IL NUOVO CIMENTO VOL. 109 B, N. 8 Agosto 1994

Generalized Mean Fields and Quasi-Particle Interactions in the Hubbard Model.

A. L. KUZEMSKY (*) (**)
Dipartimento di Fisica Teorica dell'Università di Salerno - I-84081 Baronissi (SA), Italia

(ricevuto il 10 Dicembre 1993; approvato il 12 Maggio 1994)

Summary. — The self-consistent theory of the correlation effects in transition metals and their compounds (TMC) and disordered binary alloys has been developed using the Hubbard model and random Hubbard model. In order to obtain the interpolation solution for the quasi-particle spectrum, which is valid for both the atomic and band limits, the novel Irreducible Green's Function (IGF) method has been used. This method permits to calculate the quasi-particle spectra of many-particle systems with complicated spectra and strong interaction in a very natural and compact way. The essence of the method is deeply related with the notion of the Generalized Mean Fields (GMFs), which determines the elastic-scattering corrections. The inelastic-scattering corrections lead to the damping of the quasi-particles and is 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).

PACS 05.30 – Quantum statistical mechanics.
PACS 05.30.Fk – Fermion systems and electron gas.
PACS 11.15.Tk – Other nonperturbative techniques.
PACS 71.10 – Electron states: General theories and computational techniques (including many-body perturbation theory, density-functional theory, atomic sphere approximation methods, Fourier decomposition methods, etc.).
PACS 71.20.Ad – Electron states: Developments in mathematical and computational techniques.

1. – Introduction.

The study of the excitations in many-body systems has been one of the most important and interesting subjects in the last few decades. The quantum field-theoretical techniques

(*) E-mail: kuzemsky@theor.jinrc.dubna.su.
(**) Permanent address: Department of Statistical Mechanics, Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Head Post Office Box 79, 101000 Moscow, Russia.

have been widely applied to the statistical treatment of a large number of interacting particles. Many-body calculations are often done for model systems of statistical mechanics using the perturbation expansion. The basic procedure in many-body theory is to find the relevant unperturbed Hamiltonian and then take into account the small-perturbation operator. This procedure, which works well for the weakly interacting systems, needs the suitable reformulation for the many-body systems with complicated spectra and strong interaction.

The most characteristic feature of the recent advancement in basic research on electronic properties of solids is the development of a variety of a 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 are very well known and the electrons can be represented in a way such that they weakly interact with each other, in these materials the electrons interact strongly and moreover their spectra are complicated, *i.e.* they 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 it exists at all. Therefore, the theoretical studies of the Highly Correlated Electron Systems (HCES) are very important and actual [1]. The principal importance 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 the electrons. In spite of experimental and theoretical achievements [2], still it remains much to be understood concerning such systems.

Recent theoretical investigations of HCES have brought forth the 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 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. The essence of our consideration of the dynamical properties of many-body systems with strong interaction is related closely with the field-theoretical approach and has the advantage of using the Green's functions language and the Dyson equation. It is possible to say that our method tends to emphasize the fundamental and central role of the Dyson equation for the single-particle dynamics of the many-body systems at finite temperature. This approach has been suggested as essential for various many-body systems and we believe that it bears the real physics of Highly Correlated Systems [3, 4].

2. – Irreducible Green's Functions method.

In this section, we will discuss briefly the novel non-perturbative approach for the 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 an 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?» [5] (cf. [6]). The formulation of the Anderson model [5] and closely related Hubbard model [7,8] dates really a better understanding of the electronic correlations in solids, especially if the relevant electrons are modelled better by tight-binding approximation. Both of the models, Anderson's and Hubbard's, are often referred to as the simplest models of magnetic metals and alloys. This naive perception contradicts the enormous amount of papers which has been published 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 manifests 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) method for the interpolation solution of the single-band Hubbard model. A number of other approaches has been proposed and our approach is in many respects an additional and incorporates the logic of development of the many-body techniques [9].

Let me first sketch this logic. The study of the quasi-particle excitations in solids has been one of the most fascinating subjects for many years. The considerable progress in studying the spectra of elementary excitations and thermodynamic properties of many-body systems has been for the 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 [9] 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.

To clarify the foregoing, let us consider the retarded GF of the form

$$G^{\mathrm{r}} = \langle\langle A(t), B(t') \rangle\rangle = -i\vartheta(t-t')\langle [A(t)\, B(t')]_{\eta} \rangle, \qquad \eta = \pm 1 . \tag{1}$$

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:

$$\omega G(\omega) = \langle [A, A^{+}]_{\eta} \rangle + \langle\langle [A, H] \;\; | A^{+} \rangle\rangle_{\omega} . \tag{2}$$

The essence of the method is as follows [3]. 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 terms 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,

$$^{\mathrm{ir}}\langle\langle [A, H] \;\; | A^{+} \rangle\rangle = \langle\langle [A, H]_{-} - zA \,| A^{+} \rangle\rangle . \tag{3}$$

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

$$\langle [[A, H]^{\mathrm{ir}}, A^{+}]_{\eta} \rangle = 0 . \tag{4}$$

From the condition (4) one can find

$$z = \frac{\langle [[A, H]_-, A^+]_\eta \rangle}{\langle [A, A^+]_\eta \rangle} = \frac{M_1}{M_0} . \tag{5}$$

Here M_0 and M_1 are the zeroth- and first-order moments of the spectral density. Therefore, the irreducible GF (3) is 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 translated into the language of retarded and advanced GFs. This procedure extracts all relevant (for the problem under consideration) mean-field contributions and puts them into the generalized mean-field GFs, which here are defined as

$$G^0(\omega) = \frac{\langle [A, A^+]_\eta \rangle}{(\omega - z)} . \tag{6}$$

To calculate the IGF ${}^{\mathrm{ir}}\langle\langle [A, H]_-(t), A^+(t') \rangle\rangle$ in (2), we have to write the equation of motion after differentiation with respect to the second time variable t'. The condition (4) removes 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:

$$G = G^0 + G^0 P G^0 . \tag{7}$$

The scattering operator P is given by

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

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

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

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 $M = (P)^{\mathrm{p}}$. 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 the 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 the constraint (4)) transformed into the Dyson equation for the two-time thermal GF. This is a very remarkable result, which deserves to be underlined, because the traditional form of the GF method [10, 11] did not include namely this point. The projection operator technique [12] has essentially the same

philosophy, but by 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 [3]. 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 the scheme presented above gives just a general idea of the IGF method. The specific method of introducing IGFs depends on the form of the 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 quasi-particle 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. 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 GFs in accordance with a given algebra. The Hubbard model is a very suitable tool for the application of this approach as it will be demonstrated below.

The present paper deals with many points of my own works on electron correlation effects. It reflects the evolution of my own understanding of the physics of HCES and the influence of more recent theoretical investigations in this field. As a result, the present considerations are addressing a number of new issues, which have not been mentioned previously.

3. – Hubbard model.

