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Itinerant antiferromagnetism of correlated lattice fermions

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Abstract

The problem of finding of the ferromagnetic and antiferromagnetic "symmetry broken" solutions of the correlated lattice fermion models beyond the mean-field approximation has been investigated. The calculation of the quasiparticle excitation spectra with damping for the single and multi-orbital Hubbard model has been performed in the framework of the equation-of-motion method for two-time temperature Green's functions within a non-perturbative approach. A unified scheme for the construction of generalized mean fields (elastic scattering corrections) and self-energy (inelastic scattering) in terms of Dyson equation has been generalized in order to include the presence of the "source fields". The damping of quasiparticles, which reflects the interaction of the single- particle and collective degrees of freedom has been calculated. The "symmetry broken" dynamical solutions of the Hubbard model, which corresponds to various types of itinerant antiferromagnetism has been discussed. This approach complement previous studies and clarify the nature of the concepts of itinerant antiferromagnetism and "spin-aligning field" of correlated lattice fermions.

1. Introduction

The problem of the adequate description of the strongly correlated lattice fermions has been studied intensely during the last decade, especially in context of heavy fermions and high-Tc superconductivity [1–3]. The behaviour and the true nature of the electronic states and their quasiparticle dynamics is of central importance to the understanding of the magnetism in metals and Mott–Hubbard metal–insulator transition in oxides, the heavy fermions in rare-earths compounds and the high-temperature superconductivity (HTSC) in cuprates. Recently, there has been considerable interest in identifying the microscopic origin of these states [4]. Antiferromagnetic correlations

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may play an important role in the possible scenario of normal and superconducting behaviour of these compounds. Some of the experimental and theoretical results show that antiferromagnetic spin fluctuations are really involved in the problem. This idea has stirred a great deal of discussion in recent times [5]. An appealing but phenomenological picture of HTSC, known as nearly antiferromagnetic Fermi liquids (NAFL) approach, has been developed to explain many anomalous properties of cuprates [6]. This approach predicts the detailed phase diagram for cuprates [6] and presents arguments which suggest that the physical origin of the pseudogap found in quasiparticle spectrum below critical temperature is the formation of a precursor to a spin-density-wave state. While the NAFL's scenario is appealing, it has aparently not yet been derived from fully microscopic consideration. The problem of the role of antiferromagnetic spin fluctuations for HTSC has recently been the subject of many papers (for recent review, see e.g. Ref. [7]). These investigations call for a better understanding of the nature of solutions (especially magnetic) to the Hubbard and related correlated models [8–11]. The microscopic theory of the itinerant ferromagnetism and antiferromagnetism [12,13] of strongly correlated fermions on a lattice at finite temperatures is one of the important issues of recent efforts in the field [14–17]. In some papers the spin-density-wave (SDW) spectrum was only used without careful and complete analysis of the quasiparticle spectra of correlated lattice fermions. The aim of this paper is to investigate the intrinsic nature of the "symmetry broken" (ferro- and antiferromagnetic) solutions of the Hubbard model at finite temperatures from the many-body point of view. In the previous papers we set up the formalism and derived the equations for the quasiparticle spectra with damping within single- and multi-orbital Hubbard model for the uniform paramagnetic case. In this paper we apply the formalism to consider the ferromagnetic and antiferromagnetic solutions. It is the purpose of this paper to explore more fully the notion of generalized mean fields (GMF) [10] which may arise in the system of correlated lattice fermions to justify and understand the "nature" of the local staggered mean fields which fix the antiferromagnetic ordering. The present work brings together the formulation of the itinerant antiferromagnetism of various papers. For this aim we rederive the SDW spectra by the irreducible Green's functions (IGF) method [18] taking into account the damping of quasiparticles. This alternative derivation has a close resemblance to that of the BCS theory of superconductivity for transition metals [19,20] with using the Nambu representation (cf. [21]). This aspect of the theory is connected with the concept of broken symmetry, which is discussed in detail for the present case. The advantage of the Green's function method is the relative ease with which temperature effects may be calculated.

2. Itinerant antiferromagnetism

The antiferromagnetic state is characterized by a spatially changing component of magnetization which varies in such a way that the net magnetization of the system is zero. The concept of antiferromagnetism of localized spins which is based on the

Heisenberg model and two-sublattice Neel ground state is relatively well-founded contrary to the antiferromagnetism of delocalized or itinerant electrons. The itinerant-electron picture is the alternative conceptual picture for magnetism [22].

We now sketch the main ideas of the concept of itinerant antiferromagnetism. The simplified band model of an antiferromagnet has been formulated by Slater [23] within single-particle Hartree–Fock (H–F) approximation. In this approach he used the "exchange repulsion" to keep electrons with parallel spins away from each other and to lower the Coulomb interaction energy. Some authors consider it as a prototype of the Hubbard model. However, the exchange repulsion was taken proportional to the number of electrons with the same spins only and the energy gap between two subbands was proportional to the difference of electrons with up and down spins. In the antiferromagnetic many-body problem there is an additional "symmetry broken" aspect. For antiferromagnet, contrary to ferromagnet, the one-electron H–F potential can violate the translational crystal symmetry. The period of the antiferromagnetic spin structure L is greater than the lattice constant a. To introduce the two-sublattice picture for itinerant model one should assume that $L=2a$ and that the spins of outer electrons on neighbouring atoms are reversed to each other. In other words, the alternating (H–F) potential $v_{i\sigma} = -\sigma v \exp(iQR_i)$ where $Q=(\pi/2,\pi/2)$ corresponds to a two-sublattice AFM structure. To justify an antiferromagnetic ordering with alternating up and down spin structure we must admit that in effect two different charge distributions will arise concentrated on atoms of sublattices A and B. This is the picture which accounts well for quasilocalized magnetic behaviour.

