Quasiparticle Many-Body Dynamics of Highly Correlated Electronic Systems

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Abstract

The self-consistent theory of the correlation effects in Highly Correlated Systems(HCS) is presented. The novel Irreducible Green's Functions(IGF) method is discused in detail for the Hubbard model and random Hubbard model. The interpolative solution for the quasiparticle spectrum, which is valid for both the atomic and band limit is obtained. The (IGF) method permits to calculate the quasiparticle spectra of many-particle systems with the complicated spectra and strong interaction in a very natural and compact way. The essence of the method deeply related with the notion of the Generalized Mean Fields (GMF), which determine the elastic scattering corrections. The inelastic scattering corrections leads to the damping of the quasiparticles and are the main topic of the present consideration. The calculation of the damping has been done in a self-consistent way for both limits. For the random Hubbard model the weak coupling case has been considered and the self-energy operator has been calculated using the combination of the IGF method and Coherent Potential Approximation (CPA). The other applications of the method to s-f model, Anderson model, Heisenberg antiferromagnet, electron-phonon interaction models and quasiparticle tunneling are discussed briefly.

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1 Introduction

The study of the Highly Correlated Electron Systems has attracted much attention recently, especially after discovery of copper oxide superconductors and the new class of heavy fermion compounds, coexisting with magnetism [1] - [6]. Although much work has been performed during last years it is worthy to remind that the investigation of the excitations in many-body systems has been one of the most important and interesting subject for last few decades. The quantum field theoretical techniques have been widely applied to statistical treatment of a large number of interacting particles. Many-body calculations are often done for model systems of statistical mechanics using perturbation expansion. The basic procedure in many-body theory [7] is to find relevant unperturbed Hamiltonian and then take into account the small perturbation operator. This procedure, which work well for the weakly interacting systems, needs the suitable reformulation for the many-body systems with complicated spectra and strong interaction. For many practically interesting cases the standard schemes of perturbation expansion must be reformulated greatly [8] - [12]. The most characteristic feature of the recent advancement in basic research on electronic properties of solids is development of variety of the new class of materials with unusual properties: high T_c superconductors, heavy fermion compounds, diluted magnetic semiconductors etc. Contrary to the simple metals, where the fundamentals very well known and the electrons can be represented in a way such that they weakly interact with each other(c.f. [13]), in these materials the electrons interact strongly and moreover their spectra are complicated, i.e. have many branches etc. This gives rise to interesting phenomena such as magnetism, metal-insulator transition in oxides, heavy fermions etc., but the understanding of what is going on is in many cases only partial if exist at all. Therefore the theoretical studies of the Highly Correlated Electron Systems (HCS) are very important and actual. A principle importance of of these studies is concerned with a fundamental problem of electronic solid state theory, namely with the tendency of 3d electrons in TMC and 4f electrons in rare-earth metal compounds (REC) and alloys to exhibit both localized and delocalized behaviour. The interesting electronic and magnetic properties of these substances are intimately related to this dual behaviour of electrons. In spite of experimental and theoretical achievements [1] - [6], still it remains much to be understood concerning such systems. Recent theoretical investigations of HCS have brought forth significant variety of the approaches which are trying to solve these controversial problems. It seems appropriate to point out that a number of perturbation-theory or mean-field theory approaches which have been proposed in the past few years, are in fact questionable or inadequate. In order to match such a trend we need to develop a systematic theory of the Highly Correlated Systems, to describe from the first principles of the condensed matter theory and statistical mechanics the physical properties of this class of the materials. In the present paper we will present the approach which allows one to describe completely the quasi-particle spectra with damping in a very natural way. This approach has been suggested as essential for various many-body systems and we believe that it bear the real physics of Highly Correlated Systems [14], [15]. The essence of our consideration of the dynamical properties of many-body system with strong interaction is related closely with the field theoretical approach and use the advantage of the Green's

functions language and the Dyson equation. It is possible to say that our method tend to emphasize the fundamental and central role of the Dyson equation for the single-particle dynamics of the many-body systems at finite temperature.
Just this point differ our IGF approach from the complimentary many-body approach which is based on the moment expansion for the spectral functions. It was developed in a very detail by W.Nolting [16] - [20].

2 Irreducible Green's Functions Method

In this Section, we will discuss briefly the novel nonperturbative approach for description of the many-body dynamics of the HCES. At this point it is worthwhile to underline that it is essential to apply an adequate method in order to solve a concrete physical problem; the final solution should contain a correct physical reasoning in a most natural way. The list of many-body techniques that have been applied to strongly correlated systems is extensive. The problem of adequate description of many-body dynamics for the case of very strong Coulomb correlations has been explicitly raised by Anderson, who put the direct question: "... whether a real many-body theory would give answers radically different from the Hartree-Fock results?" [21] (c.f. [22]). The formulation of the Anderson model[21] and closely related Hubbard model [23], [24] dates really a better understanding of the electronic correlations in solids, especially if the relevant electrons are modelled better by tight-binding approximation [25],[26]. Both of the models, Anderson and Hubbard, are often referred to as simplest models of magnetic metals and alloys. This naive perception contradicts the enormous amount of papers which has been publishing during the last decades and devoted to attacking the Anderson/Hubbard model by many refined theoretical techniques. As is well known now, the simplicity of the Anderson/Hubbard model manifest itself in the dynamics of a two-particle scattering. Nevertheless, as to the true many-body dynamics, there is still no simple and compact description. In this paper it will be attempted to justify the use of a novel Irreducible Green's Functions (IGF) for the interpolation solution of the single-band Hubbard model and other basic solid state models as s-f model [27], [28], Anderson model [29],[30], Heisenberg antiferromagnet [31] and strong electron-phonon interaction model in modified tight-binding approximatiom(MTBA) for normal and superconducting metals [32] and alloys [33], [34]. A number of other approaches has been proposed and the our approach is in many respect an additional and incorporate the logic of development of the many-body techniques. The considerable progress in studying the spectra of elementary excitations and thermodynamic properties of many-body systems has been for most part due to the development of the temperature dependent Green's Functions methods. We have developed the helpful reformulation of the two-time GFs method which is especially adjusted [35] for the correlated fermion systems on a lattice. The very important concept of the whole method are the **Generalized Mean Fields**. These GMFs have a complicated structure for the strongly correlated case and are not reduced to the functional of the mean densities of the electrons, when we calculate excitations spectra at finite temperature. To clarify the foregoing, let us consider the retarded GF of the form

$$G^r = << A(t), B(t') >> = -i\theta(t-t') < [A(t)B(t')]_\eta >, \eta = \pm 1. \qquad (1)$$

As an introduction of the concept of IGFs let us describe the main ideas of this approach in a symbolic form. To calculate the retarded GF $G(t-t')$ let us write down the equation of motion for it:

$$\omega G(\omega) = < [A, A^+]_\eta > + << [A, H]_- \mid A^+ >>_\omega . \qquad (2)$$

The essence of the method is as follows [14]. It is based on the notion of the *"IRREDUCIBLE"* parts of GFs (or the irreducible parts of the operators, out of which the GF is constructed) in term of which it is possible, without recourse to a truncation of the hierarchy of equations for the GFs, to write down the exact Dyson equation and to obtain an exact analytical representation for the self-energy operator. By definition we introduce the irreducible part **(ir)** of the GF

$$^{ir} << [A, H]_- | A^+ >> = << [A, H]_- - zA | A^+ >> . \qquad (3)$$

The unknown constant z is defined by the condition (or constraint)

$$< [[A, H]^{ir}_-, A^+]_\eta > = 0 \qquad (4)$$

From the condition (4) one can find:

$$z = \frac{< [[A, H]_-, A^+]_\eta >}{< [A, A^+]_\eta >} = \frac{M_1}{M_0} \qquad (5)$$

Here M_0 and M_1 are the zeroth and first order moments of the spectral density. Therefore, irreducible GF (3) are defined so that it cannot be reduced to the lower-order ones by any kind of decoupling. It is worthy to note that the irreducible correlation functions are well known in statistical mechanics. In the diagrammatic approach the irreducible vertices are defined as the graphs that do not contain inner parts connected by the G^0-line. With the aid of the definition (3) these concepts are translating into the language of retarded and advanced GFs. This procedure extract all relevant (for the problem under consideration) mean field contributions and puts them into the generalized mean-field GF, which here are defined as

$$G^0(\omega) = \frac{< [A, A^+]_\eta >}{(\omega - z)}. \qquad (6)$$

To calculate the IGF $^{ir} << [A, H]_-(t), A^+(t') >>$ in (2), we have to write the equation of motion after differentiation with respect to the second time variable t'. The condition (4) remove the inhomogeneous term from this equation and is the very crucial point of the whole approach. If one introduces an irreducible part for the right-hand side operator as discussed above for the "left" operator, the equation of motion (2) can be exactly rewritten in the following form

$$G = G^0 + G^0 P G^0. \qquad (7)$$

The scattering operator P is given by

$$P = (M_0)^{-1} \quad {}^{ir} << [A, H]_- | [A^+, H]_- >>^{ir} (M_0)^{-1}. \tag{8}$$

The structure of the equation (7) enables us to determine the self-energy operator M, in complete analogy with the diagram technique

$$P = M + MG^0 P. \tag{9}$$

From the definition (9) it follows that we can say that the self-energy operator M is defined as a proper (in diagrammatic language "connected") part of the scattering operator $M = (P)^p$. As a result, we obtain the exact Dyson equation for the thermodynamic two-time Green's Functions:

$$G = G^0 + G^0 M G, \tag{10}$$

which has well known formal solution of the form

$$G = [(G^0)^{-1} - M]^{-1}.$$

Thus, by introducing irreducible parts of GF (or the irreducible parts of the operators, out of which the GF is constructed) the equation of motion (2) for the GF can be exactly (but using constraint (4)) transformed into Dyson equation for the two-time thermal GF. This is very remarkable result, which deserve the underlining, because of the traditional form of the GF method did not included namely this point. The projection operator technique [36] has essentially the same philosophy, but with using the constraint (4) in our approach we emphasize the fundamental and central role of the Dyson equation for the calculation of the single-particle properties of the many-body systems. It is important to note, that for the retarded and advanced GFs the notion of the proper part is symbolic in nature [14]. However, because of the identical form of the equations for the GFs for all three types (advanced, retarded and causal), we can convert in each stage of calculations to causal GFs and, thereby, confirm the substantiated nature of definition (9)! We therefore should speak of an analog of the Dyson equation. Hereafter we will drop this stipulation, since it will not cause any misunderstanding. It should be emphasized that scheme presented above give just an general idea of the IGF method. The specific method of introducing IGFs depends on the form of operator A, the type of the Hamiltonian and the conditions of the problem. The general philosophy of the IGF method lies in the separation and identification of elastic scattering effects and inelastic ones. This last point is quite often underestimated and both effects are mixed. However, as far as the right definition of quasiparticle damping is concerned, the separation of elastic and inelastic scattering processes is believed to be crucially important for the many-body systems with complicated spectrum and strong interaction. Recent paper [37] emphasizes especially that the anomalous damping of electrons (or holes) distinguishes cuprate superconductors from ordinary metals. From a technical point of view the elastic (GMF) renormalizations can exhibit a quite non-trivial structure. To obtain this structure correctly, one must construct the full GF from the complete algebra of the relevant operators and develop a special projection procedure for higher-order GF in accordance with a given algebra. The Hubbard model is a very suitable tool for the applying of this approach [35],[38].