The model Hamiltonian which is usually referred to as Hubbard Hamiltonian [7,8]

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

includes the intra-atomic 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 take into account both these effects simultaneously. Thus, the Hamiltonian (11) is specified by two parameters: U and the effective electron bandwidth

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

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

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

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

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

which has been calculated by Hubbard [7, 13], has the characteristic two-pole functional structure

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

where

$$F_{\sigma}^{-1}(\omega) = \frac{\omega - (n_{-\sigma}^{+} E_{-} + n_{-\sigma}^{-} E_{+}) - \lambda}{(\omega - E_{+} - n_{-\sigma}^{-}\lambda)(\omega - E_{-} - n_{\sigma}^{+}\lambda) - n_{\sigma}^{+} n_{-\sigma}^{-} \lambda^2} \tag{14}$$

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

$$F_{\sigma}^{-1}(\omega) \approx \frac{n_{-\sigma}^{-}}{\omega - E_{-} - n_{-\sigma}^{+}\lambda} + \frac{n_{-\sigma}^{+}}{\omega - E_{+} - n_{-\sigma}^{-}\lambda},$$

which corresponds to the two shifted subbands with the gap

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

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

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

The latter solution corresponds to the single band, centred at the energy $\omega \approx n_{-\sigma}^{+} U$.

The two-pole functional structure of the single-particle GF is very easy to understand within the formalism which describes the motion of electrons in binary alloys

[13,14]. If one introduces the two types of scattering potentials $t_{\pm} \approx (\omega - E_{\pm})^{-1}$, then the two kinds of the t-matrix T_+ and T_- appear which satisfy the following system of equations:

$$\begin{cases} T_+ = t_+ + t_+ G^0_{+\,+} T_+ + t_+ G^0_{+\,-} T_- , \\ T_- = t_- + t_- G^0_{-\,-} T_- + t_- G^0_{-\,+} T_+ , \end{cases}$$

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:

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

$$= \frac{t_{\mp}^{-1} G^0_{\pm}}{(t_+^{-1} - G^0_{+\,+})(t_-^{-1} - G^0_{-\,-}) - G^0_{-\,+} G^0_{+\,-}} .$$

Thus, by comparing this functional two-pole structure and well-known «Hubbard III» solution [13]

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

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

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

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

$$Y_\sigma = F_\sigma(\omega) - G_{0\sigma}^{-1}(\omega), \qquad G_{0\sigma}(\omega) = N^{-1} \sum_k G_{k\sigma}(\omega).$$

If we put $A_\sigma(\omega) = 0$, we immediatedly obtain the «Hubbard I» solution [7]. The «alloy analogy» approximation corresponds to $A_\sigma(\omega) \approx Y_\sigma(\omega)$. Note that the «Hubbard III» self-energy operator $\Sigma_\sigma(\omega)$ is local, *i.e.* it does not depend on quasi-momentum. Another drawback of this solution is the 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 the Hubbard model has been proposed by Roth [15]. She clarified microscopically the origination of the two-pole solution of the single-particle GF, which was a 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 TMC. Thus the use of the sophisticated many-body technique is required for the calculation of the excitation spectra at finite temperature. The last point should be underlined, because the suitable modification of the Density Functional Approximation [16,17] could give the reasonable description of the ground-state properties of TMC. We shall show here that the use of the IGF method permits 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 shorter) to discuss these concepts for weakly and strongly correlated cases separately. For the first time we must construct the suitable state vector space of the many-body system [10]. 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 [18]. This concept originates in perturbation theory and finds support for weakly interacting many-particle systems. For the strongly correlated case, this approach needs the suitable reformulation (cf. [19]) and, namely, in this point the right definition of the GMFs is vital.

Let us consider the weakly correlated Hubbard model (11). In many respects, 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 $a_{i\sigma}^{\dagger}$ and annihilation $a_{i\sigma}$ second quantized operators with the properties

$$a_i^{\dagger}\Psi^{(0)} = \Psi_i^{(1)}, \qquad a_i\Psi^{(1)} = \Psi^{(0)},$$

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

are suitable variables for the description of the considered 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 quasi-particles. For a translationary invariant system, to describe the low-lying excitations of the system in terms of quasi-particles [20], one has to choose eigenstates such that they all correspond to definite momentum. For the single-band Hubbard model (11) the exact transformation reads

$$a_{k\sigma} = N^{-1/2}\sum_i \exp[-i\vec{k}\vec{R}_i]\, a_{i\sigma}.$$

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

$$H = \sum_{k\sigma}\varepsilon(k)\, a_{k\sigma}^{\dagger}a_{k\sigma} + (U/2N)\sum_{pqrs} a_{p+r-q\sigma}^{\dagger}a_{p\sigma}a_{q-\sigma}^{\dagger}a_{r-\sigma}. \tag{16}$$

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

$$G_{k\sigma}(t-t') = \langle\langle a_{k\sigma}, a_{k\sigma}^{\dagger}\rangle\rangle = -i\theta(t-t')\langle[a_{k\sigma}(t), a_{k\sigma}^{\dagger}(t')]_+\rangle = \frac{1}{2\pi}\cdot \tag{17}$$

$$\cdot\int_{-\infty}^{+\infty} d\omega \exp[-i\omega t]\, G_{k\sigma}(\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega \exp[-i\omega t]\frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{d\omega'}{\omega-\omega'}(\exp[\beta\omega']+1)A_{k\sigma}(\omega'),$$

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

$$(\omega - \varepsilon(k))\, G_{k\sigma}(\omega) = 1 + (U/)N \sum_{pq} \langle\langle a_{k+p\sigma} a^{\dagger}_{p+q-\sigma} a_{q-\sigma} | a^{\dagger}_{k\sigma} \rangle\rangle_{\omega} . \tag{18}$$

Let us introduce, by definition, an «irreducible» GF in the following way:

$$^{\mathrm{ir}}\langle\langle a_{k+p\sigma} a_{p+q-\sigma} a_{q-\sigma} | a^{\dagger}_{k\sigma} \rangle\rangle_{\omega} = \langle\langle a_{k+p\sigma} a^{\dagger}_{p+q-\sigma} a_{q-\sigma} | a^{\dagger}_{k\sigma} \rangle\rangle_{\omega} - \delta_{p,0} \langle n_{q-\sigma} \rangle G_{k\sigma} . \tag{19}$$

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

$$G_{k\sigma}(\omega) = G^{\mathrm{MF}}_{k\sigma}(\omega) + G^{\mathrm{MF}}_{k\sigma}(\omega)(U/N) \sum_{pq}^{\mathrm{ir}} \langle\langle a_{k+p\sigma} a^{\dagger}_{p+q-\sigma} a_{q-\sigma} | a^{\dagger}_{k\sigma} \rangle\rangle_{\omega} . \tag{20}$$

Here we have introduced the notations

$$G^{\mathrm{MF}}_{k\sigma}(\omega) = (\omega - \varepsilon(k\sigma))^{-1} , \qquad \varepsilon(k\sigma) = \varepsilon(k) + (U/N) \sum_{q} \langle n_{q-\sigma} \rangle . \tag{21}$$