The earlier theories of itinerant antiferromagnetism were proposed by des Cloizeaux [24] and especially Overhauser [25] (in context of the investigation of the ground state of nuclear matter). Then Overhauser [26] have applied this approach for the explanation of the anomalous properties of dilute Cu–Mn alloys, have suggested an antiferromagnetic mechanism that requires neither two-body interactions between paramagnetic solute spins, nor a sublattice structure (cf. [27]). Such a mechanism may be recognized by considering a new type of excited state of the conduction electron gas. He invented the static SDW which allow the total charge density of the gas to remain spatially uniform. Overhauser [25–29] suggested that the H–F ground state of a three-dimensional electron gas is not necessarily a Slater determinant of plane waves. Alternative sets of one-particle states can lead to a lower ground-state energy. Among these alternatives to the plane-wave state are the SDW and CDW ground states for which the one-electron Hamiltonians have the form

$$H = (p^2/2m) - G(\sigma_x \cos Qz + \sigma_y \sin Qz) \tag{1}$$

(spiral SDW; $Q = 2k_F z$) and

$$H = (p^2/2m) - 2G\cos(Qr) \tag{2}$$

(CDW; $Q = 2k_F z$). The periodic potentials in above expressions leads to a corresponding variation in the electronic spin and charge densities, accompanied by a compensating variation of the background. The effect of Coulomb interaction on the magnetic properties of the electron gas in Overhauser's approach renders the paramagnetic plane-wave state of the free-electron-gas model unstable within the H–F approximation. The long-range components of the Coulomb interaction are most important in creating this instability [29]. It was demonstrated [28] that a non-uniform static SDW is lower in energy than the uniform (paramagnetic state) in the Coulomb gas within the H–F approximation for certain electron density.

The H–F is the simplest approximation but neglects the important dynamical part. To include the dynamics one should take into consideration the correlation effects. The role of correlation corrections which seems to suppress SDW state as well as the role of shielding and screening were not fully clarified [30,31]. Overhauser remarked that SDW ground states do not occur for δ-function interactions, whatever their strength. This question was investigated further in Ref. [32]. An instability of the paramagnetic Hartree-Fock state against a state with different orbitals for different spins was interpreted as a magnetic phase transition. It is important to note that in the Slater's and des Cloiseaux's models an electron moving in a crystal does not change its spin. In these models the main processes are related with pairing of electrons having the same spins, one from each of the two sublattices. In the Overhauser's approach to itinerant antiferromagnetism the combination of the electronic states with different spins (which pairs opposite spins) is used to describe the SDW state with period Q. The first approach is obviously valid only in the simple commensurate two-sublattice case and the later is applicable to the more general case of an incommensurate spiral spin state. The general SDW state have the form

$$\Psi_{p\sigma} = \chi_{p\sigma}\cos(\theta_p/2) + \chi_{p+Q-\sigma}\sin(\theta_p/2) \tag{3}$$

The average spin for helical or spiral spin arrangement changes its direction in $(x–y)$ plane. For the spiral SDW states a spatial variation of magnetization correspond to $\boldsymbol{Q} = (\pi/a)(1,1)$. The antiferromagnetic phase of chromium [33,34] and its alloys has been satisfactorily explained in terms of the SDW within a two-band model [35]. It is essential to note that chromium becomes antiferromagnetic in a unique manner. The antiferromagnetism is established in a more subtle way from among the spins of the itinerant electrons than the magnetism of collective band electrons in metals like iron and nickel. The essential feature of chromium which makes possible the formation of the SDW is the existence of "nested" portions of the Fermi surface [34]. The formation of bound electron–hole pairs takes place between particles of opposite spins; the condensed state exhibits the SDW.

The recent attempt to describe antiferromagnetic insulator at $T=0$ using a one-electron approach was made in Ref. [36]. To do this, the authors proposed to overcome the inadequacies of standard local-spin-density theory by adding a spin-dependent magnetic pseudopotential to Kohn–Sham equations.

For the Hubbard model [37] the qualitative phase diagram was calculated by Penn [38]. Unfortunately, his work gives a clear physical picture but do not emphasize the lattice character of the tight binding or Wannier fermions as well as the essence of the anomalous spin-flip averages. The Hubbard model is a simplified but workable model for the correlated lattice fermions and the applicability of the SDW Overhauser concept to highly correlated tight binding electrons on a lattice deserve the careful analysis within this model. In earlier papers [39–42] the single- and multi-orbital Hubbard model have been inspected with respect to antiferromagnetic solutions in the mean-field approximation mainly.

3. Hubbard model

The Hubbard model has been widely recognised as a workable model for a study of the correlated itinerant electron systems. For the sake of completeness we shall discuss the single-orbital and multi-orbital cases separately.

