k}) U_{\lambda_1\nu}(\vec{k}) U_{\lambda_1\lambda_3}(\vec{p}) U^{+}_{\lambda_2\lambda_1}(\vec{p}) \langle a_{p\lambda_3} a^{+}_{p\lambda_2\sigma} \rangle -$$

$$- \frac{U'}{N} \sum_{p} \sum_{\substack{\lambda_1\lambda_2 \\ \lambda_3\lambda_4}} (1-\delta_{\lambda_1\lambda_2}) U^{+}_{\alpha\lambda_1}(\vec{k}) U_{\lambda_1\nu}(\vec{k}) U_{\lambda_2\lambda_3}(\vec{p}) U^{+}_{\lambda_4\lambda_2}(\vec{p}) \langle a_{p\lambda_3-\sigma} a^{+}_{p\lambda_4-\sigma} \rangle. \qquad (A.6)$$

Of course, when we apply the substitution $U_{\lambda_1\lambda_2}(\vec{k}) = \delta_{\lambda_1\lambda_2}$, or in other words, take transformations (24) instead of (23), we obtain for $E^{\alpha\nu}_{\sigma}(\vec{k})$ the formula given by Eq.(31) of the main text. Expression for self-energy for the same Hamiltonian and for pair decoupling of correlation functions is given as follows:

$$M^{\alpha\beta}_{\sigma}(\vec{k},\omega) = (-\frac{1}{\pi})^3 N^{-2} \sum_{\mu\nu} \sum_{\lambda\lambda_1 \ldots \lambda_7} \sum_{pq} U^{+}_{\alpha\lambda}(\vec{k}) U_{\lambda_1\beta}(\vec{k}) U_{\lambda\lambda_2}(\vec{k}+\vec{p}) U^{+}_{\lambda_1\nu}(\vec{p}+\vec{q}) \times$$

$$U_{\nu\lambda_4}(\vec{q}) U^{+}_{\lambda_5\lambda_1}(\vec{k}+\vec{p}) U^{+}_{\lambda_6\mu}(\vec{q}) U_{\mu\lambda_7}(\vec{p}+\vec{q}) \iiint_{-\infty}^{\infty} \frac{d\omega_1\, d\omega_2\, d\omega_3}{\omega+\omega_1-\omega_2-\omega_3} N(\omega_1,\omega_2,\omega_3) \times$$

$$\times \{ A^{\lambda\nu}_{\mu\lambda_1} [\mathrm{Im} G^{\mu\nu}_{p+q\sigma}(\omega_1)\, \mathrm{Im} G^{\nu\mu}_{q\sigma}(\omega_2)\, \mathrm{Im} G^{\lambda\lambda_1}_{k+p\sigma}(\omega_3) +$$

$$+ \mathrm{Im} G^{\mu\nu}_{p+q\sigma}(\omega_1) \cdot \mathrm{Im} G^{\nu\lambda_1}_{q\sigma}(\omega_2) \cdot \mathrm{Im} G^{\lambda\mu}_{k+p\sigma}(\omega_3)] + \qquad (A.7)$$

$$+ B^{\lambda\mu}_{\mu\lambda_1} \mathrm{Im} G^{\mu\nu}_{p+q-\sigma}(\omega_1)\, \mathrm{Im} G^{\nu\mu}_{q-\sigma}(\omega_2)\, \mathrm{Im} G^{\lambda\lambda_1}_{k+p\sigma}(\omega_3) \},$$

where

$$N(\omega_1,\omega_2,\omega_3) = n(\omega_1)[1-n(\omega_2)-n(\omega_3)] + n(\omega_2)n(\omega_3)$$

$$A^{\lambda\nu}_{\mu\lambda_1} = (1-\delta_{\lambda\nu})(1-\delta_{\mu\lambda_1})(U'-I)^2 \qquad (A.8)$$

$$B^{\lambda\nu}_{\mu\lambda_1} = [U\delta_{\lambda\nu} + U'(1-\delta_{\lambda\nu})][U\delta_{\mu\lambda_1} + U'(1-\delta_{\mu\lambda_1})].$$

For the approximation $U_{\lambda_1\lambda_2} \sim \delta_{\lambda_1\lambda_2}$ and for a simple Hubbard model we obtain the limiting case found by Kuzemsky [31].