In this paper, for brevity, we confine ourselves by considering the paramagnetic solutions only, *i.e.* $\langle n_{\sigma} \rangle = \langle n_{-\sigma} \rangle$. In order to calculate the higher-order GF in the right-hand side 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 $(\mathrm{d}/\mathrm{d}t')^{\mathrm{ir}} \langle\langle A(t), a^{\dagger}_{k\sigma}(t') \rangle\rangle$. For the Fourier components, this is written in the form

$$(\omega - \varepsilon(k))\, ^{\mathrm{ir}}\langle\langle A | a^{\dagger}_{k\sigma} \rangle\rangle_{\omega} = \langle ^{\mathrm{ir}}[A, a^{\dagger}_{k\sigma}]_{+} \rangle + (U/N) \sum_{rs}^{\mathrm{ir}} \langle\langle A | a^{\dagger}_{r-\sigma} a_{r+s-\sigma} a_{k+s\sigma} \rangle\rangle_{\omega} . \tag{22}$$

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

$$\langle [^{\mathrm{ir}}(a_{k+p\sigma} a^{\dagger}_{p+q-\sigma} a_{q-\sigma}), a^{\dagger}_{k\sigma}]_{+} \rangle = \tag{23}$$

$$= \langle [a_{k+p\sigma} a^{\dagger}_{p+q-\sigma} a_{q-\sigma} - \langle a^{\dagger}_{p+q-\sigma} a_{q-\sigma} \rangle a_{k+p\sigma}, a^{\dagger}_{k\sigma}]_{+} \rangle = 0 .$$

If one introduces the irreducible part for the right-hand side operators by analogy with expression (19), the equation of motion (20) can be exactly rewritten in the form (7)

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

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

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

$$= \frac{U^2}{N^2} \sum_{pqrs}^{\mathrm{ir}} \langle\langle a_{k+p\sigma} a^{\dagger}_{p+q-\sigma} a_{q-\sigma} | a^{\dagger}_{r-\sigma} a_{r+s-\sigma} a^{\dagger}_{k+s\sigma} \rangle\rangle^{\mathrm{ir}}_{\omega} .$$

To define the self-energy operator according to (9), one must separate the «proper»

part in the following way:

$$D^{\mathrm{ir}}_{k\sigma}(p, q|r, s; \omega) = L^{\mathrm{ir}}_{k\sigma}(p, q|r, s; \omega) + \tag{26}$$

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

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

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

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

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

where the self-energy operator M is given by

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

$$= \frac{U^2}{N^2} \sum_{pqrs}{}^{\mathrm{ir}} \langle\langle a_{k+p\sigma} a^\dagger_{p+q-\sigma} a_{q-\sigma} | a^\dagger_{k+s\sigma} a^\dagger_{r-\sigma} a_{r+s-\sigma} \rangle\rangle^{\mathrm{ir}}.$$

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. [4]). 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 the self-energy operator, as will be shown in detail below. The formal solution of the Dyson equation (28) defines the right reference frame for the formation of the quasi-particle spectrum due to 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 at 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 the self-energy M (29), we have to evaluate approximatively 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 [10, 11]:

$$\langle\langle a_{k+p\sigma} a^\dagger_{p+q-\sigma} a_{q-\sigma} | a^\dagger_{k+s\sigma} a^\dagger_{r-\sigma} a_{r+s-\sigma} \rangle\rangle_\omega = \tag{30}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega'}{\omega - \omega'} (\exp[\beta\omega'] + 1) \int_{-\infty}^{+\infty} \exp[i\omega' t] \cdot$$

$$\cdot \langle a^\dagger_{k+s\sigma}(t) a^\dagger_{r-\sigma}(t) a_{r+s-\sigma}(t) a_{k+p\sigma} a^\dagger_{p+q-\sigma} a_{q-\sigma} \rangle.$$

Further insight is gained if we select the suitable relevant «trial» approximation for the correlation function in the right-hand side of (30). In this paper we show that the earlier formulations, based on the decoupling or/and diagrammatic methods can be arrived at by our technique but in a self-consistent way. Clearly the choice of the relevant trial approximation for the 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 quasi-particles:

$$(31)\quad \langle a^{\dagger}_{k+s\sigma}(t)\, a^{\dagger}_{r\,-\sigma}(t)\, a_{r+s-\sigma}(t)\, a_{k+p\sigma} a^{\dagger}_{p+q-\sigma} a_{q-\sigma}\rangle^{\mathrm{ir}} \approx$$

$$\approx \langle a^{\dagger}_{k+p\sigma}(t)\, a_{k+p\sigma}\rangle \langle a^{\dagger}_{q-\sigma}(t)\, a_{q-\sigma}\rangle \langle a_{p+q\,-\sigma}(t)\, a^{\dagger}_{p+q\,-\sigma}\rangle \hat{\delta}_{k+s,k+p}\, \hat{\delta}_{r,q}\, \hat{\delta}_{r+s,p+q}\,.$$

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

$$(32)\quad M_{\sigma}(k,\omega) = \frac{U^2}{N^2} \sum_{pq} \int \frac{\mathrm{d}\omega_1\, \mathrm{d}\omega_2\, \mathrm{d}\omega_3}{\omega + \omega_1 - \omega_2 - \omega_3} \cdot$$

$$\cdot [n(\omega_2)\, n(\omega_3) + n(\omega_1)(1 - n(\omega_2) - n(\omega_3))]\, g_{p+q-\sigma}(\omega_1)\, g_{k+p\sigma}(\omega_2)\, g_{q\,-\sigma}(\omega_3)\,,$$

where we have used the notations

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

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, in the right-hand side 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:

$$(33)\quad g_{k\sigma}(\omega) \approx \hat{\delta}(\omega - \varepsilon(k\sigma))\,.$$

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

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

The numerical calculations of the real and imaginary parts of the self-energy (34) have been performed [21] for the model density of states of the FCC lattice. The calculations were done taking the dispersion law

$$\varepsilon(k) = E_0 + 4t\left(\cos\frac{ak_x}{2}\cos\frac{ak_y}{2} + \cos\frac{ak_x}{2}\cos\frac{ak_z}{2} + \cos\frac{ak_z}{2}\cos\frac{ak_y}{2}\right),$$

with the appropriate set of metal parameters, which approximatively represent the ones for d-bands in transition metals. In fig. 1 the typical behaviour of the real and imaginary parts of the self-energy $M_{\sigma}(k,\omega)$ is shown. This picture proves that the conventional one-electron approximation of the band theory is not always a