3 Hubbard Model

The model Hamiltonian which is usually referred to as Hubbard Hamiltonian

$$H = \sum_{ij\sigma} t_{ij} a^{+}_{i\sigma} a_{j\sigma} + U/2 \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} \tag{11}$$

includes the intraatomic Coulomb repulsion U and the one-electron hopping energy t_{ij}. The electron correlation forces electrons to localize in the atomic orbitals, which are modelled here by the complete and orthogonal set of the Wannier wave functions $[\phi(\vec{r} - \vec{R}_j)]$. On the other hand, the kinetic energy is reduced when electrons are delocalized. The main difficulty of the right solution of the Hubbard model is the necessity to taking into account of the both these effects simultaneously. Thus, the Hamiltonian (11) is specified by two parameter: U and effective electron bandwidth

$$\Delta = (N^{-1} \sum_{ij} |t_{ij}|^2)^{1/2}.$$

The band energy of Bloch electrons $\epsilon(\vec{k})$ is defined as follows

$$t_{ij} = N^{-1} \sum_{\vec{k}} \epsilon(\vec{k}) \exp[i\vec{k}(\vec{R}_i - \vec{R}_j],$$

where the N is the number of the lattice sites. It is convenient to count the energy from the center of gravity of the band, i.e. $t_{ii} = \sum_k \epsilon(k) = 0$. The effective electron bandwidth Δ and Coulomb intrasite integral U define completely the different regimes in 3 dimension depending on parameter $\gamma = \Delta/U$. It is usually a rather difficult task to find interpolation solution for the dynamical properties of the Hubbard model. To solve this problem with a reasonably accuracy and describe correctly an interpolating solution from "band" limit ($\gamma \gg 1$) to "atomic" limit ($\gamma \to 0$) one need more sophisticated approach than usual procedures which have been developed for description of the interacting electron-gas-problem. We evidently have to to improve the early Hubbard's theory taking account of variety of possible regimes for the model depending on electronic density, temperature and values of γ. The single-electron GF

$$G_{ij\sigma}(\omega) = << a_{i\sigma}|a^{+}_{j\sigma} >>= N^{-1} \sum_{\vec{k}} G_{\sigma}(\vec{k}, \omega) \exp[-i\vec{k}(\vec{R}_i - \vec{R}_j)], \tag{12}$$

which has been calculated by Hubbard [23], [39], has the characteristic two-pole functional structure

$$G_{\sigma}(k, \omega) = [F_{\sigma}(\omega) - \epsilon(k)]^{-1} \tag{13}$$

where

$$F^{-1}_{\sigma}(\omega) = \frac{\omega - (n^{+}_{-\sigma} E_{-} + n^{-}_{-\sigma} E_{+}) - \lambda}{(\omega - E_{+} - n^{-}_{-\sigma}\lambda)(\omega - E_{-} - n^{+}_{-\sigma}\lambda) - n^{+}_{-\sigma} n^{-}_{-\sigma} \lambda^2} \tag{14}$$

andλ is the certain function which depends on parameters of the Hamiltonian. If λ is small ($\lambda \to 0$) then expression (14) take the form:

$$F^{-1}_{\sigma}(\omega) \approx \frac{n^{-}_{-\sigma}}{\omega - E_{-} - n^{+}_{-\sigma}\lambda} + \frac{n^{+}_{-\sigma}}{\omega - E_{+} - n^{-}_{-\sigma}\lambda},$$

which correspond to the two shifted subbands with the gap

$$\omega_1 - \omega_2 = (E_+ - E_-) + (n^-_{-\sigma} - n^+_{-\sigma})\lambda = U + \lambda 2n^+_{-\sigma}.$$

Here $n^+ = n$ and $n^- = 1 - n$; $E_+ = U$, $E_- = 0$. If λ is very big then we obtain

$$F_\sigma^{-1}(\omega) \approx \frac{\lambda}{[(\omega - E_-)n^-_{-\sigma} + (\omega - E_+)n^+_{-\sigma}]\lambda} = \frac{1}{\omega - (n^+_{-\sigma}E_+ - n^-_{-\sigma}E_-)}.$$

This latter solution correspond to the single band, centered at the energy $\omega \approx n^+_{-\sigma}U$. The two- pole functional structure of the single-particle GF is very easy to understand within formalism which describe the motion of electrons in binary alloys [39], [40]. If one introduce the two types of the scattering potentials $t_\pm \approx (\omega - E_\pm)^{-1}$ then the two kinds of the t-matrix T_+ and T_- appears which satisfy the following system of equations:

$$T_+ = t_+ + t_+G^0_{++}T_+ + t_+G^0_{+-}T_-$$

$$T_- = t_- + t_-G^0_{--}T_- + t_-G^0_{-+}T_+,$$

where $G^0_{\alpha\beta}$ is the bare propagator between the sites with the energies $E_\pm$. The solution of this system has the following form

$$T_\pm = \frac{t_\pm + t_\pm G^0_\pm t_\pm}{(1 - t_+G^0_{++})(1 - t_-G^0_{--}) - G^0_{-+}G^0_{+-}t_+t_-} = \frac{t^{-1}_\mp + G^0_\pm}{(t^{-1}_+ - G^0_{++})(t^{-1}_- - G^0_{--}) - G^0_{-+}G^0_{+-}}. \tag{15}$$

Thus, by comparing this functional two-pole structure and well-known "Hubbard III" solution [39]

$$\Sigma_\sigma(\omega) = \omega - F_\sigma(\omega)$$

it is possible to identify the "scattering corrections" and "resonance broadening corrections" in the following way:

$$F_\sigma(\omega) = \frac{\omega(\omega - U) - (\omega - Un_{-\sigma})A_\sigma(\omega)}{\omega - U(1 - n_{-\sigma}) - A_\sigma(\omega)}$$

$$A_\sigma(\omega) = Y_\sigma(\omega) + Y_{-\sigma}(\omega) - Y^*_{-\sigma}(U - \omega)$$

$$Y_\sigma = F_\sigma(\omega) - G^{-1}_{0\sigma}(\omega); G_{0\sigma}(\omega) = N^{-1}\sum_k G_{k\sigma}(\omega)$$

If we put $A_\sigma(\omega) = 0$ we immediately obtain the "Hubbard I" solution [23]. The "alloy analogy" approximation correspond to $A_\sigma(\omega) \approx Y_\sigma(\omega)$. Note, that the "Hubbard III" self-energy operator $\Sigma_\sigma(\omega)$ is local, i.e. do not depend on quasimomentum. The another drawback of this solution is very inconvenient functional representation of the elastic and inelastic scattering processes. The conceptually new approach to the theory of very strong but finite electron correlation for Hubbard model has been proposed by Roth [41]. She clarified microscopically the origination of the two-pole solution of the single-particle GF, what was the very unusual fact from the point of view of the standard Fermi-liquid approach, showing that the naive one-electron approximation of the band structure calculations is not valid for the description of the electron correlations in HCS . Thus the use of sophisticated many-body technique is required for the calculation of the excitation spectra at finite temperature. This last point should be underlined, because of the suitable modification of the Density Functional Approximation [42], [43],[44] could give the reasonable description of the ground-state properties of HCS. We shall show here, following the papers [35],[38] that the use of the IGF method permit to improve substantially both solutions, Hubbard's and Roth's, by defining the correct Generalized Mean Fields for the Hubbard model.