Let us now consider the tight-binding approximation following [47]. The tight-binding degenerate bands are constructed from localized atomic orbitals $\varphi_{\alpha}(\vec{r}-\vec{R}_i)$ in the following well-known way [47]:

$$\Psi_{\lambda}(\vec{r},\vec{k}) = N^{-1/2} \sum_{i\alpha} \exp[i\vec{k}\vec{R}_i] V^{\lambda_1\alpha}(\vec{k})\, \varphi_{\alpha}(\vec{r}-\vec{R}_i), \qquad (A.9)$$

where we denote atomic orbitals by α, β indices and energy bands by λ, λ_1 indices. This equation gives the required (exact) expansion of the Bloch function in the general case of several bands. The main point of that expansion is the replacement of the expansion coefficients $\exp[i\vec{k}\cdot\vec{R}_i]$ (appropriate for the one-band case) by more complicated ones. The coefficients $V^{\lambda\alpha}(\vec{k})$ give the required mixture of atomic orbitals to

yield the Bloch states. Formula (A.9) may be inverted by writing for the atomic orbital state

$$\varphi_\alpha(\vec{r}-\vec{R}_i)=N^{-1/2}\sum_{\lambda k}\exp[-i\vec{k}\vec{R}_i]U^{\alpha\lambda}(\vec{k})\Psi_\lambda(\vec{k},\vec{r}), \tag{A.10}$$

where matrices U , V yield the relations:

$$\begin{aligned}&\sum_{\lambda k}U^{\alpha\lambda}(\vec{k})V^{\lambda\lambda_1}(\vec{k})\exp[i\vec{k}(\vec{R}_i-\vec{R}_j)]=\delta_{\alpha\alpha_1}\delta_{ij}\cdot N,\\&\sum_{\alpha i}V^{\lambda_1\alpha}(\vec{p})U^{\alpha\lambda_2}(\vec{q})\exp[i\vec{R}_i(\vec{p}-\vec{q})]=\delta_{\lambda_1\lambda_2}\delta_{\vec{p}\,\vec{q}}\cdot N.\end{aligned} \tag{A.11}$$

Here we have, because of non-orthonormalized atomic orbitals, overlap integrals

$$R^{\alpha\beta}_{ij}=N^{-1}\sum_{\lambda k}\exp[i\vec{k}(\vec{R}_i-\vec{R}_j)]U^{*\alpha\lambda}(\vec{k})U^{\beta\lambda}(\vec{k}). \tag{A.12}$$

Now we can introduce the formalism of second quantization with operators $a^+_{k\lambda\sigma}$, $a_{k\lambda\sigma}$ for the creation and annihilation of electrons with wave vector $\vec{k}$ spin σ for band labelled by index λ or with operators $a^+_{i\alpha\sigma}$, $b_{i\alpha\sigma}$ for the creation and annihilation of electrons described by function $\varphi_\alpha(\vec{r}-\vec{R}_i)$ and spin σ. Note that because of non-orthonormalized atomic orbitals $\varphi_\alpha(\vec{r}-\vec{R}_i)$ now we have $b^+_{i\alpha\sigma}\neq a^+_{i\alpha\sigma}$. In such a case we can still work with the Hamiltonian written in terms of $a^+_{i\alpha\sigma}b_{i\alpha\sigma}$ but some operators, for example, $a^+_{i\alpha\sigma}b_{i\alpha\sigma}$ have to be handled with a certain care (they are not Hermitian)[46]. For that reason, one often make the approximation