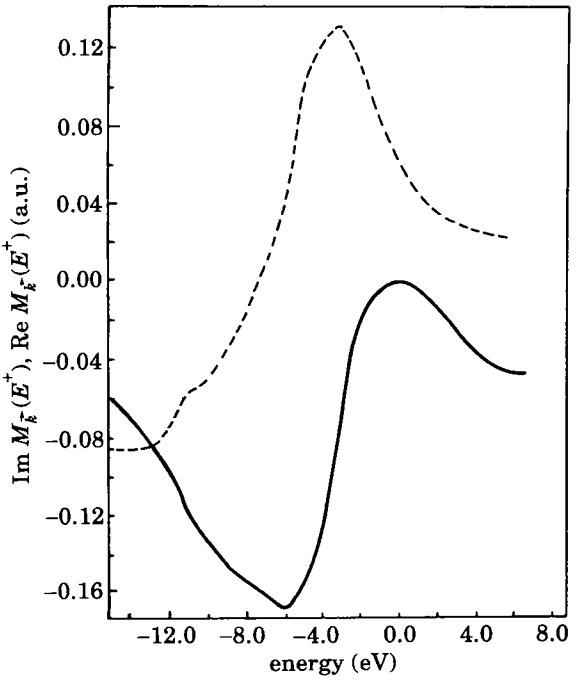

Fig. 1. – Real and imaginary parts of self-energy calculated for the point Γ of the Brillouin zone ($k = (0, 0, 0)$) and for FCC crystal lattice with parameters close to the nickel metal. --- $\mathrm{Re}\, M_k(E^+)$, —— $\mathrm{Im}\, M_k(E^+)$, $E_{\mathrm{Fermi}} = 0.0$ eV, band limits = $(-4.0, +1.2)$.

sufficiently good approximation for transition metals like nickel. An adequate description of electronic quasi-particle spectra in transition metals like nickel requires including electron-electron scattering processes in a self-consistent way.

The simple formula (32) derived above for the self-energy operator is typical in showing the role of correlation effects in the formation of quasi-particle spectrum of the Hubbard model. It is instructive to examine other types of the possible trial solutions for the six-operator correlation function in eq. (30). The approximation which we propose now reflects the interference between the one-particle branch of the spectrum and the collective one:

$$\langle a^{\dagger}_{k+s\sigma}(t)\, a^{\dagger}_{r-\sigma}(t)\, a_{r+s-\sigma}(t)\, a_{k+p\sigma} a^{\dagger}_{p+q-\sigma} a_{q-\sigma}\rangle^{\mathrm{ir}} \approx \tag{35}$$

$$\approx \langle a^{\dagger}_{k+s\sigma}(t)\, a_{k+p\sigma}\rangle \langle a^{\dagger}_{r-\sigma}(t)\, a_{r+s-\sigma}(t)\, a^{\dagger}_{p+q-\sigma} a_{q-\sigma}\rangle +$$

$$+ \langle a_{r+s-\sigma}(t)\, a^{\dagger}_{p+q-\sigma}\rangle \langle a^{\dagger}_{k+s\sigma}(t)\, a^{\dagger}_{r-\sigma}(t)\, a_{k+p\sigma} a_{q-\sigma}\rangle +$$

$$+ \langle a^{\dagger}_{r-\sigma}(t)\, a_{q-\sigma}\rangle \langle a^{\dagger}_{k+s\sigma}(t)\, a_{r+s-\sigma}(t)\, a_{k+p\sigma} a^{\dagger}_{p+q-\sigma}\rangle .$$

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 quasi-particle spectra with damping requires the suitable incorpor-

ation 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 correlated systems are magnetic or have very well developed magnetic fluctuations. We follow the above steps and calculate the self-energy operator (29) as

$$(36)\quad M_\sigma(\vec{k}, \omega) = \frac{U^2}{N} \int_{-\infty}^{\infty} d\omega_1 \, d\omega_2 \frac{1 + N(\omega_1) - n(\omega_2)}{\omega - \omega_1 - \omega_2} \cdot$$

$$\cdot \sum_{i,j} \exp[-i\vec{k}(\vec{R}_i - \vec{R}_j)] \left(-\frac{1}{\pi} \operatorname{Im} \langle\langle S_i^+ | S_j^\mp \rangle\rangle_{\omega_1} \right) \left(-\frac{1}{\pi} \operatorname{Im} \langle\langle a_{i-\sigma} | a_{j-\sigma}^\dagger \rangle\rangle_{\omega_2} \right),$$

where the following notations have been used:

$$S_i^+ = a_{i\uparrow}^\dagger a_{i\downarrow}, \qquad S_i^- = a_{i\downarrow}^\dagger a_{i\uparrow},$$

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

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

$$(37)\quad M_\sigma(k, \omega) = \frac{U^2}{N} \sum_q \int d\omega' \left(\operatorname{ctg} \frac{\omega - \omega'}{2T} + \operatorname{tg} \frac{\omega'}{2T} \right) \cdot$$

$$\cdot \left(-\frac{1}{\pi} \operatorname{Im} \chi^{\mp\pm}(k - q, \omega - \omega') g_{q\sigma}(\omega') \right).$$

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 quasi-momentum; in other words, the approximative procedure does not break the momentum conservation law. It is important, because the poles $\omega(k, \sigma) = \varepsilon(k, \sigma) - i\Gamma(k)$ of the GF (28) are determined by the equation

$$(38)\quad \omega - \varepsilon(k\sigma) - \operatorname{Re}[M_\sigma(k, \omega)] - i \operatorname{Im}[M_\sigma(k, \omega)] = 0.$$

It may be shown quite generally that Luttinger's definition of the true Fermi surface [20] 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 quasi-momentum, the definition of the Fermi surface is a little more complicated than 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). Very recently, this approximation has been applied to the single-band Hubbard model (11) for the calculation of the density of states for CuO_2 clusters [22]. The following definition of UHFA has been used:

$$(39)\quad n_{i-\sigma} a_{i\sigma} = \langle n_{i-\sigma} \rangle a_{i\sigma} - \langle a_{i-\sigma}^\dagger a_{i\sigma} \rangle a_{i-\sigma}.$$

Thus, in addition to the standard HF term, the new, the so-called «spin-flip» terms, are retained. This example clearly shows 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 $\langle a^{\dagger}_{i-\sigma} a_{i,\sigma}\rangle = 0$, because of the rotational symmetry of the Hubbard model. So, in ref. [22] the effective Hamiltonian H_{eff} has been defined. We have analysed in detail [23] the proper definition of the irreducible GFs which include the «spin-flip» terms. The definition (19) must be modified in the following way:

$$(40) \quad {}^{\text{ir}}\langle\langle a_{k+p\sigma} a_{p+q-\sigma} a_{p+q-\sigma} | a^{\dagger}_{k\sigma}\rangle\rangle_{\omega} = \langle\langle a_{k+p\sigma} a^{\dagger}_{p+q-\sigma} a_{q-\sigma} | a^{\dagger}_{k\sigma}\rangle\rangle_{\omega} -$$

$$- \delta_{p,0}\langle n_{q-\sigma}\rangle G_{k\sigma} - \langle a_{k+p\sigma} a^{\dagger}_{p+q-\sigma}\rangle \langle\langle a_{q-\sigma} | a^{\dagger}_{k\sigma}\rangle\rangle_{\omega} .$$

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

$$\begin{pmatrix} \langle\langle a_{i\sigma} | a^{\dagger}_{i\sigma}\rangle\rangle & \langle\langle a_{i\sigma} | a^{\dagger}_{i-\sigma}\rangle\rangle \\ \langle\langle a_{i-\sigma} | a^{\dagger}_{i\sigma}\rangle\rangle & \langle\langle a_{i-\sigma} | a^{\dagger}_{i-\sigma}\rangle\rangle \end{pmatrix}.$$

In fact, this approximation has been investigated earlier by Kishore and Joshi [24]. They clearly pointed out that they assumed that the system is magnetized in the x-direction instead of the conventional z-axis. Very recently, the detailed and clear reconsideration of the HF and UHF approximations in comparison with the Density Functional Theory has been given in paper [25].