4 Hubbard Model. Weak Correlation

The concept of the GMFs and the relevant algebra of operators from which GFs are constructed are the central ones to our treatment of electron correlation in solids. It will be convenient (and much more shorter) to discuss these concepts for weakly and strongly correlated cases separately. For the first time we must to construct the suitable state vector space of the many-body system [45]. The fundamental assumption implies that the states of a system of interacting particles can be expanded in terms of the states of non-interacting particles [45]. This concept originate in perturbation theory and finds support for weakly interacting many-particle systems(c.f. [5]). For the strongly correlated case this approach needs the the suitable reformulation (cf. [46]) and namely in this point the right definition of the GMFs is vital. Let us consider the weakly correlated Hubbard model (11). In many respect this case is similar to the ordinary interacting electron gas but with very local, singular interaction. It will be shown below that the usual creation $a^+_{i\sigma}$ and annihilation $a_{i\sigma}$ second quantized operators with the properties

$$a^+_i \Psi^{(0)} = \Psi^{(1)}_i ; a_i \Psi^{(1)} = \Psi^{(0)}$$

$$a_i \Psi^{(0)} = 0; a_j \Psi^{(1)}_i = 0, (i \neq j)$$

are suitable variables for the description of the considering systems. Here $\Psi^{(0)}$ and $\Psi^{(1)}$ are the vacuum and single-particle states respectively. The question now is how to describe our system in terms of the quasiparticles. For a translationally invariant system, to describe the low-lying excitations of the system in terms of quasiparticles [45], one has to choose eigenstates such that they all correspond to definite momentum. For the single-band

Hubbard model (11) the exact transformation reads

$$a_{\vec{k}\sigma} = N^{-1/2} \sum_i \exp(-i\vec{k}\vec{R}_i) a_{i\sigma}$$

Note, that for degenerate bands model the more general transformation is necessary. Then the Hubbard Hamiltonian (11) in the Bloch vector state space are given by

$$H = \sum_{k\sigma} \epsilon(k) a^+_{k\sigma} a_{k\sigma} + U/2N \sum_{pqr} \sum_{\sigma} a^+_{p+r-q\sigma} a_{p\sigma} a^+_{q-\sigma} a_{r-\sigma} \tag{16}$$

If the interaction is weak, the algebra of the relevant operators is very simple: it is an algebra of the non-interacting fermion system ($a_{k\sigma}, a^+_{k\sigma}, n_{k\sigma} = a^+_{k\sigma} a_{k\sigma}$). For the calculation of the electronic quasiparticle spectrum of the Hubbard model in this limit let us consider the single-electron GF, which are defined as

$$\begin{aligned} G_{k\sigma}(t-t') = << a_{k\sigma}, a^+_{k\sigma} >> = -i\theta(t-t') < [a_{k\sigma}(t), a^+_{k\sigma}(t')]_+ > = \\ 1/2\pi \int_{-\infty}^{+\infty} d\omega \exp(-i\omega t) G_{k\sigma}(\omega) = \\ 1/2\pi \int_{-\infty}^{+\infty} d\omega \exp(-i\omega t) 1/2\pi \int_{-\infty}^{+\infty} \frac{d\omega'}{\omega - \omega'} (\exp(\beta\omega') + 1) A_{k\sigma}(\omega') \end{aligned} \tag{17}$$

where $\beta = (kT)_{-1}$ and $A_{k\sigma}(\omega)$ is the spectral intensity. The equation of motion for the Fourier transform of the GF $G_{k\sigma}(\omega)$ has the form

$$(\omega - \epsilon_k) G_{k\sigma}(\omega) = 1 + U/N \sum_{pq} << a_{k+p\sigma} a^+_{p+q-\sigma} a_{q-\sigma} | a^+_{k\sigma} >>_\omega \tag{18}$$

Let us introduce, by definition, an "irreducible" GF in the following way

$$\begin{aligned} {}^{ir} << a_{k+p\sigma} a^+_{p+q-\sigma} a_{q-\sigma} | a^+_{k\sigma} >>_\omega = \\ << a_{k+p\sigma} a^+_{p+q-\sigma} a_{q-\sigma} | a^+_{k\sigma} >>_\omega - \delta_{p,0} < n_{q-\sigma} > G_{k\sigma} \end{aligned} \tag{19}$$

The irreducible (ir) GF in (19) is defined in such a way that it cannot be reduced to GF of lower order with respect to the number of fermion operators by an arbitrary pairing of operators or, in another words, by any kind of decoupling. Substituting (19) in (18) we obtain

$$G_{k\sigma}(\omega) = G^{MF}_{k\sigma}(\omega) + G^{MF}_{k\sigma}(\omega) U/N \sum_{pq} {}^{ir} << a_{k+p\sigma} a^+_{p+q-\sigma} a_{q-\sigma} | a^+_{k\sigma} >>_\omega \tag{20}$$

Here we have introduced the notations

$$G^{MF}_{k\sigma}(\omega) = (\omega - \epsilon(k\sigma))^{-1}; \epsilon(k\sigma) = \epsilon(k) + U/N \sum_q < n_{q-\sigma} > \tag{21}$$

In this paper, for brevity, we confine ourself by considering the paramagnetic solutions only, i.e. $< n_\sigma > = < n_{-\sigma} >$. In order to calculate the higher-order GF on the r.h.s. of (20) we have to write the equation of motion obtained by means of differentiation with

respect to the second variable t'. Constraint (4) allows us to remove the inhomogeneous term in this equation for $\frac{d}{dt'}^{ir} << A(t), a^{+}_{k\sigma}(t') >>$.
For the Fourier components, this is written in the form

$$(\omega - \epsilon(k))^{ir} << A|a^{+}_{k\sigma} >>_{\omega} = <^{ir} [A, a^{+}_{k\sigma}]_{+} > +$$
$$U/N \sum_{rs}{}^{ir} << A|a^{+}_{r-\sigma} a_{r+s-\sigma} a_{k+s\sigma} >>_{\omega} \ . \tag{22}$$

The anticommutator in (22) is calculated on the basis of the definition of the irreducible part

$$< [^{ir}(a_{k+p\sigma} a^{+}_{p+q-\sigma} a_{q-\sigma}), a^{+}_{k\sigma}]_{+} >=$$
$$< [a_{k+p\sigma} a^{+}_{p+q-\sigma} a_{q-\sigma} - < a^{+}_{p+q-\sigma} a_{q-\sigma} > a_{k+p\sigma}, a^{+}_{k\sigma}]_{+} >= 0 \tag{23}$$

If one introduces irreducible part for the r.h.s. operators by analogy with expression (19), the equation of motion (20) can be exactly rewritten in the form (7)

$$G_{k\sigma}(\omega) = G^{MF}_{k\sigma}(\omega) + G^{MF}_{k\sigma}(\omega) P_{k\sigma}(\omega) G^{MF}_{k\sigma}(\omega) \tag{24}$$

where we have introduced the following notation for the operator P (8)

$$P_{k\sigma}(\omega) = \frac{U^2}{N^2} \sum_{pqrs} D^{ir}_{k\sigma}(p, q|r, s, ; \omega) =$$
$$= \frac{U^2}{N^2} \sum_{pqrs}{}^{ir} << a_{k+p\sigma} a^{+}_{p+q-\sigma} a_{q-\sigma} | a^{+}_{r-\sigma} a_{r+s-\sigma} a^{+}_{k+s\sigma} >>^{ir}_{\omega} \tag{25}$$

To define the self-energy operator according to the (9) one must separate the "proper" part by the following way

$$D^{ir}_{k\sigma}(p, q|r, s; \omega) = L^{ir}_{k\sigma}(p, q|r, s; \omega)$$
$$+ \frac{U^2}{N^2} \sum_{r's'p'q'} L^{ir}_{k\sigma}(p, q|r's'; \omega) G^{MF}_{k\sigma}(\omega) D^{ir}_{k\sigma}(p', q'|r, s; \omega) \tag{26}$$

Here $L^{ir}_{k\sigma}(p, q|r, s; \omega)$ is the "proper" part of the GF $D^{ir}_{k\sigma}(p, q|r, s; \omega)$, which in accordance with the definition (19) cannot be reduced to the lower-order one by any type of decoupling. Using (9) we find

$$G_{k\sigma} = G^{MF}_{k\sigma}(\omega) + G^{MF}_{k\sigma}(\omega) M_{\sigma}(k, \omega) G_{k,\sigma}(\omega) \tag{27}$$

Equation (27) is the Dyson equation for the single-particle two-time thermal GF. According to (10) it has the formal solution

$$G_{k\sigma}(\omega) = [\omega - \epsilon(k\sigma) - M_{\sigma}(k, \sigma)]^{-1} \tag{28}$$

where the self-energy operator M is given by

$$M_{\sigma}(k, \omega) = \frac{U^2}{N^2} \sum_{pqrs} L^{ir}_{k\sigma}(p, q|r, s; \omega) =$$
$$\frac{U^2}{N^2} \sum_{pqrs}{}^{ir} << a_{k+p\sigma} a^{+}_{p+q-\sigma} a_{q-\sigma} | a^{+}_{k+s\sigma} a^{+}_{r-\sigma} a_{r+s-\sigma} >>^{ir} \tag{29}$$

The latter expression (29) is an exact representation (no decoupling has been made till now) for the self-energy in terms of higher-order GFs up to second order in U (for the consideration of the higher order equations of motion see Ref. [15]). Thus, in contrast to the standard equation-of-motion approach the determination of the full GF has been reduced to the calculation of the mean-field GF G^{MF} and the self-energy operator M. The main reason for this method of calculation is that the decoupling is only introduced into self-energy operator, as it will shown in a detail below. The formal solution of the Dyson equation (28) define the right reference frame for the formation of the quasiparticle spectrum due to the its own (formal solution) correct functional structure. In the standard equation-of-motion approach such a structure could be lost by using decoupling approximations **before** arriving to the correct functional structure of the formal solution of the Dyson equation. This is a crucial point of the IGF method. The energies of the electronic states in the mean-field approximation are given by the poles of G^{MF} (21). Now let us consider the damping effects and finite lifetimes. To find an explicit expression for self-energy M (29), we have to evaluate approximately the higher-order GF in (21). It will be shown below that the IGF method can be used to derive the damping in a self-consistent way simply and more generally than other formulations. First, it is convenient to write down the GF in (29) in terms of correlation functions by using the well-known spectral theorem [45]:

$$\begin{aligned}
&<< a_{k+p\sigma}a^{+}_{p+q-\sigma}a_{q-\sigma}|a^{+}_{k+s\sigma}a^{+}_{r-\sigma}a_{r+s-\sigma}>>_{\omega}= \\
&\frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{d\omega'}{\omega-\omega'}(\exp(\beta\omega')+1)\int_{-\infty}^{+\infty}\exp(i\omega' t) \\
&< a^{+}_{k+s\sigma}(t)a^{+}_{r-\sigma}(t)a_{r+s-\sigma}(t)a_{k+p\sigma}a^{+}_{p+q-\sigma}a_{q-\sigma}>
\end{aligned} \tag{30}$$