3.1. Multi-orbital Hubbard model

To demonstrate the advantage of our approach we shall consider the quasiparticle spectrum of the lattice fermions for degenerate band model. Let us start with the second quantized form of the Hamiltonian taking the set of the Wannier functions $[\phi_\lambda(r-R_i)]$. Here λ is the band index ($\lambda = 1,2,\ldots,5$)

$$H = \sum_{ij\mu\nu\sigma} t_{ij}^{\mu\nu} a_{i\mu\sigma}^{+} a_{j\nu\sigma} + \frac{1}{2} \sum_{ij,mn} \sum_{\alpha\beta\gamma\delta\sigma\sigma'} \langle i\alpha, j\beta | W | m\gamma, n\delta \rangle a_{i\alpha\sigma}^{+} a_{j\beta\sigma'}^{+} a_{m\gamma\sigma'} a_{n\delta\sigma} . \tag{4}$$

For a degenerate d-band the second quantized form of the total Hamiltonian in the Wannier-function representation then is reduced to the following model Hamiltonian:

$$H = H_1 + H_2 + H_3 . \tag{5}$$

The kinetic energy operator is given by

$$H_1 = \sum_{ij} \sum_{\mu\nu\sigma} t_{ij}^{\mu\nu} a_{i\mu\sigma}^{+} a_{j\nu\sigma} . \tag{6}$$

The term H_2 describes one-centre Coulomb interactions

$$\begin{aligned} H_2 = {} & \frac{1}{2} \sum_{i\mu\sigma} U_{\mu\mu} n_{i\mu\sigma} n_{i\mu-\sigma} + \frac{1}{2} \sum_{i\mu\nu} \sum_{\sigma\sigma'} V_{\mu\nu} n_{i\mu\sigma} n_{i\nu\sigma'} (1-\delta_{\mu\nu}) \\ & - \frac{1}{2} \sum_{i\mu\nu\sigma} I_{\mu\nu} n_{i\mu\sigma} n_{i\nu\sigma} (1-\delta_{\mu\nu}) + \frac{1}{2} \sum_{i\mu\nu\sigma} I_{\mu\nu} a_{i\mu\sigma}^{+} a_{i\mu-\sigma}^{+} a_{i\nu-\sigma} a_{i\nu\sigma} (1-\delta_{\mu\nu}) \\ & - \frac{1}{2} \sum_{i\mu\nu\sigma} I_{\mu\nu} a_{i\mu\sigma}^{+} a_{i\mu-\sigma} a_{i\nu-\sigma}^{+} a_{i\nu\sigma} (1-\delta_{\mu\nu}) . \end{aligned} \tag{7}$$

In addition to the intrasite intraorbital interaction $U_{\mu\mu}$ which is the only interaction present in the single-orbital Hubbard model, this term contains three more kinds of interorbital interactions.

The last term H_3 describes the direct intersite exchange interaction

$$H_3 = -\frac{1}{2} \sum_{ij\mu} \sum_{\sigma\sigma'} J_{ij}^{\mu\mu} a_{i\mu\sigma}^{+} a_{i\mu-\sigma'} a_{j\mu\sigma'}^{+} a_{j\mu\sigma} . \tag{8}$$

The definition of various integrals in H is obvious. It is reasonable to assume that

$$U_{\mu\mu} = U, \quad V_{\mu\nu} = V, \quad I_{\mu\nu} = I, \quad J_{ij}^{\mu\mu} = J_{ij} . \tag{9}$$

This Hamiltonian differ slightly from the analogous Hamiltonian of Ref. [40] where the only intrasite interaction terms of the second-quantized Hamiltonian of the d-band were taken into consideration.

3.2. Single-orbital Hubbard model

The model Hamiltonian which is usually referred to as Hubbard Hamiltonian [36]

$$H = \sum_{ij\sigma} t_{ij} a_{i\sigma}^{+} a_{j\sigma} + U/2 \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} \tag{10}$$

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 $[\phi(\boldsymbol{r} - \boldsymbol{R}_j)]$. (The Wannier representation, which is unitary transformation of the Bloch representation is an important background of the Hubbard model. It is well known that in one dimension the Wannier functions decrease exponentially but less is known about two and three dimensional cases.) 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 in taking into account both of these effects simultaneously. Thus, Hamiltonian (10) is specified by two parameter: U and effective electron bandwidth

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

The important third “player” is the Pauli principle.

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

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

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 three 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. We evidently have 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. It was the purpose of the papers [3,10] to find the electronic quasiparticle spectra in a wide temperature and parameters of the model range and to account explicitly for the contribution of damping of the electronic states when calculating the various characteristics of the model. In the past years many theoretical papers have been published, in which the approximative dynamical solution of models (5) and (10) have been investigated by means of various advanced methods of many-body theory. Despite the considerable contributions to development of the many-body theory and to our better understanding of the physics of the correlated electron systems, the fully consistent dynamical analytical solution of the Hubbard model is still lacking. To solve this problem with a reasonable accuracy and describe correctly an interpolating solution one needs more sophisticated approach than usual procedures which have been developed for description of the interacting electron-gas problem.