5. – Hubbard model. Strong correlation.

When studying the electronic quasi-particle 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 leads to the necessity of the redefinition of the single-particle states. Due to the strong correlation, the initial algebra of the operators is transformed into the 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 [26, 27]. It is very important to underline that the transformation into the new algebra of relevant operators reflects some important internal symmetries of the problem and nowadays this way of thinking is formulated in the elegant and very powerful technique of the classification of the integrable models [28, 29] and exactly soluble models (see also [30]).

ii) The single-electron GF, which describes the dynamical properties, must have a two-pole functional structure, giving, in the atomic limit, when the hopping integral tends to zero, the exact two-level atomic solution.

iii) The GMFs have, in the 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 [13, 19, 27] 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:

$$\begin{cases} d_{i\alpha\sigma} = n^{\alpha}_{i\,-\sigma} a_{i\sigma}, \quad (\alpha = \pm); \qquad n^{+}_{i\sigma} = n_{i\sigma}, \quad n_{i\sigma} = (1 - n_{i\sigma}), \\ \sum n^{\alpha}_{i\sigma} = 1; \qquad n^{\alpha}_{i\sigma} n^{\beta}_{i\sigma} = \delta_{\alpha\beta} n^{\alpha}_{i\sigma}, \quad \sum_{\alpha} d_{i\alpha\sigma} = a_{i\sigma}. \end{cases} \tag{41}$$

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

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

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

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

It is possible to interpret [7, 13], both contribution in this equation, as *alloy analogy* and *resonance broadening corrections*. The usefulness of the new algebra of the operator has been emphasized by Matsumoto and Umezawa in the context of thermo field dynamics [31] and recently for the consideration of the strong electron correlation in the high-T_c superconductors [32, 33]. The reformulation of the many-body diagrammatic technique [34] for the correlated systems underlines the same aspect of the problem.

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:

$$G_{ij\sigma}(\omega) = \sum_{\alpha\beta} \langle\langle d_{j\alpha\sigma} | d^{\dagger}_{j\beta\sigma} \rangle\rangle_{\omega} = \sum_{\alpha\beta} F^{\alpha\beta}_{ij\sigma}(\omega). \tag{43}$$

The equation of motion for the auxiliary matrix GF

$$F^{\alpha\beta}_{ij\sigma}(\omega) = \begin{pmatrix} \langle\langle d_{i+\sigma} | d^{\dagger}_{j+\sigma} \rangle\rangle_{\omega} & \langle\langle d_{i+\sigma} | d^{\dagger}_{j\,-\sigma} \rangle\rangle_{\omega} \\ \langle\langle d_{i-\sigma} | d^{\dagger}_{j+\sigma} \rangle\rangle_{\omega} & \langle\langle d_{i-\sigma} | d^{\dagger}_{j-\sigma} \rangle\rangle_{\omega} \end{pmatrix}. \tag{44}$$

has the following form:

$$(\boldsymbol{E}\boldsymbol{F}_{ij\sigma}(\omega) - \boldsymbol{I}\delta_{ij})_{\alpha\beta} = \sum_{l \neq i} t_{il} \langle\langle n^{\alpha}_{i\,-\sigma} a_{l\sigma} + \alpha a_{i\sigma} b_{il\,-\sigma} | d^{\dagger}_{j\beta\sigma} \rangle\rangle_{\omega}, \tag{45}$$

where the following matrix notations have been used:

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

In accordance with the general method of sect. 2, we introduce by definition the IGF matrix:

$$(47)\quad \boldsymbol{D}^{\mathrm{ir}}_{il,j}(\omega) = \begin{pmatrix} \langle\langle Z_{11} \mid d^{\dagger}_{j+\sigma}\rangle\rangle_{\omega} & \langle\langle Z_{12} \mid d^{\dagger}_{j-\sigma}\rangle\rangle_{\omega} \\ \langle\langle Z_{21} \mid d^{\dagger}_{j+\sigma}\rangle\rangle_{\omega} & \langle\langle Z_{22} \mid d^{\dagger}_{j-\sigma}\rangle\rangle_{\omega} \end{pmatrix} - \\ - \sum_{\alpha'} \left(\begin{bmatrix} A^{+\alpha'}_{il} \\ A^{-\alpha'}_{il} \end{bmatrix} [F^{\alpha'+}_{ij\sigma} + F^{\alpha'-}_{ij\sigma}] - \begin{bmatrix} B^{-\alpha'}_{li} \\ B^{-\alpha'}_{li} \end{bmatrix} [F^{\alpha'+}_{lj\sigma} + F^{\alpha'-}_{lj\sigma}] \right).$$

Here the following notations have been used:

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

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

$$(48)\quad \langle [(\boldsymbol{D}^{\mathrm{ir}}_{il,j})_{\alpha\beta},\, d^{+}_{j\beta\sigma}]_{+} \rangle = 0\,.$$

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

$$(49)\quad \begin{cases} [A_{il}]_{\alpha\beta} = \alpha(\langle d^{\dagger}_{i\beta} a_{l-\sigma}\rangle + \langle d_{i-\beta-\sigma} a^{\dagger}_{l-\sigma}\rangle)(n^{\beta}_{-\sigma})^{-1}\,, \\ [B_{li}]_{\alpha\beta} = [\langle n^{\beta}_{l-\sigma} n^{\alpha}_{i-\sigma}\rangle + \alpha\beta(\langle a_{i\sigma} a^{\dagger}_{i-\sigma} a_{l-\sigma} a^{\dagger}_{l\sigma}\rangle - \langle a_{i\sigma} a_{i-\sigma} a^{\dagger}_{l-\sigma} a^{\dagger}_{l\sigma}\rangle)](n^{\beta}_{-\sigma})^{-1}\,, \end{cases}$$

As previously, we introduce now the GMF GF $\boldsymbol{F}^{0}_{ij\sigma}$ 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

$$(50)\quad \begin{pmatrix} F^{0++}_{k\sigma} & F^{0+-}_{k\sigma} \\ F^{0-+}_{k\sigma} & F^{0--}_{k\sigma} \end{pmatrix} = \begin{pmatrix} \dfrac{n^{+}_{-\sigma} b}{ab - cd} & \dfrac{n^{-}_{-\sigma} d}{ab - cd} \\ \dfrac{n^{+}_{-\sigma} c}{ab - cd} & \dfrac{n^{-}_{-\sigma} a}{ab - cd} \end{pmatrix}.$$