Further insight is gained if we select the suitable relevant "trial" approximation for the correlation function on the r.h.s. of (30). In this paper we show that the earlier formulations, based on the decoupling or/and diagrammatic methods can be arrive at from our technique but in a self- consistent way. Clearly that the choice of the relevant trial approximation for correlation function in (30) can be done in many ways. For example, the reasonable and workable one may be the following "pair approximation", which is especially good for the low density of the quasiparticles:

$$\begin{aligned}
&< a^{+}_{k+s\sigma}(t)a^{+}_{r-\sigma}(t)a_{r+s-\sigma}(t)a_{k+p\sigma}a^{+}_{p+q-\sigma}a_{q-\sigma}>^{ir}\approx \\
&< a^{+}_{k+p\sigma}(t)a_{k+p\sigma}>< a^{+}_{q-\sigma}(t)a_{q-\sigma}>< a_{p+q-\sigma}(t)a^{+}_{p+q-\sigma}> \\
&\delta_{k+s,k+p}\delta_{r,q}\delta_{r+s,p+q}
\end{aligned} \tag{31}$$

Using (30) and (31) in (29) we obtain the approximate expression for the self-energy operator in a self-consistent form (the self-consistency means that we express approximately the self-energy operator in terms of the initial GF and, in principle, one can obtain the required solution by suitable iteration procedure):

$$\begin{aligned}
M_{\sigma}(k,\omega) = \frac{U^2}{N^2}\sum_{pq}\int\frac{d\omega_1 d\omega_2 d\omega_3}{\omega+\omega_1-\omega_2-\omega_3} \\
[n(\omega_2)n(\omega_3)+n(\omega_1)(1-n(\omega_2)-n(\omega_3))]g_{p+q-\sigma}(\omega_1)g_{k+p\sigma}(\omega_2)g_{q-\sigma}(\omega_3)
\end{aligned} \tag{32}$$

where we have used the notations

$$g_{k\sigma}(\omega) = -\frac{1}{\pi} Im G_{k\sigma}(\omega + i\varepsilon); n(\omega) = [\exp(\beta\omega) + 1]^{-1}$$

The equations (28) and (32) form a closed self-consistent system of equations for the single-electron GF for the Hubbard model, but for weakly correlated limit only. In principle, we may use, on the r.h.s. of (32) any workable first iteration-step form of the GF and find a solution by repeated iteration. It is most convenient to choose as the first iteration step the following simple one-pole approximation:

$$g_{k\sigma}(\omega) \approx \delta(\omega - \epsilon(k\sigma)) \tag{33}$$

Then, using (33) in (32), we get for the self-energy an explicit and simple expression

$$M_\sigma(k,\omega) = \frac{U^2}{N^2} \sum_{pq} \frac{n_{p+q-\sigma}(1 - n_{k+p\sigma} - n_{q-\sigma}) + n_{k+p\sigma} n_{q-\sigma}}{\omega + \epsilon(p+q\sigma) - \epsilon(k+p\sigma) - \epsilon(q\sigma)} \tag{34}$$

The numerical calculations of the typical behaviour of real and imaginary parts of the self-energy (34) have been performed [47] for the model density of states of the FCC lattice. These calculations and many other [48] - [50] prove that the conventional one-electron approximation of the band theory is not always a sufficiently good approximation for transition metals like nickel. The simple formula (32) derived above for the self-energy operator are typical in showing the role of correlation effects in the formation of quasiparticle spectrum of the Hubbard model. It is instructive to examine other types of the possible trial solutions for the six-operator correlation function in the eqn.(30). The approximation which we propose now reflects the interference between the one-particle branch of the spectrum and the collective one:

$$\begin{gathered} < a^+_{k+s\sigma}(t) a^+_{r-\sigma}(t) a_{r+s-\sigma}(t) a_{k+p\sigma} a^+_{p+q-\sigma} a_{q-\sigma} >^{ir} \approx \\ < a^+_{k+s\sigma}(t) a_{k+p\sigma} >< a^+_{r-\sigma}(t) a_{r+s-\sigma}(t) a^+_{p+q-\sigma} a_{q-\sigma} > + \\ < a_{r+s-\sigma}(t) a^+_{p+q-\sigma} >< a^+_{k+s\sigma}(t) a^+_{r-\sigma}(t) a_{k+p\sigma} a_{q-\sigma} > + \\ < a^+_{r-\sigma}(t) a_{q-\sigma} >< a^+_{k+s\sigma}(t) a_{r+s-\sigma}(t) a_{k+p\sigma} a^+_{p+q-\sigma} > \end{gathered} \tag{35}$$

It is visible now that the three contributions in this trial solution describe the self-energy corrections that take into account the collective motions of electron density, the spin density and the density of "doubles", respectively. The essential feature of this approximation is connected with the fact that correct calculation of the single-electron quasiparticle spectra with damping require the suitable incorporating of the influence of the collective degrees of freedom on the single-particle ones. The most interesting contribution is related with the spin degrees of freedom because of correlated system are the magnetic or have very well developed magnetic fluctuations. We follows the above steps and calculate the self-energy operator (29) as

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

$$\sum_{i,j} \exp[-i\vec{k}(\vec{R}_i - \vec{R}_j)](-\frac{1}{\pi} Im << S_i^{\pm}|S_j^{\mp} >>_{\omega_1})$$
$$(-\frac{1}{\pi} Im << a_{i-\sigma}|a^{+}_{j-\sigma} >>_{\omega_2}) \tag{36}$$

where the following notations have been used:

$$S_i^+ = a^+_{i\uparrow}a_{i\downarrow}; S_i^- = a^+_{i\downarrow}a_{i\uparrow}$$

$$N(\omega) = [\exp(\beta\omega) - 1]^{-1}.$$

It is possible to rewrite (37) in a more convenient way now

$$M_\sigma(k,\omega) = \frac{U^2}{N}\sum_q \int d\omega'(\cot\frac{\omega-\omega'}{2T} + \tan\frac{\omega'}{2T})$$
$$(-\frac{1}{\pi} Im\chi^{\mp\pm}(k-q,\omega-\omega')g_{qsigma}(\omega')). \tag{37}$$

The equations (28) and (37) form again another self-consistent system of equations for the single-particle GF of the Hubbard model. Note, that both expressions for the self-energy depend on quasimomentum; in other words the approximate procedure do not broke the momentum conservation law. It is important, because of the poles $\omega(k,\sigma) = \epsilon(k,\sigma) - i\Gamma(k)$ of the GF (28) are determined by the equation

$$\omega - \epsilon(k\sigma) - Re[M_\sigma(k,\omega)] - iIm[M_\sigma(k,\omega)] = 0 \tag{38}$$

It may be shown quite generally that the Luttinger's definition of the true Fermi surface [7] is valid in the framework of our theory. It is worthy to note that for electrons in a crystal where there is a band index, as well as quasimomentum, the definition of the Fermi surface are a little more complicated then the single-band one. Before the single particle energies and Fermi surface are known, one must carry out a diagonalization in the band index. In order to give a complete picture of the GMFs let us discuss briefly the interesting question of the correct definition of the so-called unrestricted Hartree-Fock approximation (UHFA). Recently, this approximation has been applied for the single-band Hubbard model (11) for the calculation of the density of states for CuO_2 clusters [51]. The following definition of UHFA has been used:

$$n_{i-\sigma}a_{i\sigma} =< n_{i-\sigma} > a_{i\sigma}- < a^+_{i-\sigma}a_{i\sigma} > a_{i-\sigma} \tag{39}$$

Thus, in addition to the standard HF term, the new, the so-called "spin-flip" terms, are retained. This example clearly show that the nature of the mean-fields follows from the essence of the problem and should be defined in a proper way. It is clear, however, that the definition (39) broke the rotational symmetry of the Hubbard Hamiltonian. For the single- band Hubbard Hamiltonian the averaging $< a^+_{i-\sigma}a_{i,\sigma} >= 0$ because of the rotational symmetry of the Hubbard model. So, in Ref. [51] the effective Hamiltonian H_{eff} has been defined. We have analysed in detail the proper definition of the irreducible

GFs which include the "spin-flip" terms. The definition (19) must be modified in the following way:

$$^{ir} << a_{k+p\sigma}a^+_{p+q-\sigma}a_{q-\sigma}|a^+_{k\sigma} >>_\omega = << a_{k+p\sigma}a^+_{p+q-\sigma}a_{q-\sigma} >>_\omega - \\ \delta_{p,0} < n_{q-\sigma} > G_{k\sigma} - < a_{k+p\sigma}a^+_{p+q-\sigma} >< < a_{q-\sigma}|a^+_{k\sigma} >>_\omega \quad (40)$$

From this definition follows that such a type of introduction of the IGF broaden the initial algebra of the operator and initial set of the GFs. That means that "actual" algebra of the operators must include the spin-flip terms at the beginning, namely: ($a_{i\sigma}$, $a^+_{i\sigma}$, $n_{i\sigma}$, $a^+_{i\sigma}a_{i-\sigma}$). The corresponding initial GF will have the form

$$\begin{pmatrix} << a_{i\sigma}|a^+_{j\sigma} >> & << a_{i\sigma}|a^+_{j-\sigma} >> \\ << a_{i-\sigma}|a^+_{j\sigma} >> & << a_{i-\sigma}|a^+_{j-\sigma} >> \end{pmatrix}$$

In fact, this approximation has been investigated earlier by Kishore and Joshi [52]. They clearly pointed out that they assumed that the system is magnetized in x direction instead of conventional z axis.