4. Irreducible Green's functions method

Recent theoretical investigations of strongly correlated electron systems have brought forth significant variety of approaches. To describe from the first principles of the condensed matter theory and statistical mechanics the physical properties of strongly correlated systems we need to develop a systematic theory of quasiparticle spectra.

In this paper we will use 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 bears the real physics of strongly correlated electron systems [10,18]. 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 tends to emphasize the fundamental and central role of the Dyson equation for the single-particle dynamics of the many-body systems at finite temperatures.

In this section, we will discuss briefly this novel non-perturbative approach for description of the many-body dynamics of strongly correlated systems. A number of other approaches has been proposed and our approach is in many respects 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 [3] 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 temperatures. To clarify the foregoing, let us consider the retarded GF of the form

$$G^r = \langle\langle A(t), B(t') \rangle\rangle = -i\theta(t-t')\langle [A(t)B(t')]_\eta \rangle, \quad \eta = \pm 1 . \tag{11}$$

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

$$\omega G(\omega) = \langle [A, A^+]_\eta \rangle + \langle\langle [A, H]_- | A^+ \rangle\rangle_\omega . \tag{12}$$

The essence of the method is as follows [18]: 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

$$^{ir}\langle\langle [A,H]_- | A^+ \rangle\rangle = \langle\langle [A,H]_- - zA | A^+ \rangle\rangle \, . \tag{13}$$

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

$$\langle [[A,H]_-^{ir}, A^+]_\eta \rangle = 0 \, . \tag{14}$$

From condition (14) one can find

$$z = \frac{\langle [[A,H]_-, A^+]_\eta \rangle}{\langle [A,A^+]_\eta \rangle} = \frac{M_1}{M_0} \, . \tag{15}$$

Here M_0 and M_1 are the zeroth and first-order moments of the spectral density. Therefore, irreducible GF 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 definition (13) these concepts are translating 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 GF, which here are defined as

$$G^0(\omega) = \frac{\langle [A,A^+]_\eta \rangle}{(\omega - z)} \, . \tag{16}$$

To calculate the IGF $^{ir}\langle\langle [A,H]_-(t), A^+(t') \rangle\rangle$ in (12), we have to write the equation of motion after differentiation with respect to the second time variable t'. Condition (14) 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 (12) can be exactly rewritten in the following form:

$$G = G^0 + G^0 P G^0 \, . \tag{17}$$

The scattering operator P is given by

$$P = (M_0)^{-1} \quad ^{ir}\langle\langle [A,H]_- | [A^+,H]_- \rangle\rangle^{ir} (M_0)^{-1} \, . \tag{18}$$

The structure of Eq. (17) enables us to determine the self-energy operator M, in complete analogy with the diagram technique

$$P = M + M G^0 P \, . \tag{19}$$

From definition (19) 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:

$$G = G^0 + G^0 MG \,, \tag{20}$$

which has well-known formal solution of the form

$$G = [(G^0)^{-1} - M]^{-1} \,. \tag{21}$$

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 (12) for the GF can be exactly (but using constraint (14)) transformed into Dyson equation for the two-time thermal GF. This is a very remarkable result, which deserve the underlining, because the traditional form of the GF method did not include namely this point. The projection operator technique has essentially the same philosophy, but with using constraint (14) 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 [18]. 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 (19)! 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 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 spectra and strong interaction. Recently, it was emphasized 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. It is necessary to emphasize that there is an intimate connection between adequate introductions of mean fields and internal symmetries of the Hamiltonian.

5. Symmetry broken solutions

In many-body interacting systems, symmetry is important in classification of the different phases and in understanding the phase transitions between them [43–49]. According to Bogolubov [43] (cf. [48]) in each condensed phase, in addition to the normal process, there is an anomalous process (or processes) which can take place because of the long-range internal field, with a corresponding propagator. The anomalous propagators for interacting many-fermion system corresponding to the ferromagnetic (FM) and antiferromagnetic (AFM) long-range ordering are given by

$$\begin{aligned} FM &: G_{fm} \sim \langle\langle a_{k\sigma}; a^{+}_{k-\sigma}\rangle\rangle \,, \\ AFM &: G_{afm} \sim \langle\langle a_{k+Q\sigma}; a^{+}_{k+Q'\sigma'}\rangle\rangle \,. \end{aligned} \tag{22}$$

In the SDW case, a particle picks up momentum $Q - Q'$ from scattering against the periodic structure of the spiral (nonuniform) internal field, and has its spin changed from σ to σ' by the spin-aligning character of the internal field. The long-range-order (LRO) parameters are:

$$\begin{aligned} FM &: m = 1/N \sum_{k\sigma} \langle a^{+}_{k\sigma} a_{k-\sigma}\rangle \,, \\ AFM &: M_Q = \sum_{k\sigma} \langle a^{+}_{k\sigma} a_{k+Q-\sigma}\rangle \,. \end{aligned} \tag{23}$$

It is important to note that the long-range order parameters are the functions of the internal field, which is itself a function of the order parameter. There is a more mathematical way of formulating this assertion. According to the paper [14], the phrase “symmetry breaking” means that the state fails to have the symmetry that the Hamiltonian has. True broken symmetry can arise only if there are infinitesimal “source fields” present. Indeed, for the rotationally and translationally invariant Hamiltonian the suitable source terms should be added:

$$\begin{aligned} FM &: \varepsilon \mu_B H_x \sum_{k\sigma} a^{+}_{k\sigma} a_{k-\sigma} \,, \\ AFM &: \varepsilon \mu_B H \sum_{kQ} a^{+}_{k\sigma} a_{k+Q-\sigma} \,, \end{aligned} \tag{24}$$

where $\varepsilon \to 0$ at the end of calculations.