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

$$(51)\quad \begin{cases} \left.\begin{matrix} a \\ b \end{matrix}\right\} = \Big(\omega - E_{\pm} - N^{-1} \sum_{p} \varepsilon(p)(A^{\pm\pm}(-p) - B^{\pm\pm}(p-q))\Big), \\ \left.\begin{matrix} c \\ d \end{matrix}\right\} = N^{-1} \sum_{p} \varepsilon(p)(A^{\mp\pm}(-p) - B^{\mp\pm}(p-q))\,. \end{cases}$$

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

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

Here we have introduced the following notations:

$$\left.\begin{matrix}\lambda_1(k)\\ \lambda_2(k)\end{matrix}\right\} = \frac{1}{n^{\mp}_{\sigma}} \sum_p \varepsilon(p)(A^{\pm\pm}(-p) - B^{\pm\pm}(p-k)), \tag{53}$$

$$\begin{cases}\left.\begin{matrix}\lambda_3(k)\\ \lambda_4(k)\end{matrix}\right\} = \frac{1}{n^{\mp}_{\sigma}} \sum_p \varepsilon(p)(A^{\pm\mp}(-p) - B^{\pm\mp}(p-k)), \\ \lambda(k) = (n^{-}_{-\sigma})^2(\lambda_1 + \lambda_3) + (n^{+}_{-\sigma})^2(\lambda_2 + \lambda_4). \end{cases} \tag{54}$$

From eq. (52) it is obvious that our two-pole solution is more general than the «Hubbard III» [13] and Roth [15] 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 includes a great number of intermediate scattering processes (cf. the interesting analysis in ref. [35]).

The spectrum of the mean-field quasi-particle excitations follows from the poles of the GF (52) and consists of two branches:

$$\left.\begin{matrix}\omega_1(k)\\ \omega_2(k)\end{matrix}\right\} = 1/2[(E_+ - E_- + a_1 + b_1) \pm \sqrt{E_+ + E_- - a_1 - b_1)^2 - 4cd}], \tag{55}$$

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

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

For a deeper insight into the functional structure of the solution (52) and for comparison with the other solutions we rewrite (50) in the following form:

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

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

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

$$\approx \frac{n^{-}_{-\sigma}}{\omega - E_- - n^{-}_{-\sigma}W^{-}_{-\sigma}(k)} + \frac{n^{+}_{-\sigma}}{\omega - E_+ - n^{-}_{-\sigma}W^{+}_{-\sigma}(k)},$$

where

$$(59)\quad n^{+}_{-\sigma} n^{-}_{-\sigma} W^{\pm}_{-\sigma}(k) = N^{-1} \sum_{ij} t_{ij} \exp[-ik(R_i - R_j)] \cdot$$

$$\cdot(\langle\langle a^{\dagger}_{i-\sigma} n^{\pm}_{i\sigma} a_{j-\sigma}\rangle + \langle a_{i-\sigma} n^{\mp}_{i\sigma} a^{\dagger}_{j-\sigma}\rangle\rangle) + (\langle n^{\mp}_{j-\sigma} n^{\pm}_{i-\sigma}\rangle + \langle a_{i\sigma} a^{\dagger}_{i-\sigma} a_{j-\sigma} a^{\dagger}_{j\sigma}\rangle - \langle a_{i\sigma} a_{i-\sigma} a^{\dagger}_{j-\sigma} a^{\dagger}_{j\sigma}\rangle\rangle)),$$

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 non-trivial structure of the mean-field renormalizations (59), which is crucial to understand the physics of strongly correlated systems. It is important to emphasize that this complicated form of the GMF namely is 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, mainly from the point of view of the real nature of the physics of HCES. This physics clearly shows 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 [7] from our GMF solution (52). If we approximate (59) as

$$(60)\quad n^{+}_{-\sigma} n^{-}_{-\sigma} W^{\pm}(k) \approx N^{-1} \sum_{ij} t_{ij} \exp[-ik(R_i - R_j)] \langle n^{\pm}_{j-\sigma} n^{\mp}_{i-\sigma}\rangle$$

and make the additional approximation, namely

$$\langle n_{j-\sigma} n_{i-\sigma}\rangle \approx n^2_{-\sigma},$$

the solution (52) goes over into the «Hubbard I» solution,

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

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

As regards our solution (52), the second important aspect is that the parameters $\lambda_i(k)$ do not depend on frequency, *i.e.* they depend 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 in the right-hand side 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:

$$(62)\quad \boldsymbol{F}_{k\sigma}(\omega) = \boldsymbol{F}^0_{k\sigma}(\omega) + \boldsymbol{F}^0_{k\sigma}(\omega) \boldsymbol{P}_{k\sigma}(\omega) \boldsymbol{F}^0_{k\sigma}(\omega).$$

Here the scattering operator P (8) has the form

$$(63)\quad \boldsymbol{P}_{q\sigma}(\omega) = \boldsymbol{I}^{-1} \left[\sum_{lm} t_{il} t_{mj} \langle\langle \boldsymbol{D}^{\mathrm{ir}}_{il,j} | \boldsymbol{D}^{\mathrm{ir},\dagger}_{i,mj} \rangle\rangle_{\omega} \right]_q \boldsymbol{I}^{-1}.$$

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

$$\boldsymbol{F} = \boldsymbol{F}^0 + \boldsymbol{F}^0\boldsymbol{M}\boldsymbol{F}\,. \tag{64}$$

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 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 the Dyson equation,

$$G_\sigma(k,\omega) = \left(\frac{1}{n^-_\sigma}(a - n^-_\sigma M^{+\,+}_\sigma(k,\omega)) + \frac{1}{n^-_{-\sigma}}(b - n_{-\sigma} M_\sigma{}^{-}(k,\omega)) + \right. \tag{65}$$

$$\left. + \frac{1}{n^+_{-\sigma}}(d + n^+_{-\sigma} M^{+\,-}_\sigma(k,\omega)) + \frac{1}{n^-_{-\sigma}}(c + n^-_{-\sigma} M^{-\,+}_\sigma(k,\omega)) \right) \cdot$$

$$\cdot [\det((F^0_{k\sigma}(\omega))^{-1} - M_\sigma(k,\omega))]^{-1}\,.$$

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

$$G = \frac{\omega - (n^+ E_+ + n^- E_-) - L}{(\omega - E_+ - n^- L_1)(\omega - E_- - n^- L_2) - n^- n^+ L_3 L_4}\,, \tag{66}$$

where

$$\begin{cases} L_1(k,\omega) = \lambda_1(k) - \dfrac{n^+_{-\sigma}}{n^-_{-\sigma}} M^{+\,+}_\sigma(k,\omega)\,, \\ L_2(k,\omega) = \lambda_2(k) - \dfrac{n^-_\sigma}{n^+_{-\sigma}} M^{-\,-}_\sigma(k,\omega)\,, \\ L_3(k,\omega) = \lambda_3(k) + \dfrac{n_{-\sigma}}{n^+_\sigma} M^{+}_\sigma(k,\omega)\,, \\ L_4(k,\omega) = \lambda_4(k) + \dfrac{n^+_\sigma}{n_{-\sigma}} M_\sigma{}^{+}(k,\omega)\,, \\ L(k,\omega) = \lambda(k) + n^+_{-\sigma} n_{-\sigma}(M^{+\,+} + M^{-\,-} - M^{-\,+} - M^{+\,-})\,. \end{cases} \tag{67}$$