5 Hubbard Model. Strong Correlation

When studying the electronic quasiparticle spectrum of the strongly correlated systems, one must take care of at least three facts of major importance:
(i) The ground state is reconstructed radically as compared with the weakly correlated case. Namely this fact lead to the necessity of the redefinition of the single-particle states. Due to the strong correlation, the initial algebra of the operators are transformed into new algebra of the complicated operators. In principle, in terms of the new operators the initial Hamiltonian may be rewritten as bilinear form and the generalized Wick theorem can be formulated [53], [54]. It is very important to underline, that the transformation to the new algebra of relevant operators reflect some important internal symmetries of the problem and nowadays this way of thinking are formulating in elegant and very powerful technique of the classification of the integrable models [55], [56] and exactly soluble models (see also[57]).
(ii) The single-electron GF, which describe the dynamical properties, must have two-pole functional structure, giving in the atomic limit, when hopping integral tends to zero, the exact two-level atomic solution.
(iii) The GMFs have, in general case, a very non-trivial structure. The GMFs functional cannot be expressed in terms of the functional of the mean particles density.
In this section we consider large, but finite, Coulomb repulsion. The inspiring ideas of papers [39], [46], [54] where the problem of the relevant algebra of the operators has been considered, are central to our consideration here. Following this approach we consider the new set of relevant operators:

$$d_{i\alpha\sigma} = n^\alpha_{i-\sigma}a_{i\sigma}, (\alpha = \pm); n^+_{i\sigma} = n_{i\sigma}, n^-_{i\sigma} = (1 - n_{i\sigma}); \\ \sum n^\alpha_{i\sigma} = 1; n^\alpha_{i\sigma}n^\beta_{i\sigma} = \delta_{\alpha\beta}n^\alpha_{i\sigma}; \sum_\alpha d_{i\alpha\sigma} = a_{i\sigma} \quad (41)$$

The new operators $d_{i\alpha\sigma}$ and $d^{+}_{j\beta\sigma}$ have complicated commutation rules, namely

$$[d_{i\alpha\sigma}, d^{+}_{j\beta\sigma}]_{+} = \delta_{ij}\delta_{\alpha\beta}n^{\alpha}_{i-\sigma}$$

The convenience of the new operators follows immediately if one write down the equation of motion for them

$$[d_{i\alpha\sigma}, H]_{-} = E_{\alpha}d_{i\alpha\sigma} + \sum_{ij} t_{ij}(n^{\alpha}_{i-\sigma}a_{j\sigma} + \alpha a_{i\sigma}b_{ij-\sigma})$$
$$b_{ij\sigma} = (a^{+}_{i\sigma}a_{j\sigma} - a^{+}_{j\sigma}a_{i\sigma}). \tag{42}$$

It is possible to interpret [23], [39] both contribution in this equation as *alloy analogy* and *resonance broadening correction*. Let us consider the single-particle GF (12) in the Wannier basis. Using the new operator algebra it is possible to rewrite identically GF (12) in the following way

$$G_{ij\sigma}(\omega) = \sum_{\alpha\beta} << d_{i\alpha\sigma}|d^{+}_{j\beta\sigma} >>_{\omega} = \sum_{\alpha\beta} F^{\alpha\beta}_{ij\sigma}(\omega) \tag{43}$$

The equation of motion for the auxiliary matrix GF

$$F^{\alpha\beta}_{ij\sigma}(\omega) = \begin{pmatrix} << d_{i+\sigma}|d^{+}_{j+\sigma} >>_{\omega} & << d_{i+\sigma}|d^{+}_{j-\sigma} >>_{\omega} \\ << d_{i-\sigma}|d^{+}_{j+\sigma} >>_{\omega} & << d_{i-\sigma}|d^{+}_{j-\sigma} >>_{\omega} \end{pmatrix} \tag{44}$$

have the following form

$$(\mathbf{E}\mathbf{F}_{ij\sigma}(\omega) - \mathbf{I}\delta_{ij})_{\alpha\beta} = \sum_{l\neq i} t_{il} << n^{\alpha}_{i-\sigma}a_{l\sigma} + \alpha a_{i\sigma}b_{il-\sigma}|d^{+}_{j\beta\sigma} >>_{\omega} \tag{45}$$

Where the following matrix notations have been used

$$\mathbf{E} = \begin{pmatrix} (\omega - E_{+}) & 0 \\ 0 & (\omega - E_{-}) \end{pmatrix}; \mathbf{I} = \begin{pmatrix} n^{+}_{-\sigma} & 0 \\ 0 & n^{-}_{-\sigma} \end{pmatrix}. \tag{46}$$

In accordance with the general method of Section 2 we introduce by definition the matrix IGF:

$$\mathbf{D}^{ir}_{il,j}(\omega) = \begin{pmatrix} << Z_{11}|d^{+}_{j+\sigma} >>_{\omega} & << Z_{12}|d^{+}_{j-\sigma} >>_{\omega} \\ << Z_{21}|d^{+}_{j+\sigma} >>_{\omega} & << Z_{22}|d^{+}_{j-\sigma} >>_{\omega} \end{pmatrix} -$$
$$\sum_{\alpha'}(\begin{bmatrix} A^{+\alpha'}_{il} \\ A^{-\alpha'}_{il} \end{bmatrix}[F^{\alpha'+}_{ij\sigma}\ F^{\alpha'-}_{ij\sigma}] - \begin{bmatrix} B^{+\alpha'}_{li} \\ B^{-\alpha'}_{li} \end{bmatrix}[F^{\alpha'+}_{lj\sigma}\ F^{\alpha'-}_{lj\sigma}]) \tag{47}$$

Here the notations have been used:

$$Z_{11} = Z_{12} = n^{+}_{i-\sigma}a_{l\sigma} + a_{i\sigma}b_{il-\sigma};\ Z_{21} = Z_{22} = n^{-}_{i-\sigma}a_{l\sigma} - a_{i\sigma}b_{il-\sigma}$$

It is worth to underline that the definition (47) are in heart of the whole our approach to description of the strong correlation in the Hubbard model. The coefficients A and B are determined from the constraint (4), namely

$$< [(\mathbf{D}^{ir}_{il,j})_{\alpha\beta}, d^{+}_{j\beta\sigma}]_{+} >= 0 \tag{48}$$

After some algebra we obtain from (48) ($i \neq j$)

$$
\begin{aligned}
[A_{il}]_{\alpha\beta} &= \alpha(< d^{+}_{i\beta-\sigma} a_{l-\sigma} > + < d_{i-\beta-\sigma} a^{+}_{l-\sigma} >)(n^{\beta}_{-\sigma})^{-1} \\
[B_{li}]_{\alpha\beta} &= [< n^{\beta}_{l-\sigma} n^{\alpha}_{i-\sigma} > + \alpha\beta(< a_{i\sigma} a^{+}_{i-\sigma} a_{l-\sigma} a^{+}_{l\sigma} > - \\
&\qquad < a_{i\sigma} a_{i-\sigma} a^{+}_{l-\sigma} a^{+}_{l\sigma} >)](n^{\beta}_{-\sigma})^{-1}
\end{aligned} \tag{49}
$$

As previously, we introduce now the GMF GF $\mathbf{F}^{0}_{ij\sigma}$ in analogy with (6), however, as it is clear from (47), the actual definition of the GMF GF is very non-trivial. After the Fourier transformation we get

$$
\begin{pmatrix} F^{0++}_{k\sigma} & F^{0+-}_{k\sigma} \\ F^{0-+}_{k\sigma} & F^{0--}_{k\sigma} \end{pmatrix} = \frac{1}{ab - cd} \begin{pmatrix} n^{+}_{-\sigma} b & n^{-}_{-\sigma} d \\ n^{+}_{-\sigma} c & n^{-}_{-\sigma} a \end{pmatrix} \tag{50}
$$

The coefficients a, b, c, d are equal to

$$
\begin{aligned}
\begin{matrix} a \\ b \end{matrix} &= (\omega - E_{\pm} - N^{-1} \sum_{p} \epsilon(p)(A^{\pm\pm}(-p) - B^{\pm\pm}(p-q))) \\
\begin{matrix} c \\ d \end{matrix} &= N^{-1} \sum_{p} \epsilon(p)(A^{\mp\pm}(-p) - B^{\mp\pm}(p-q))
\end{aligned} \tag{51}
$$

Then, using the definition (43) we find the final expression for the GMF GF

$$
G^{MF}_{\sigma}(k,\omega) = \frac{\omega - (n^{+}_{-\sigma} E_{-} + n^{-}_{-\sigma} E_{+}) - \lambda(k)}{(\omega - E_{+} - n^{-}_{-\sigma}\lambda_1(k))(\omega - E_{-} - n^{+}_{-\sigma}\lambda_2(k)) - n^{-}_{-\sigma} n^{+}_{-\sigma} \lambda_3(k)\lambda_4(k)} \tag{52}
$$

Here we have introduced the following notations:

$$
\begin{matrix} \lambda_1(k) \\ \lambda_2(k) \end{matrix} = \frac{1}{n^{\mp}_{-\sigma}} \sum_{p} \epsilon(p)(A^{\pm\pm}(-p) - B^{\pm\pm}(p-k)) \tag{53}
$$

$$
\begin{matrix} \lambda_3(k) \\ \lambda_4(k) \end{matrix} = \frac{1}{n^{\mp}_{-\sigma}} \sum_{p} \epsilon(p)(A^{\pm\mp}(-p) - B^{\pm\mp}(p-k)) \tag{54}
$$

$$
\lambda(k) = (n^{-}_{-\sigma})^2(\lambda_1 + \lambda_3) + (n^{+}_{-\sigma})^2(\lambda_2 + \lambda_4)
$$

From the equation (52) it is obvious that our two-pole solution is more general than "Hubbard III" [39] and Roth[41] solutions. Our solution has the correct non-local structure, taking into account the non-diagonal scattering matrix elements more accurately. Those matrix elements describe the virtual "recombination" processes and reflect the extremely complicated structure of the single-particle state, which virtually include a great number of intermediate scattering processes (c.f. interesting analysis in Ref. [58]).
The spectrum of the mean-field quasiparticle excitations follows from the poles of the GF (52) and consist of two branches

$$
\omega_{\substack{1\\2}}(k) = 1/2[(E_{+} - E_{-} + a_1 + b_1) \pm \sqrt{(E_{+} + E_{-} - a_1 - b_1)^2 - 4cd}] \tag{55}
$$

where $a_1(b) = \omega - E_{\pm} - a(b)$. Thus the Spectral Intensity $A_{k\sigma}(\omega)$ of the GF (52) consist of two peaks, which separated by the distance

$$
\omega_1 - \omega_2 = \sqrt{(U - a_1 - b_1)^2 - cd} \approx U(1 - \frac{a_1 - b_1}{U}) + O(\gamma) \tag{56}
$$