Broken symmetry solutions of the Overhauser type (3) imply that the vector Q is a measure of the inhomogeneity or breaking of translational symmetry. It is interesting to note the remark of paper [47] (cf. [49]) about antiferromagnetism, for which “a staggered magnetic field plays the role of symmetry-breaking field. No mechanism can generate a real staggered magnetic field in an antiferromagnetic material”. The Hubbard model is a very interesting tool for the analysing of this concept [42–52].

Penn [38] shown that antiferromagnetic state and more complicated states (e.g. ferrimagnetic) can be made eigenfunctions of the self-consistent field equations within an “extended” mean-field approach, assuming that the “anomalous” averages $\langle a^{+}_{i\sigma} a_{i-\sigma}\rangle$ determine the behaviour the system on the same footing as “normal” density of quasiparticles $\langle a^{+}_{i\sigma} a_{i\sigma}\rangle$. It is clear, however, that these “spin-flip” terms broke the rotational symmetry of the Hubbard Hamiltonian. For the single-band Hubbard Hamiltonian the averaging $\langle a^{+}_{i-\sigma} a_{i,\sigma}\rangle = 0$ because of the rotational symmetry of the Hubbard model. The including of the “anomalous” averages lead to unrestricted H–F approximation. The rigorous definition of the unrestricted Hartree–Fock approximation (UHFA) has been done recently in Ref. [14]. This approximation has been applied also for the single-band Hubbard model (10) for the calculation of the density of states. The following definition of UHFA has been used:

$$n_{i-\sigma}a_{i\sigma} = \langle n_{i-\sigma}\rangle a_{i\sigma} - \langle a^{+}_{i-\sigma}a_{i\sigma}\rangle a_{i-\sigma}\ . \tag{25}$$

Thus, in addition to the standard H–F 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. So, one need the properly defined effective Hamiltonian H_{eff}. We shall analyse below in detail the proper definition of the irreducible GFs which include the "spin-flip" terms. For single-orbital Hubbard model this definition should be modified in the following way:

$$\begin{aligned} {}^{ir}\langle\langle a_{k+p\sigma}a^{+}_{p+q-\sigma}a_{q-\sigma}|a^{+}_{k\sigma}\rangle\rangle \omega &= \langle\langle a_{k+p\sigma}a^{+}_{p+q-\sigma}a_{q-\sigma}|a^{+}_{k\sigma}\rangle\rangle_{\omega} - \delta_{p,0}\langle n_{q-\sigma}\rangle G_{k\sigma} \\ &\quad -\langle a_{k+p\sigma}a^{+}_{p+q-\sigma}\rangle\langle\langle a_{q-\sigma}|a^{+}_{k\sigma}\rangle\rangle_{\omega}\ . \end{aligned} \tag{26}$$

From this definition it follows that such way of introduction of the IGF broaden the initial algebra of the operators and initial set of the GFs. This 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

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

With this definition we introduce the so-called anomalous (off-diagonal) GFs which fix the relevant vacuum and select the proper symmetry broken solutions. In fact, this approximation has been investigated earlier by Kishore and Joshi [51]. They clearly pointed out that they assumed that the system is magnetized in the x direction instead of conventional z-axis. The detailed investigation and classification of the magnetic and non-magnetic symmetry broken solutions of the three-band extended Hubbard model for CuO_2 planes of high-T_c superconductors was made in Ref. [52] within mean-field approximation.

6. Dynamical properties

In many-body interacting systems the quasiparticle dynamics can be quite non-trivial. Here the problem of the adequate description of the many-body dynamics of the multi-orbital Hubbard model will be discussed in the framework of equation-of-motion appproach for two-time thermodynamic Green's functions. Our main motivation was the intention to formulate the consistent theory of dynamical properties of the Hubbard model taking into account the symmetry broken (magnetic) solutions.

This formulation gives to us an opportunity to emphasize some important issues about the relevant dynamical solutions of the strongly correlated models of fermions on a lattice and to formulate in a more sharp form the ideas of the method of the irreducible Green's functions (IGF) [18]. This IGF method allows one to describe the quasiparticle spectra with damping of the strongly correlated electron systems in a very general and natural way and to construct the relevant dynamical solution in a self-consistent way on the level of Dyson equation without decoupling the chain of the equation of motion for the GFs.