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:

$$M^{\alpha,\beta}_\sigma(k,\omega) \sim \langle D^{\mathrm{ir}\,\dagger}_{mj,\beta}(t) D^{\mathrm{ir}}_{il,\alpha} \rangle\,. \tag{68}$$

For the approximative calculation of the self-energy we propose to use the following

trial solution:

$$(69)\quad \langle D^{\mathrm{ir}\dagger}(t) D^{\mathrm{ir}}\rangle \approx \langle a^{\dagger}_{m\sigma}(t) a_{l\sigma}\rangle\langle n^{\beta}_{j-\sigma}(t) n^{\alpha}_{i-\sigma}\rangle + \langle a^{\dagger}_{m\sigma}(t) n^{\alpha}_{i-\sigma}\rangle\langle n^{\beta}_{j-\sigma}(t) a_{l\sigma}\rangle +$$
$$+ \beta\langle b^{\dagger}_{mj-\sigma}(t) a_{l\sigma}\rangle\langle a^{\dagger}_{j\sigma}(t) n^{\alpha}_{i-\sigma}\rangle + \beta\langle b^{\dagger}_{mj\ \sigma}(t) n^{\alpha}_{i\ \sigma}\rangle\langle a^{\dagger}_{j\sigma}(t) a_{l\sigma}\rangle +$$
$$+ \alpha\langle a^{\dagger}_{m\sigma}(t) a_{i\sigma}\rangle\langle n^{\beta}_{j\ \sigma}(t) b_{il-\sigma}\rangle + \alpha\langle a^{\dagger}_{m\sigma}(t) b_{il-\sigma}\rangle\langle n^{\beta}_{j-\sigma}(t) b_{il\ \sigma}\rangle +$$
$$+ \alpha\beta\langle b^{\dagger}_{mj-\sigma}(t) a_{i\sigma}\rangle\langle a^{\dagger}_{j\sigma}(t) b_{il-\sigma}\rangle + \alpha\beta\langle b^{\dagger}_{mj-\sigma}(t) b_{il-\sigma}\rangle\langle a^{\dagger}_{j\sigma}(t) a_{i\sigma}\rangle .$$

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. To this aim we retain the first contribution in (69)

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

Equations (70) and (64) constitute 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

$$(71)\quad [\boldsymbol{IMI}]_{\alpha\beta} \approx \sum_q |\varepsilon(k-q)|^2 K^{\alpha\beta}_q \left[\frac{n_{-\sigma}}{\omega - U - \varepsilon(k-q) n_{-\sigma}} + \frac{1 - n_{-\sigma}}{\omega - \varepsilon(k-q)(1 - n_{-\sigma})} \right].$$

On the basis of the self-energy operator (71) we can explicitly find the energy shift and damping due to inelastic scattering of the quasi-particles, 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 the IGF method for the 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 $A_x B_{1-x}$ transition metal alloys is based upon a certain generalization of the Hubbard model, including random diagonal and off-diagonal elements caused by substitutional disorder in binary alloys. The electron-electron interaction plays an important role for various aspects of behaviour in alloys, *e.g.*, in the weak localisation

in Ti-Al alloys [36]. There are certain aspects of the high-T_c superconductivity where disorder plays a role and very recently in the paper [37] the fictitious alloy resulting from the random distribution of magnetic molecular fields has been treated within the single-site Coherent Potential Approximation (CPA) [38]. The CPA has been refined and developed in many papers (*e.g.*, [39, 40]) and till now [41] it is 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 [42] 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

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

Contrary to the periodic model (11), the atomic-level energy ε_i^{ν}, the hopping integrals $t_{ij}^{\nu\mu}$ as well as the intra-atomic 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 a 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)

$$(\omega - \varepsilon_i) \langle\langle a_{i\sigma} | a_{j\sigma}^{\dagger} \rangle\rangle_{\omega} = \delta_{ij} + \sum_n t_{in} \langle\langle a_{n\sigma} | a_{j\sigma}^{\dagger} \rangle\rangle_{\omega} + U_i \langle\langle a_{i\,-\sigma} a_{i\sigma} | a_{j\sigma}^{\dagger} \rangle\rangle_{\omega} . \tag{74}$$

In the present paper, for brevity, we will confine ourselves to 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:

$$^{\mathrm{ir}}\langle\langle n_{i\,-\sigma} a_{i\sigma} | a_{j\sigma}^{\dagger} \rangle\rangle = \langle\langle n_{i\,-\sigma} a_{i\sigma} | a_{j\sigma}^{\dagger} \rangle\rangle - \langle n_{i\,-\sigma} \rangle \langle\langle a_{i\sigma} | a_{j\sigma}^{\dagger} \rangle\rangle . \tag{75}$$

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

$$\sum_n [(\omega - \varepsilon_i - U_i \langle n_{i\,-\sigma} \rangle) \delta_{ij} - t_{in}] \langle\langle a_{n\sigma} | a_{j\sigma}^{\dagger} \rangle\rangle_{\omega} = \delta_{ij} + U_i (^{\mathrm{ir}}\langle\langle n_{i\,-\sigma} a_{i\sigma} | a_{j\sigma}^{\dagger} \rangle\rangle_{\omega}) . \tag{76}$$

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

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

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

$$
(78)\qquad \begin{cases} \sum_m H_{im\sigma} G^0_{mj\sigma}(\omega) = \delta_{ij}\,, \\ P_{mn\sigma} = M_{mn\sigma} + \sum_{ij} M_{mi\sigma} G^0_{ij\sigma} P_{jn\sigma}\,, \\ H_{im\sigma} = (\omega - \varepsilon_i - U_i \langle n_{i-\sigma}\rangle)\,\delta_{im} - t_{im}\,, \\ P_{mn\sigma}(\omega) = U_m ({}^{\mathrm{ir}}\langle\langle n_{m-\sigma} a_{m\sigma} | n_{n-\sigma} a^+_{n\sigma}\rangle\rangle^{\mathrm{ir}}_{\omega})\, U_n\,. \end{cases}
$$