For the deeper insight into the functional structure of the solution (52) and to compare with the other solutions we rewrite the (50) in the following form

$$\mathbf{F}^0_{k\sigma}(\omega) = \begin{pmatrix} (\frac{a}{n^+_{-\sigma}} - \frac{db^{-1}c}{n^+_{-\sigma}})^{-1} & \frac{d}{a}(\frac{b}{n^-_{-\sigma}} - \frac{da^{-1}c}{n^-_{-\sigma}})^{-1} \\ \frac{c}{b}(\frac{a}{n^+_{-\sigma}} - \frac{db^{-1}c}{n^+_{-\sigma}})^{-1} & (\frac{b}{n^-_{-\sigma}} - \frac{db^{-1}c}{n^-_{-\sigma}})^{-1} \end{pmatrix} \tag{57}$$

from which we obtain for the $G^{MF}_\sigma(k,\omega)$

$$G^{MF}_\sigma(k,\omega) = \frac{n^+_{-\sigma}(1+cb^{-1})}{a - db^{-1}c} + \frac{n^-_{-\sigma}(1+da^{-1})}{b - ca^{-1}d} \approx \\ \frac{n^-_{-\sigma}}{\omega - E_- - n^+_{-\sigma}W^-_{-\sigma}(k)} + \frac{n^+_{-\sigma}}{\omega - E_+ - n^-_{-\sigma}W^+_{-\sigma}(k)} \tag{58}$$

where

$$n^+_{-\sigma}n^-_{-\sigma}W^\pm_{-\sigma}(k) = N^{-1}\sum_{ij} t_{ij}\exp(-ik(R_i - R_j)) \\ \Big((< a^+_{i-\sigma}n^\pm_{i\sigma}a_{j-\sigma} > + < a_{i-\sigma}n^\mp_{i\sigma}a^+_{j-\sigma} >) + \\ (< n^\pm_{j-\sigma}n^\pm_{i-\sigma} > + < a_{i\sigma}a^+_{i-\sigma}a_{j-\sigma}a^+_{j\sigma} > - < a_{i\sigma}a_{i-\sigma}a^+_{j-\sigma}a^+_{j\sigma} >)\Big) \tag{59}$$

are the shifts for the upper and lower splitted subbands due to the elastic scattering of the carriers in the Generalized Mean Field. Namely $W^\pm$ are the functionals of the GMF. The most important feature of the present solution of the strongly correlated Hubbard model is a very nontrivial structure of the mean-field renormalizations (59), which is crucial to understanding the physics of strongly correlated systems. It is important to emphasize that namely this complicated form of the GMF are only relevant to the essence of the physics under consideration. The attempts to reduce the functional of the GMF to the simpler functional of the average density of electrons are incorrect namely from the point of view of the real nature of the physics of HCS. This physics clearly show that the mean-field renormalizations cannot be expressed as a functional of the electron mean density. To explain this statement let us derive the “Hubbard I” solution [23] from our GMF solution (52). If we approximate (59) as

$$n^+_{-\sigma}n^-_{-\sigma}W^\pm(k) \approx N^{-1}\sum_{ij} t_{ij}\exp(-ik(R_i - R_j)) < n^\pm_{j-\sigma}n^\pm_{i-\sigma} > \tag{60}$$

and makes the additional approximation, namely

$$< n_{j-\sigma}n_{i-\sigma} > \approx n^2_{-\sigma}$$

then solution (52) goes over into the “Hubbard I” solution

$$G^0_\sigma(k,\omega) \approx \frac{n_{-\sigma}}{\omega - U - \epsilon(k)n_{-\sigma}} + \frac{1 - n_{-\sigma}}{\omega - \epsilon(k)(1 - n_{-\sigma})} \tag{61}$$

This solution, as it is well known, is unrealistic from the many points of view.

As regards to our solution (52), the second important aspect is that the parameters $\lambda_i(k)$ do not depend on frequency, i.e. depends essentially on the elastic scattering processes. Such a dependence on frequency arises due to inelastic scattering processes which are contained in our self-energy operator and we proceed now with the derivation of the explicit expression for it.
To calculate the high-order GF on the r.h.s. of (45) we should use the second time variable (t') differentiation of it again. If one introduces irreducible parts for the right-hand-side operators by analogy with expression (47), the equation of motion (45) can be rewritten exactly in the following form

$$\mathbf{F}_{k\sigma}(\omega) = \mathbf{F}^0_{k\sigma}(\omega) + \mathbf{F}^0_{k\sigma}(\omega)\mathbf{P}_{k\sigma}(\omega)\mathbf{F}^0_{k\sigma}(\omega) \tag{62}$$

Here the scattering operator P (8) has the form

$$\mathbf{P}_{q\sigma}(\omega) = \mathbf{I}^{-1}[\sum_{lm} t_{il}t_{mj} << \mathbf{D}^{ir}_{il,j}|\mathbf{D}^{ir+}_{i,mj} >>_\omega]_q\mathbf{I}^{-1} \tag{63}$$

In accordance with the definition (9) we write down the Dyson equation

$$\mathbf{F} = \mathbf{F}^0 + \mathbf{F}^0\mathbf{M}\mathbf{F} \tag{64}$$

The self-energy operator M is defined by Eq. (9). Let us note again that the self-energy corrections, according to (10), contribute to the full GF as an additional terms. This is an essential advantage in comparison with the "Hubbard III" solution and other two-pole solutions. For the full GF we find, using the formal solution of Dyson equation

$$\begin{aligned} G_\sigma(k,\omega) = \Bigg(&\frac{1}{n^+_{-\sigma}}(a - n^+_{-\sigma}M^{++}_\sigma(k,\omega)) + \frac{1}{n^-_{-\sigma}}(b - n^-_{-\sigma}M^{--}_\sigma(k,\omega)) \\ &+ \frac{1}{n^+_{-\sigma}}(d + n^+_{-\sigma}M^{+-}_\sigma(k,\omega)) + \frac{1}{n^-_{-\sigma}}(c + n^-_{-\sigma}M^{-+}_\sigma(k,\omega))\Bigg) \\ &[\det\Big((F^0_{k\sigma}(\omega))^{-1} - M_\sigma(k,\omega)\Big)]^{-1} \end{aligned} \tag{65}$$

After some algebra we can rewrite this expression in the following form, which is essentially new and, in a certain sense, are the central result of the present theory

$$G = \frac{\omega - (n^+E_- + n^-E_+) - L}{(\omega - E_+ - n^-L_1)(\omega - E_- - n^+L_2) - n^-n^+L_3L_4} \tag{66}$$

where

$$\begin{aligned} L_1(k,\omega) &= \lambda_1(k) - \frac{n^+_{-\sigma}}{n^-_{-\sigma}}M^{++}_\sigma(k,\omega); \\ L_2(k,\omega) &= \lambda_2(k) - \frac{n^-_{-\sigma}}{n^+_{-\sigma}}M^{--}_\sigma(k,\omega); \\ L_3(k,\omega) &= \lambda_3(k) + \frac{n^-_{-\sigma}}{n^+_{-\sigma}}M^{+-}_\sigma(k,\omega); \\ L_4(k,\omega) &= \lambda_4(k) + \frac{n^+_{-\sigma}}{n^-_{-\sigma}}M^{-+}_\sigma(k,\omega); \\ L(k,\omega) &= \lambda(k) + n^+_{-\sigma}n^-_{-\sigma}(M^{++} + M^{--} - M^{-+} - M^{+-}) \end{aligned} \tag{67}$$

Thus, now we have to find the explicit expressions for the elements of the self-energy matrix M. To proceed we should use the spectral theorem again, as in Eq. (30), to express the GF in terms of correlation functions

$$M^{\alpha,\beta}_{\sigma}(k,\omega) \sim < D^{ir+}_{mj,\beta}(t) D^{ir}_{il,\alpha} > \tag{68}$$

For the approximate calculation of the self-energy we propose to use the following trial solution

$$\begin{aligned}
< D^{ir+}(t) D^{ir} > \approx < a^{+}_{m\sigma}(t) a_{l\sigma} >< n^{\beta}_{j-\sigma}(t) n^{\alpha}_{i-\sigma} > \\
+ < a^{+}_{m\sigma}(t) n^{\alpha}_{i-\sigma} >< n^{\beta}_{j-\sigma}(t) a_{l\sigma} > + \beta < b^{+}_{mj-\sigma}(t) a_{l\sigma} >< a^{+}_{j\sigma}(t) n^{\alpha}_{i-\sigma} > \\
+\beta < b^{+}_{mj-\sigma}(t) n^{\alpha}_{i-\sigma} >< a^{+}_{j\sigma}(t) a_{l\sigma} > + \alpha < a^{+}_{m\sigma}(t) a_{i\sigma} >< n^{\beta}_{j-\sigma}(t) b_{il-\sigma} > \\
+\alpha < a^{+}_{m\sigma}(t) b_{il-\sigma} >< n^{\beta}_{j-\sigma}(t) b_{il-\sigma} > \\
+\alpha\beta < b^{+}_{mj-\sigma}(t) a_{i\sigma} >< a^{+}_{j\sigma}(t) b_{il-\sigma} > \\
+\alpha\beta < b^{+}_{mj-\sigma}(t) b_{il-\sigma} >< a^{+}_{j\sigma}(t) a_{i\sigma} >
\end{aligned} \tag{69}$$

It is quite natural to interpret the contributions in this expression in terms of scattering, resonance-broadening and interference corrections of different types. For example, let us consider the simplest approximation. For this aim we retain the first contribution in (69)

$$\begin{aligned}
[\mathbf{IMI}]_{\alpha\beta} = \int_{-\infty}^{+\infty} \frac{d\omega'}{\omega - \omega'} (\exp(\beta\omega') + 1) \\
\int_{-\infty}^{+\infty} \frac{dt}{2\pi} \exp(i\omega' t) N^{-1} \sum_{ijlm} exp(-ik(R_i - R_j)) t_{il} t_{mj} \\
\int d\omega_1 n(\omega_1) \exp(i\omega_1 t) g_{ml\sigma}(\omega_1) \left(-\frac{1}{\pi} Im K^{\alpha\beta}_{ij}(\omega_1 - \omega') \right).
\end{aligned} \tag{70}$$

Equations (70) and (64) are the self-consistent system of equations for the single-particle Green's function. For a simple estimation, for the calculation of the self-energy (70) it is possible to use any initial relevant approximation of the two-pole structure. As an example we take the expression (61). We then obtain

$$\begin{aligned}
[\mathbf{IMI}]_{\alpha\beta} \approx \sum_q |\epsilon(k-q)|^2 K^{\alpha\beta}_q \\
[\frac{n_{-\sigma}}{\omega - U - \epsilon(k-q) n_{-\sigma}} + \frac{1 - n_{-\sigma}}{\omega - \epsilon(k-q)(1 - n_{-\sigma})}]
\end{aligned} \tag{71}$$

On the basis of the self-energy operator (71) we can explicitly find the energy shift and damping due to inelastic scattering of the quasiparticles, which is a great advantage of the present approach. It is clear from the present consideration that for the systematic construction of the approximate solutions we need to calculate the collective correlation functions of the electron density and spin density and the density of doubles, but this problem must be considered separately.