The interplay and the competition of the kinetic energy and potential energy affects substantially the electronic spectrum. The renormalized electron energies are temperature dependent and the electronic states have a finite life times. These effects are most suitable accounted for by the Green's functions method. We shall use the (IGF) method of Section 4. To give a more instructive discussion let us consider the single-particle GF of lattice fermions, which is defined as

$$G^{\mu\nu}_{\sigma\sigma'}(ij;t-t') = \langle\langle a_{i\mu\sigma}(t), a^{+}_{j\nu\sigma'}(t')\rangle\rangle = -i\theta(t-t')\langle[a_{i\mu\sigma}(t), a^{+}_{j\nu\sigma'}(t')]_{+}\rangle$$
$$= 1/2\pi \int_{-\infty}^{+\infty} \mathrm{d}\omega \exp(-i\omega t) G^{\mu\nu}_{\sigma\sigma'}(ij;\omega)\,. \tag{27}$$

Actually, this GF is a matrix (10×10) in the joint tensor product vector space of spin and orbital momentum. The diagonal elements of this matrix GF are normal propagators, while the off-diagonal elements are anomalous. The equation of motion for the Fourier transform of the GF has the form

$$\begin{aligned}\sum_{m\alpha} A^{\mu\alpha}(im) G^{\alpha\nu}_{\sigma\sigma'}(mj;\omega) = \delta_{ij}\delta_{\mu\nu}\delta_{\sigma\sigma'} + \sum_{m\alpha} [&B^{\mu\alpha}_{1}(im)\langle\langle a_{m\mu\sigma} n_{m\alpha\sigma} | a^{+}_{j\nu\sigma'}\rangle\rangle \\ &+ B^{\mu\alpha}_{2}(im)\langle\langle a_{m\mu\sigma} n_{m\alpha-\sigma} | a^{+}_{j\nu\sigma'}\rangle\rangle \\ &+ B^{\mu\alpha}_{3}(im)(\langle\langle a_{i\mu\sigma} n_{m\mu\sigma} | a^{+}_{j\nu\sigma'}\rangle\rangle \\ &+ \langle\langle a_{i\mu-\sigma} a^{+}_{m\mu-\sigma} a_{m\mu\sigma} | a^{+}_{j\nu\sigma'}\rangle\rangle)]\,.\end{aligned} \tag{28}$$

Here we have introduced the notations

$$\begin{aligned} &A^{\mu\alpha}(im) = \omega\delta_{mi}\delta_{\mu\alpha} - t^{\mu\alpha}_{im}, \quad B^{\mu\alpha}_{1}(im) = (V-I)\delta_{im}(1-\delta_{\mu\alpha})\,, \\ &B^{\mu\alpha}_{2} = [U\delta_{\mu\alpha} + V(1-\delta_{\mu\alpha})]\delta_{im}, \quad B^{\mu\alpha}_{3}(im) = J_{im}(1-\delta_{im})\delta_{\mu\alpha}\,. \end{aligned} \tag{29}$$

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

$$\begin{aligned}({}^{ir}\langle\langle a_{i\beta\sigma} a^{+}_{m\alpha\sigma_1} a_{m\alpha\sigma_1} | a^{+}_{j\nu\sigma'}\rangle\rangle) = \langle\langle a_{i\beta\sigma} a^{+}_{m\alpha\sigma_1} a_{m\alpha\sigma_1} | a^{+}_{j\nu\sigma'}\rangle\rangle - \langle n_{m\alpha\sigma_1}\rangle\delta_{mi}\langle\langle a_{i\beta\sigma} | a^{+}_{j\nu\sigma'}\rangle\rangle \\ - \langle a_{i\beta\sigma} a^{+}_{m\alpha\sigma_1}\rangle\langle\langle a_{m\alpha\sigma_1} | a^{+}_{j\nu\sigma'}\rangle\rangle\,.\end{aligned} \tag{30}$$

According to (14), the following constraint should be valid:

$$\langle[(a_{i\beta\sigma} n_{m\alpha\sigma_1})^{(ir)}, a^{+}_{j\nu\sigma'}]_{+}\rangle = 0\,. \tag{31}$$

Substituting (30) in (28) we obtain the following equation of motion in the matrix (in spin space) form:

$$\begin{aligned}\sum_{m\alpha} F^{\mu\alpha}(im) G^{\alpha\nu}(mj;\omega) = 1 + \sum_{m\alpha} [&L^{\mu\alpha}_{1}(il) D^{\mu\alpha\,\nu}_{1}(mj) + L^{\mu\alpha}_{2}(im) D^{\mu\alpha,\nu}_{2}(mj) \\ &+ L^{\mu\alpha}_{3}(im)(R^{\alpha\nu}_{1}(im,j) + R^{\alpha\nu}_{2}(im,j))]\,,\end{aligned} \tag{32}$$

where

$$F^{\mu\alpha}(im)=\begin{pmatrix} E_{11}^{\mu\alpha}(im) & E_{12}^{\mu\alpha}(im) \\ E_{21}^{\mu\alpha}(im) & E_{22}^{\mu\alpha}(im) \end{pmatrix}, \quad 1=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\delta_{\mu\nu}\delta_{ij}\,, \tag{33}$$

$$L_1^{\mu\alpha}(im)=\begin{pmatrix} B_1^{\mu\alpha}(im) & B_2^{\mu\alpha} \\ 0 & 0 \end{pmatrix}, \quad L_2^{\mu\alpha}(im)=\begin{pmatrix} 0 & 0 \\ B_1^{\mu\alpha}(im) & B_2^{\mu\alpha}(il) \end{pmatrix},$$

$$L_3^{\mu\alpha}(im)=\begin{pmatrix} B_3^{\mu\alpha}(im) & 0 \\ 0 & B_3^{\mu\alpha}(im) \end{pmatrix}$$