In order to calculate the self-energy operator M self-consistently, we have to express it approximatively 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):

$$
(79)\qquad \begin{cases} M^{(\nu)}_{mn\sigma}(\omega) = U_m U_n \dfrac{1}{2\pi^4} \int R(\omega_1, \omega_2, \omega_3) \cdot \\ \qquad\qquad \cdot \operatorname{Im} G^{(\nu)}_{mn-\sigma}(\omega_1) \operatorname{Im} G^{(\nu)}_{mn-\sigma}(\omega_2) \operatorname{Im} G^{(\nu)}_{mn\sigma}(\omega_3)\,, \\ R = -\dfrac{\mathrm{d}\omega_1\,\mathrm{d}\omega_2\,\mathrm{d}\omega_3}{\omega + \omega_1 - \omega_2 - \omega_3} \dfrac{(1 - n(\omega_1))\, n(\omega_2)\, n(\omega_3)}{n(\omega_2 + \omega_3 - \omega_1)}\,. \end{cases}
$$

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) depend 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 $\bar{G}$, then 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 [38], namely we take

$$
(80)\qquad \bar{G}^0_{mn\sigma}(\omega) = N^{-1} \sum_k \frac{\exp[ik(R_m - R_n)]}{\omega - \Sigma^\sigma(\omega) - \varepsilon(k)}\,.
$$

Here $\varepsilon(k) = \sum_{n=1}^{z} t_{n,0} \exp[ikR_n]$, z is the number of nearest neighbours 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

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

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

$$\bar{M} \approx (\overline{U_m U_n})(\overline{\mathrm{Im}\, G})(\overline{\mathrm{Im}\, G})(\overline{\mathrm{Im}\, G}) .$$

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

$$\text{(82)} \qquad \begin{cases} \overline{U_m U_n} = U_2 + (U_1 - U_2)\,\delta_{mn} , \\ U_1 = x^2 U_A^2 + 2x(1-x)\,U_A U_B + (1-x)^2 U_B^2 , \\ U_2 = x U_A^2 + (1-x)\,U_B^2 . \end{cases}$$

The averaged value for the self-energy is

$$\text{(83)} \qquad \bar{M}_{mn\sigma}(\omega) = \frac{U_2}{2\pi^4} \int R(\omega_1, \omega_2, \omega_3)\, \mathrm{Im}\, \bar{G}_{nm-\sigma}(\omega_1)\, \mathrm{Im}\, \bar{G}_{mn\,-\sigma}(\omega_2)\, \mathrm{Im}\, \bar{G}_{mn\sigma}(\omega_3) +$$

$$+ \frac{U_1 - U_2}{2\pi^4}\, \delta_{mn} \int R(\omega_1, \omega_2, \omega_3)\, \mathrm{Im}\, \bar{G}_{nm\,-\sigma}(\omega_1)\, \mathrm{Im}\, \bar{G}_{mn\,-\sigma}(\omega_2)\, \mathrm{Im}\, \bar{G}_{mn\sigma}(\omega_3) .$$

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 the Dyson equation and Fourier-transforming the resulting expressions according to the above rules, we obtain

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

where

$$\text{(85)} \qquad \bar{M}_\sigma(k, \omega) = \frac{1}{2\pi^4} \sum_{pq} \int R(\omega_1, \omega_2, \omega_3) N^{-2}\, \mathrm{Im}\, \bar{G}_{p-q-\sigma}(\omega_1)\, \mathrm{Im}\, \bar{G}_{q-\sigma}(\omega_2) \cdot$$

$$\cdot \left[U_2\, \mathrm{Im}\, \bar{G}_{k+p\sigma}(\omega_3) + \frac{(U_1 - U_2)}{N} \sum_q \mathrm{Im}\, \bar{G}_{k+p\,-q}(\omega_3) \right] .$$

The simplest way to obtain the explicit solution for the self-energy $\bar{M}$ is to start with a suitable initial trial solution as 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):

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

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

$$\bar{V} = xV^A + (1-x)V^B; \qquad E_k^\sigma = \bar{\varepsilon}_i^\sigma + \varepsilon(k),$$

$$\bar{\varepsilon}_i^\sigma = x\varepsilon_A^\sigma + (1-x)\varepsilon_B^\sigma .$$

Note that the use of VCA here is by no means the solution of the correlation problem in VCA. It is only the use of 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

$$(86) \quad \bar{M}_\sigma(k,\omega) = \frac{U^2}{N^2}\sum_{pq}\frac{n(E_{p+q}^{-\sigma})[1-n(E_q^{-\sigma})-n(E_{k+p}^{\sigma})]+n(E_{k+p}^{\sigma})n(E_q^{-\sigma})}{\omega+E_{p+q}^{-\sigma}-E_q^{-\sigma}-E_{k+p}^{\sigma}} +$$

$$+\frac{(U_1-U_2)}{N^3}\sum_{pqg}\frac{n(E_{p+q}^{-\sigma})[1-n(E_q^{-\sigma})-n(E_{k+p-g}^{\sigma})]+n(E_{k+p-g}^{\sigma})n(E_q^{-\sigma})}{\omega+E_{p+q}^{-\sigma}-E_q^{-\sigma}-E_{k+p-g}^{\sigma}} .$$

It must be emphasized that eqs. (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. – 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 permits to use the convenient analytical properties of retarded and advanced GFs and gives the advantage of using the formal solution of the Dyson equation, which, in spite of required approximations for the self-energy, provides the correct functional structure of the single-electron GF. This strong point of our approach does not give the possibility of direct application of it to the calculation of the two-particle GFs. In this paper we have restricted ourselves to the idealized single-band Hubbard model, which is one of the simplest (in the sense of formulation, but not solution) and most popular models of correlated lattice fermions. We have presented here the novel method of calculation of the quasi-particle spectra for this model, as the most representative example. We hope that this explanation has been done with sufficient details to bring out their scope and power, since we believe that such techniques will be applied to a variety of many-body systems with complicated spectrum and strong interaction.

In summary, using the 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 [20], defined

for a point $(k, \omega = \varepsilon(k))$:

$$Z(k) = \frac{1}{\left(1 - \frac{\mathrm{d}M(k, \omega)}{\mathrm{d}\omega}\right)_{\omega = \varepsilon(k)}}. \tag{87}$$

The renormalization coefficient (87) is one of the most important notions for the characterization of the single-particle behaviour of the quasi-particle excitations in correlated many-body systems. For the Hubbard model, these equations provide the general microscopic description of correlation effects for both the weak and strong Coulomb correlation, representing 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 the present consideration is that the GMF for the case of strong Coulomb interaction has a quite non-trivial structure and cannot be reduced to the mean-density functional. This last statement resembles very much the situation with the strongly non-equilibrium system, where the single-particle distribution function only is not enough to describe the essence of the strongly non-equilibrium state and more complicated correlation functions must be taken into account, in accordance with general ideas of Bogoljubov and Mori-Zwanzig. The IGF method is intimately related to the projection method in this sense, which espresses the idea of a «reduced description» of the system in the most general form. This line of consideration is very promising for the development of the complete and self-contained theory of the strongly interacting many-body systems.

* * *

The author would like to express his sincere gratitude to Profs. M. Marinaro, F. Mancini and G. Scarpetta for their kind hospitality at Dipartimento di Fisica Teorica, Università di Salerno, where the present paper was written. He has benefited from discussions with many colleagues; two of them, namely P. Fulde and N. Bickers, he wants to mention especially.

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