$$R^{\alpha\beta}_{ij}\cong\delta_{\alpha\beta}\delta_{ij} \tag{A.13}$$

which is equivalent to working with matrices $U=V^+$. Now, the above described formalism given by Gutzwiller is equivalent to that one given for the tight-binding description by Marschall[47], and in his notation we have:

$$\Psi_\lambda(\vec{k},\vec{r})=N^{-1/2}\sum_{\ell\alpha}\exp[i\vec{k}\cdot\vec{R}_\ell]a^\alpha_\lambda(\vec{k})\varphi_\alpha(\vec{r}-\vec{R}_\ell) \tag{A.14}$$

$$\varphi_\alpha(\vec{r}-\vec{R}_\ell)=N^{-1/2}\sum_{k\lambda}\exp[-i\vec{k}\cdot\vec{R}_\ell]a^{\alpha*}_\lambda(\vec{k})\Psi_\lambda(\vec{k},\vec{r}),$$

where for the transformation coefficients $a^\alpha_\lambda(\vec{k})$ we have the eigenvalue equation

$$-\sum_{i\beta}t^{\alpha\beta}_{ij}a^\beta_\lambda(\vec{k})\exp[i\vec{k}\vec{R}_{ij}]=\epsilon_\lambda(\vec{k})a^\alpha_\lambda(\vec{k})\exp[i\vec{k}\vec{R}_i], \tag{A.15}$$

Such an approach for the description of electronic states has been used in paper[26]. We may clearly rewrite Eq. (A.6) in terms

of coefficients $a^\alpha_\lambda(\vec{k})$ and in the limit of the Hubbard model (only U integral is retained) the obtained result is quite the same as that one given in paper[26].

APPENDIX B

The Perturbation Theory for Self-Energy

In paper[27] it was mentioned that an expansion of self-energy to higher orders in the Coulomb integral U 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 but usual workable way. Following paper[31] we may write

$$\begin{aligned}-\frac{1}{\pi}\operatorname{Im}G^\alpha_\sigma(\vec{k},\omega)&=\frac{1}{\pi}\frac{\Gamma^\alpha_\sigma(\vec{k},\omega)}{[\omega-\tilde{E}^\alpha_\sigma(\vec{k})]^2+(\Gamma^\alpha_\sigma(\vec{k},\omega))^2}\approx\\&\approx(1-\Lambda^\alpha_\sigma(k))\delta(\omega-\tilde{E}^\alpha_\sigma(\vec{k}))+\frac{1}{\pi}\frac{\Gamma^\alpha_\sigma(\vec{k},\omega)}{(\omega-\tilde{E}^\alpha_\sigma(\vec{k}))^2},\end{aligned} \tag{B.1}$$

where

$$\Gamma^\alpha_\sigma(\vec{k},\omega)=-\operatorname{Im}M^\alpha_\sigma(\vec{k},\omega+i\epsilon) \tag{B.2}$$

$$\tilde{E}^\alpha_\sigma(\vec{k})=E^\alpha_\sigma(\vec{k})+\operatorname{Re}M^\alpha_\sigma(\vec{k},\tilde{E}^\alpha_\sigma(\vec{k})). \tag{B.3}$$

The unknown coefficient $(1-\Lambda^\alpha_\sigma(\vec{k}))$ in (B.1) must be determined from a normalization condition

$$-\frac{1}{\pi}\int_{-\infty}^{\infty}\operatorname{Im}G^\alpha_\sigma(\vec{k},\omega)\,d\omega=1. \tag{B.4}$$