and

$$\begin{aligned} E_{11}^{\mu\alpha}(im) = {} & A^{\mu\alpha}(im) - B_1^{\mu\alpha}(im)\langle a_{m\mu\uparrow}a^+_{m\alpha\uparrow}\rangle \\ & -\sum_\beta (B_1^{\mu\beta}(im)\langle n_{m\alpha\uparrow}\rangle\delta_{\mu\beta} - B_2^{\mu\beta}(im)\langle n_{i\alpha\downarrow}\rangle\delta_{\mu\beta}) \\ & -B_3^{\mu\alpha}(im)(\langle a_{i\alpha\uparrow}a^+_{m\alpha\uparrow}\rangle + \langle a_{i\alpha\downarrow}a^+_{m\alpha\downarrow}\rangle) - \sum_l B_3^{\mu\alpha}(ml)\langle n_{l\alpha\uparrow}\rangle\,, \end{aligned} \tag{34}$$

$$E_{12}^{\mu\alpha} = -B_2^{\mu\alpha}\langle a_{m\mu\uparrow}a^+_{m\alpha\downarrow}\rangle - \sum_l B_3^{\mu\alpha}\langle a^+_{l\alpha\downarrow}a_{l\alpha\uparrow}\rangle\delta_{im} \tag{35}$$

and similar expressions for E_{21} and E_{22} with reversed spin indices. The higher-order GF have the form

$$\begin{aligned} D_1 &= \begin{pmatrix} (^{(ir)}\langle\langle a_{m\mu\uparrow}n_{m\alpha\uparrow}|a^+_{j\nu\uparrow}\rangle\rangle) & (^{(ir)}\langle\langle a_{m\mu\uparrow}n_{m\mu\uparrow}|a^+_{j\nu\downarrow}\rangle\rangle) \\ (^{(ir)}\langle\langle a_{m\mu\uparrow}n_{m\alpha\downarrow}|a^+_{j\nu\uparrow}\rangle\rangle) & (^{(ir)}\langle\langle a_{m\mu\uparrow}n_{m\alpha\downarrow}|a^+_{j\nu\downarrow}\rangle\rangle) \end{pmatrix}, \\ D_2 &= \begin{pmatrix} (^{(ir)}\langle\langle a_{i\alpha\uparrow}n_{m\alpha\uparrow}|a^+_{j\nu\uparrow}\rangle\rangle) & (^{(ir)}\langle\langle a_{i\alpha\uparrow}n_{m\alpha\uparrow}|a^+_{j\nu\downarrow}\rangle\rangle) \\ (^{(ir)}\langle\langle a_{i\alpha\downarrow}n_{m\alpha\downarrow}|a^+_{j\nu\uparrow}\rangle\rangle) & (^{(ir)}\langle\langle a_{i\alpha\downarrow}n_{m\alpha\downarrow}|a^+_{j\nu\downarrow}\rangle\rangle) \end{pmatrix} \end{aligned} \tag{36}$$

and R have the following structure:

$$R = \begin{pmatrix} (^{(ir)}\langle\langle a_{m\mu\uparrow}a^+_{m\alpha\uparrow}a_{m\alpha\uparrow}|a^+_{n\nu\uparrow}\rangle\rangle) & (^{(ir)}\langle\langle a_{m\mu\uparrow}a^+_{m\alpha\uparrow}a_{m\alpha\uparrow}|a^+_{n\nu\downarrow}\rangle\rangle) \\ (^{(ir)}\langle\langle a_{m\mu\uparrow}a^+_{m\alpha\downarrow}a_{m\alpha\downarrow}|a^+_{n\nu\uparrow}\rangle\rangle) & (^{(ir)}\langle\langle a_{m\mu\uparrow}a^+_{m\alpha\downarrow}a_{m\alpha\downarrow}|a^+_{n\nu\downarrow}\rangle\rangle) \end{pmatrix}.$$

To calculate the higher-order GF D_1, D_2, R_1 and R_2, we will differentiate the r.h.s. of it with respect to the second-time variable (t'). Combining both (the first- and second-time differentiated) equations of motion we get the "exact" (no approximation have been made till now) "scattering" equation

$$G^{\mu\nu}(ij;\omega) = G_0^{\mu\nu}(ij;\omega) + \sum_{mn\alpha\beta} G_0^{\mu\alpha}(im;\omega)P^{\alpha\beta}(mn;\omega)G_0^{\beta\nu}(nj;\omega)\,. \tag{37}$$

Here we have introduced the generalized mean-field (GMF) GF G_0 according to the following definition:

$$\sum_{m\alpha} F^{\mu\alpha}(im)G_0^{\alpha\nu}(mj;\omega) = \delta_{ij}\delta_{\mu\nu}\,. \tag{38}$$

The scattering operator P has the form

$$P^{\mu\alpha}(mn;\omega) = \begin{pmatrix} P_{11}^{\mu\alpha}(mn;\omega) & P_{12}^{\mu\alpha}(mn;\omega) \\ P_{21}^{\mu\alpha}(mn;\omega) & P_{22}^{\mu\alpha}(mn;\omega) \end{pmatrix} . \tag{39}$$