6 Correlations in Random Hubbard Model

In this chapter we shall apply IGF method for consideration of the electron-electron correlations in the presence of disorder to demonstrate the advantage of our approach. The treatment of the electron motion in substitutionally disordered disordered A_xB_{1-x} transition metal alloys is based upon certain generalization of Hubbard model, including random diagonal and off-diagonal elements caused by substitutional disorder in the binary alloy. The electron-electron interaction play an important role for various aspects of behaviour in alloys, e.g. in the weak localisation in Ti-Al alloys[59] (for recent review see [60]). There are certain aspects of the High-T_c superconductivity where disorder play a role and recently it have been discussed in papers[61], [62], where the distribution of magnetic molecular fields has been treated within the single-site Coherent Potrntial Approximation(CPA) [63]. The CPA has been refined and developed in many papers (e.g. [64], [65]) and till now[66] are the most popular approximation for theoretical studying of alloys. But the simultaneous effect of disorder and electron- electron inelastic scattering has been considered for some limited cases only[67],[68] and not within the self-consistent scheme. Let us consider the Hubbard model Hamiltonian on a given configuration of alloy (ν)

$$H^{(\nu)} = H_1^{(\nu)} + H_2^{(\nu)} \tag{72}$$

where

$$\begin{aligned} H_1^{(\nu)} &= \sum_{i\sigma} \varepsilon_i^{\nu} n_{i\sigma} + \sum_{ij\sigma} t_{ij}^{\nu\mu} a_{i\sigma}^{+} a_{j\sigma} \\ H_2^{(\nu)} &= \frac{1}{2} \sum_{i\sigma} U_i^{\nu} n_{i\sigma} n_{i-\sigma} \end{aligned} \tag{73}$$

Contrary to the periodic model (11), the atomic level energy ε_i^{ν}, the hopping integrals $t_{ij}^{\nu\mu}$ as well as the intraatomic Coulomb repulsion U_i^{ν} here are the random variables, which take the values ε^{ν}, $t^{\nu\mu}$ and U^{ν}, respectively; the superscript $\nu(\mu)$ refers to the atomic species $(\nu, \mu = A, B)$ located on site i(j). The nearest-neighbour hopping integrals are included only.

To unify the IGF method and CPA into completely self-consistent scheme let us consider the single-electron GF (17) $G_{ij\sigma}$ in the Wannier representation for a given configuration (ν). The corresponding equation of motion has the form(for brevity we shall omit the superscript (ν) where its presence is clear)

$$\begin{aligned} (\omega - \varepsilon_i) << a_{i\sigma} | a_{j\sigma}^{+} >>_{\omega} = \delta_{ij} + \sum_{n} t_{in} << a_{n\sigma} | a_{j\sigma}^{+} >>_{\omega} \\ + U_i << n_{i-\sigma} a_{i\sigma} | a_{j\sigma}^{+} >>_{\omega} \end{aligned} \tag{74}$$

In the present paper, for brevity, we will confine ourselves by the weak correlation case and the diagonal disorder only. The generalization for the case of strong correlation or off-diagonal disorder is straightforward, but its length considerations preclude us from discussing at this time.

Using the definition (3), we define the IGF for a given (fixed) configuration of atoms in an alloy as follows

$$^{ir} << n_{i-\sigma} a_{i\sigma} | a^{+}_{j\sigma} >>=<< n_{i-\sigma} a_{i\sigma} | a^{+}_{j\sigma} >> - < n_{i-\sigma} ><< a_{i\sigma} | a^{+}_{j\sigma} >> \tag{75}$$

This time, contrary to (19), because of lack of translational invariance we must take into account the site dependence of $< n_{i-\sigma} >$. Then we rewrite the equation of motion (76)in the following form

$$\sum_{n} [(\omega - \varepsilon_i - U_i < n_{i-\sigma} >)\delta_{ij} - t_{in}] << a_{n\sigma} | a^{+}_{j\sigma} >>_{\omega} =$$
$$\delta_{ij} + U_i (^{ir} << n_{i-\sigma} a_{i\sigma} | a^{+}_{j\sigma} >>_{\omega}) \tag{76}$$

In accordance with the general method of Section 2, we find then the Dyson equation for a given configuration (ν)

$$G_{ij\sigma}(\omega) = G^{0}_{ij\sigma}(\omega) + \sum_{mn} G^{0}_{im\sigma}(\omega) M_{mn\sigma}(\omega) G_{nj\sigma}(\omega) \tag{77}$$

The GMF GF $G^{0}_{ij\sigma}$ and the self-energy operator M are defined as

$$\begin{aligned} \sum_{m} H_{im\sigma} G^{0}_{mj\sigma}(\omega) &= \delta_{ij} \\ P_{mn\sigma} &= M_{mn\sigma} + \sum_{ij} M_{mi\sigma} G^{0}_{ij\sigma} P_{jn\sigma} \\ H_{im\sigma} &= (\omega - \varepsilon_i - U_i < n_{i-\sigma} >)\delta_{im} - t_{im} \\ P_{mn\sigma}(\omega) &= U_m (^{ir} << n_{m-\sigma} a_{m\sigma} | n_{n-\sigma} a^{+}_{n\sigma} >>^{ir}_{\omega}) U_n \end{aligned} \tag{78}$$

In order to calculate the self-energy operator M self-consistently we have to express it approximately by the lower-order GFs. Employing the same pair approximation as (31) (now in Wannier representation) and the same procedure of calculations we arrive at the following expression for M for a given configuration (ν)

$$\begin{aligned} M^{(\nu)}_{mn\sigma}(\omega) &= U_m U_n \frac{1}{2\pi^4} \int R(\omega_1, \omega_2, \omega_3) \\ ImG^{(\nu)}_{nm-\sigma}(\omega_1) & ImG^{(\nu)}_{mn-\sigma}(\omega_2) ImG^{(\nu)}_{mn\sigma}(\omega_3); \\ R &= \frac{d\omega_1 d\omega_2 d\omega_3}{\omega + \omega_1 - \omega_2 - \omega_3} \frac{(1 - n(\omega_1)) n(\omega_2) n(\omega_3)}{n(\omega_2 + \omega_3 - \omega_1)} \end{aligned} \tag{79}$$

As we have mentioned previously, all the calculations just presented have been done for a given configuration of atoms in alloy. All the quantities in our theory (G, G^0, P, M) depends on the whole configuration of the alloy. To obtain a theory of a real macroscopic sample, we have to average over various configurations of atoms in the sample. The configurational averaging cannot be exactly made for a macroscopic sample. Hence we must resort to an additional approximation. It is obvious that self-energy M is in turn the functional of G, namely $M = M[G]$. If the process of taking configurational averaging is denoted by $\bar{G}$, than we have

$$\bar{G} = \bar{G}^0 + \overline{G^0 M G}$$

Few words are now appropriate for the description of general possibilities. The calculations of $\bar{G}^0$ can be performed with the help of any relevant available scheme. In the present work, for the sake of simplicity, we choose the single-site CPA[63], namely we take

$$\bar{G}^0_{mn\sigma}(\omega) = N^{-1} \sum_k \frac{\exp(ik(R_m - R_n))}{\omega - \Sigma^\sigma(\omega) - \epsilon(k)} \tag{80}$$

Here $\epsilon(k) = \sum_{n=1}^{z} t_{n,0} \exp(ikR_n)$, z is the number of nearest neigbours of the site 0, and the Coherent potential $\Sigma^\sigma(\omega)$ is the solution of the CPA self-consistency equations. For the $A_x B_{1-x}$ these read

$$\begin{aligned} \Sigma^\sigma(\omega) = x\varepsilon^\sigma_A + (1-x)\varepsilon^\sigma_B - (\varepsilon^\sigma_A - \Sigma^\sigma)F^\sigma(\omega, \Sigma^\sigma)(\varepsilon^\sigma_B - \Sigma^\sigma); \\ F^\sigma(\omega, \Sigma^\sigma) = \bar{G}^0_{mm\sigma}(\omega) \end{aligned} \tag{81}$$

Now, let us return to the calculation of the configurationally averaged total GF $\bar{G}$. To perform the remaining averaging in the Dyson equation we use the approximation

$$\overline{G^0 M G} \approx \bar{G}^0 \bar{M} \bar{G}$$

The calculation of $\bar{M}$ requires further averaging of the product of matrices. We again use the prescription of the factorisability there, namely

$$\bar{M} \approx \overline{(U_m U_n)}\;\overline{(ImG)}\;\overline{(ImG)}\;\overline{(ImG)}$$

However, the quantities $\overline{U_m U_n}$ entering into $\bar{M}$ are averaged here according to

$$\begin{aligned} \overline{U_m U_n} = U_2 + (U_1 - U_2)\delta_{mn} \\ U_1 = x^2 U_A^2 + 2x(1-x)U_A U_B + (1-x)^2 U_B^2 \\ U_2 = x U_A^2 + (1-x) U_B^2 \end{aligned} \tag{82}$$