Then we obtain

$$\Lambda^\alpha_\sigma(\vec{k})=\frac{U^2}{N^2}\sum_{\vec{p}\vec{q}}\frac{N^{\alpha\alpha\alpha}_\sigma(\vec{k}\vec{p}\vec{q})}{\Omega^{\alpha\alpha\alpha}_\sigma(\vec{k}\vec{p}\vec{q})-\tilde{E}^\alpha_\sigma(\vec{k})}+\frac{(U'-I)^2+(U')^2}{N^2}\sum_{\vec{p}\vec{q}\nu}\frac{N^{\nu\nu\alpha}_\sigma(\vec{k}\vec{p}\vec{q})(1-\delta_{\nu\alpha})}{\Omega^{\nu\nu\alpha}_\sigma(\vec{k}\vec{p}\vec{q})-\tilde{E}^\alpha_\sigma(\vec{k})}, \tag{B.5}$$

where

$$\Omega^{\alpha\beta\gamma}_\sigma(\vec{k}\vec{p}\vec{q})=-\epsilon_\alpha(\vec{p}+\vec{q})+\epsilon_\beta(\vec{k}+\vec{p})+\epsilon_\gamma(\vec{q}). \tag{B.6}$$

For the occupation numbers we obtain:

$$n^\alpha_\sigma=\sum_k n(\tilde{E}^\alpha_\sigma(k))+U^2N^{-2}\sum_{kpq}\frac{N^{aaa}_\sigma(kpq)}{[\Omega^{\alpha aa}_\sigma(kpq)-\tilde{E}^\alpha_\sigma(k)]^2}\times$$

$$\times [n(\Omega_\sigma^{aaa}(kpq)-n(\tilde{E}_\sigma^a(k))]+$$

$$[(U'-I)^2+(U')^2]N^{-2}\sum_{\nu kpq}\frac{N_\sigma^{\nu\nu a}(kpq)(1-\delta_{\nu a})}{[\Omega_\sigma^{\nu\nu a}(kpq)-\tilde{E}_\sigma^a(k)]^2}\times \qquad (B.7)$$

$$\times[n(\Omega_\sigma^{\nu\nu a}(kpq)-n(\tilde{E}_\sigma^a(k))].$$

The first term in eq.(B.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

$$D_\sigma^a(\omega)=N^{-2}\sum_k(1-\Lambda_\sigma^a(k))\,\delta(\omega-\tilde{E}_\sigma^a(\vec{k}))+$$

$$+N^{-1}\sum_k\{U^2N^{-2}\sum_{pq}N_\sigma^{aaa}(kpq)\,\delta(\omega-\Omega_\sigma^{aaa}(kpq))+ \qquad (B.8)$$

$$+\frac{(U'-I)^2+(U')^2}{[\omega-\tilde{E}_\sigma^a(k)]^2}N^{-2}\sum_{\nu pq}(1-\delta_{a\nu})N_\sigma^{\nu\nu a}(kpq)\,\delta(\omega-\Omega_\sigma^{\nu\nu a}(kpq)).$$

If we use eq.(B.8) for the calculation of the self-energy by substitution eq.(B.8) into the r.h.s. of eqs.(48) and (49), we straightforwardly obtain a perturbation-type expansion for the self-energy up to order U^6, $(U')^6$ and I^6.

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Таранко Р., Куземский А.Л. E17-86-34

Корреляционные эффекты и спектр элементарных возбуждений в многозонных переходных металлах

Развит новый формализм для самосогласованного расчета спектра электронных квазичастичных возбуждений и их затухания в рамках реалистической многозонной модели переходного металла. Рассмотрена обобщенная модель Хаббарда, учитывающая вырождение электронов и дополнительные типы взаимодействий /одно- и двухцентровые/. Проведены численные расчеты действительной и мнимой части массового оператора, а также спектральной плотности состояний для параметров, отвечающих никелю и кобальту.

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Taranko R., Kuzemsky A.L. E17-86-34

Correlation Effects and Electronic Quasiparticle Excitations in Multiband Transition Metals

A new self-consistent formalism for the description of electronic quasiparticle excitations in the framework of the multiband model of the transition metal has been developed by taking explicitly into account damping effects and finite lifetimes. A generalized Hubbard model of a d-band with its degeneracy fully included as well as additional parts of interactions have been considered. Numerical calculations of the real and imaginary parts of the self-energy and spectral density of states have been done for nickel and cobalt metal parameters.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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