The averaged value for the self-energy is

$$\begin{aligned} \bar{M}_{mn\sigma}(\omega) = \frac{U_2}{2\pi^4} \int R(\omega_1, \omega_2, \omega_3) Im\bar{G}_{nm-\sigma}(\omega_1) Im\bar{G}_{mn-\sigma}(\omega_2) Im\bar{G}_{mn\sigma}(\omega_3) + \\ \frac{U_1 - U_2}{2\pi^4}\delta_{mn} \int R(\omega_1, \omega_2, \omega_3) Im\bar{G}_{nm-\sigma}(\omega_1) Im\bar{G}_{mn-\sigma}(\omega_2) Im\bar{G}_{mn\sigma}(\omega_3) \end{aligned} \tag{83}$$

The averaged quantities are periodic, so we can introduce the Fourier transform of them, i.e.

$$\bar{M}_{mn\sigma}(\omega) = N^{-1} \sum_k \bar{M}_\sigma(k, \omega) \exp(ik(R_m - R_n))$$

and similar formulae for $\bar{G}$ and $\bar{G}^0$. Performing the configurational averaging of Dyson equation and Fourier transforming the resulting expressions according to the above rules, we obtain

$$\bar{G}_{k\sigma}(\omega) = (\omega - \epsilon(k) - \Sigma^\sigma(\omega) - \bar{M}_\sigma(k, \omega))^{-1} \tag{84}$$

where

$$\bar{M}_{\sigma}(k,\omega) = \frac{1}{2\pi^4}\sum_{pq}\int R(\omega_1,\omega_2,\omega_3)N^{-2}Im\bar{G}_{p-q-\sigma}(\omega_1)Im\bar{G}_{q-\sigma}(\omega_2)$$

$$[U_2 Im\bar{G}_{k+p\sigma}(\omega_3) + \frac{(U_1-U_2)}{N}\sum_{g} Im\bar{G}_{k+p-g}(\omega_3)] \tag{85}$$

The simplest way to obtain the explicit solution for the self-energy$\bar{M}$ is to start with suitable initial trial solution as it was done for the periodic case (33). For the disordered system, it is reasonable to use as the first iteration approximation the so-called Virtual Crystal Approximation(VCA):

$$\frac{-1}{\pi}Im\bar{G}^{VCA}_{k\sigma}(\omega+i\epsilon) \approx \delta(\omega - E^{\sigma}_{k})$$

where for the binary alloy A_xB_{1-x} this approximation read

$$\bar{V} = xV^A + (1-x)V^B; \quad E^{\sigma}_{k} = \bar{\varepsilon}^{\sigma}_{i} + \epsilon(k);$$

$$\bar{\varepsilon}^{\sigma}_{i} = x\varepsilon^{\sigma}_{A} + (1-x)\varepsilon^{\sigma}_{B}$$

Note, that the using of VCA here is by no means the solution of the correlation problem in VCA. It is only the using the VCA for the parametrisation of the problem, to start with VCA input parameters. After the integration of (83) the final result for the self-energy is

$$\bar{M}_{\sigma}(k,\omega) = \frac{U^2}{N^2}\sum_{pq}\frac{n(E^{-\sigma}_{p+q})[1-n(E^{-\sigma}_{q}) - n(E^{\sigma}_{k+p})] + n(E^{\sigma}_{k+p})n(E^{-\sigma}_{q})}{\omega + E^{-\sigma}_{p+q} - E^{-\sigma}_{q} - E^{\sigma}_{k+p}} +$$

$$\frac{(U_1-U_2)}{N^3}\sum_{pqg}\frac{n(E^{-\sigma}_{p+q})[1-n(E^{-\sigma}_{q}) - n(E^{\sigma}_{k+p-g})] + n(E^{\sigma}_{k+p-g})n(E^{-\sigma}_{q})}{\omega + E^{-\sigma}_{p+q} - E^{-\sigma}_{q} - E^{\sigma}_{k+p-g}} \tag{86}$$

It must be emphasized that the equations (84) - (85) give the general microscopic self-consistent description of inelastic electron-electron scattering in alloy in the spirit of the CPA. We take into account the randomness not only through the parameters of the Hamiltonian but also in a self-consistent way through the configurational dependence of the self-energy operator.

7 Electron-Lattice Interaction and MTBA

In order to understand quantitatively the electrical, thermal and superconducting properties of metals and their alloys one needs a proper description an electron-lattice interaction too [32], [69]. A systematic, self-consistent simultaneous treatment of the electron-electron and electron-phonon interaction plays an important role in recent studies of strongly correlated systems. It was argued from the different points of view that in order to understand

quantitatively the phenomenon of high-temperature superconductivity one needs a proper involving of electron-phonon interaction, too [70]- [87]. A lot of theoretical searches for the relevant mechanism of high temperature superconductivity deal with the strong electron-phonon models. This mechanism is certainly valuable for bismuthate ceramics [88] and for fullerens. Recently [89] a new family of quaternary intermetallic $LuNi_2B_2C$ compounds has been shown to display superconductivity with Tc = 16.6 K for $LuNi_2B_2C$, which, besides that studies of their physical properties are still in the early stages, suggest that electron-phonon coupling is responsible for the superconductivity.
The natural approach for the description of superconductivity in such type of compounds is MTBA [32], [69]. The papers [32], [33],[34] contain a self-consistent microscopic theory of the normal and superconducting properties of transition metals and strongly disordered binary alloys in the framework of Hubbard Model (11) and random Hubbard model (73). It is worthy to emphasize that in paper [34] a very detailed microscopic theory of strong coupling superconductivity in highly disordered transition metals alloys has been developed on the basis of IGF method within MTBA reformulated approach [33]. The Eliashberg-type strong coupling equations for highly disordered alloys has been derived. It was shown that the electron-phonon Spectral Function in alloy is modified strongly. An interesting discussion [90], [91], [92] clarified many uncertainties in this important issue (c.f. [93]- [97]).

8 Other Applications of the IGFs Method

Another important application of IGF method is related with the investigation of non-local correlations and quasiparticle interactions in Anderson model [29], [30]. A comparative study of real-many body dynamics of single-impurity, two-impurity and periodic Anderson model, especially for strong but finite Coulomb correlation, when perturbation expansion in U does not work (c.f. [98]) has permitted to characterize the true quasiparticle excitations and the role of magnetic correlations. It was shown that the physics of two-impurity Anderson model can be understood in terms of competition between of itinerant motion of carriers and magnetic correlations of the RKKY nature. The correct functional two-pole structure of the propagator has been found for the strongly correlated case. This issue is still very controversial [99] and the additional efforts must be applied in this field.
The application of the IGF method to the theory of magnetic semiconductors was very succsessfull [27], [28]. As a remarkable results of our approach let me mention the finite temperature generalization of the Shastry-Mattis theory for magnetic polaron [28], which clarified greatly the true nature of the carrier in magnetic semiconductors. There are some analogy of the Kondo-lattice type of model in [27] with the Kondo-Heisenberg model of copper oxides, however the physics are different. There is a dense system of spins interacting with smaller concentration of holes in HTSC. The application of IGF method to spin-fermion model [100] has been done by using the theory of Heisenberg antiferromagnet [31] and allows one to consider carefully the true nature of the carriers in CuO_2 planes.
And finally, the new interesting application of the IGF method for consideration of dy-

namics of quasiparticles and dynamical conductivity of single electron resonant tunneling systems has been done recently in papers [101], [102] (c.f. [103]). This reformulation of IGF method has much in common with the approach of paper [104].

9 Conclusions

In the present paper we have formulated the theory of the correlation effects using the ideas of the quantum field theory for the interacting electron system on a lattice. The main achievement of this formulation is the derivation of the Dyson equation for two-time thermodynamic retarded Green's Functions instead of causal ones. Such a formulation permit to use the convenient analytical properties of retarded and advanced GF and advantage of using the formal solution of the Dyson equation, which, in spite required approximations for the self-energy, provide the correct functional structure of the single-electron GF. This strong point of our approach do not give the possibility of direct application of it to the calculation of the two-particle GFs. In this paper we have considered in details the idealized single-band Hubbard model, which is one of the simplest (in the sense of formulation, but not solution) and most popular model of correlated lattice fermions. We have presented here the novel method of calculation of the quasiparticle spectra for this model, as the most representative example. We hope that this explanation have been done with sufficient details to bring out their scope and power, since we believe that such techniques will have application to a variety of many-body systems with complicated spectrum and strong interaction, as it was shown in Section 8.
In summary, with using IGF method we were able to obtain the closed self- consistent set of equations determining the electron GF and self-energy. These equations define the renormalization coefficient of the one-electron GF[7], defined for a point (k, $\omega = \epsilon(k)$):

$$Z(k) = \frac{1}{(1 - \frac{dM(k,\omega)}{d\omega})_{\omega=\epsilon(k)}} \tag{87}$$

The renormalization coefficient (87) is an one of the most important notion for the characterization of the single-particle behaviour of the quasiparticle excitations in correlated many-body systems. For the Hubbard model, these equations give the general microscopic description of correlation effects for both the weak and strong Coulomb correlation, determining of the complete interpolation solution of the Hubbard model. Moreover, this approach gives the workable scheme for the definition of the relevant Generalized Mean Fields written in terms of appropriate correlators. The most important conclusion to be drawn from of the present consideration is that the GMF for the case of strong Coulomb interaction have a quite non-trivial structure and cannot be reduced to the mean-density functional. This last statement resemble very much the situation with the strongly nonequilibrium system, where the single-particle distribution function only not enough to describe the essence of the strongly nonequilibrium state and more complicated correlation functions must be taken into account, in accordance with general ideas of Bogolubov and Mori-Zwanzig. The IGF method is intimately related to the projection method in this sense, which express the idea of a "reduced description" of the system in the most general form. This line of consideration is very promising for developing the complete and self-contained theory of the strongly interacting many-body systems.

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