Let us write down explicitly the first matrix element

$$\begin{aligned} P_{11}^{\alpha\beta}(mn;\omega) = \sum_{ij\mu\nu} [& B_1^{\mu\alpha}(im)(^{(ir)}\langle\langle a_{m\mu\uparrow} n_{m\alpha\uparrow} | a_{n\nu\uparrow}^{+} n_{n\beta\uparrow} \rangle\rangle^{(ir)}) B_1^{\mu\beta}(nj) \\ & + B_1^{\mu\alpha}(im)(^{(ir)}\langle\langle a_{m\mu\uparrow} n_{m\alpha\uparrow} | a_{n\nu\uparrow}^{+} n_{n\beta\downarrow} \rangle\rangle^{(ir)}) B_2^{\beta\nu}(nj) \\ & + B_2^{\mu\alpha}(im)(^{(ir)}\langle\langle a_{m\mu\uparrow} n_{m\alpha\downarrow} | a_{n\nu\uparrow}^{+} n_{n\beta\uparrow} \rangle\rangle^{(ir)}) B_1^{\beta\nu}(nj) \\ & + B_2^{\mu\alpha}(im)(^{(ir)}\langle\langle a_{m\mu\uparrow} n_{m\alpha\downarrow} | a_{n\nu\uparrow}^{+} n_{n\beta\downarrow} \rangle\rangle^{(ir)}) B_2^{\beta\nu}(nj)] . \end{aligned} \tag{40}$$

Here we presented for brevity the explicit expression for a part of Hamiltonian (5) only without last term. Using (17)–(19) we find the Dyson equation in the Wannier basis

$$G^{\mu\nu}(ij;\omega) = G_0^{\mu\nu}(ij;\omega) + \sum_{mn\alpha\beta} G_0^{\mu\alpha}(im;\omega) M^{\alpha\beta}(mn;\omega) G^{\beta\nu}(nj;\omega) . \tag{41}$$

Eq. (41) is the central result of the present consideration.

7. Quasiparticle formulation

Let us first consider how to describe our system in terms of quasiparticles. For a translationally invariant system, to describe the low-lying excitations in terms of quasiparticles one has to make a Fourier transformation

$$\begin{aligned} G^{\mu\nu}(ij;\omega) &= N^{-1} \sum_k \exp[ik(R_i - R_j)] G^{\mu\nu}(k;\omega) , \\ M^{\mu\nu}(ij;\omega) &= N^{-1} \sum_k \exp[ik(R_i - R_j)] M^{\mu\nu}(k;\omega) , \end{aligned} \tag{42}$$

$$t_{ij}^{\mu\mu} = N^{-1} \sum_k \exp[ik(R_i - R_j)] \varepsilon_\mu(k) .$$

The Dyson equation (41) in the Bloch vector space are given by

$$G^{\mu\nu}(k;\omega) = G_0^{\mu\nu}(k;\omega) + \sum_{\alpha\beta} G_0^{\mu\alpha}(k;\omega) M^{\alpha\beta}(k;\omega) G^{\beta\nu}(k;\omega) . \tag{43}$$

The renormalized energies in the mean-field approximations are the solutions of the equation

$$\sum_\alpha F^{\mu\alpha}(k) G_0^{\alpha\nu}(k;\omega) = 1\delta_{\mu\nu} . \tag{44}$$

Using (44) we find

$$E_{11}^{\alpha\nu}(k) = [\omega - \varepsilon_\alpha(k)]\delta_{\alpha\nu} - (1-\delta_{\alpha\nu})(V-I)K_{\uparrow\uparrow}^{\alpha\nu} - \sum_\mu [(1-\delta_{\alpha\mu})\delta_{\alpha\nu}(V-I)N_\uparrow^\mu + (U\delta_{\alpha\mu} + V(1-\delta_{\alpha\mu}))\delta_{\alpha\nu}N_\downarrow^\mu]\,, \tag{45}$$

$$E_{12}^{\alpha\nu}(k) = [U\delta_\alpha \nu + V(1-\delta_{\alpha\nu})]K_{\uparrow\downarrow}^{\alpha\nu}\,, \tag{46}$$

$$N_\sigma^\alpha = N^{-1}\sum_p \langle a_{p\alpha\sigma}^+ a_{p\alpha\sigma}\rangle\,, \tag{47}$$

$$K_{\sigma_1\sigma_2}^{\alpha\beta} = N^{-1}\sum_p \langle a_{p\alpha\sigma_1} a_{p\beta\sigma_2}^+\rangle\,. \tag{48}$$

For the degenerate Hubbard model ($V = I = J = 0$) we get

$$E_{11}^{\alpha\nu}(k) = [\omega - \varepsilon_\alpha(k) - UN_\downarrow^\alpha]\delta_{\alpha\nu}\,. \tag{49}$$

The spectrum of electronic low-lying excitations without damping follows from the poles of the single-particle mean-field GF

$$\begin{pmatrix} \hat{E}_{11} & \hat{E}_{12} \\ \hat{E}_{21} & \hat{E}_{22} \end{pmatrix} \begin{pmatrix} \hat{G}_{011} & \hat{G}_{012} \\ \hat{G}_{021} & \hat{G}_{022} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{50}$$

Here $\hat{G}_0$ denotes a matrix in the space of band indices. If we put the spin-flip contributions

$$\hat{E}_{12} = \hat{E}_{21} = 0\,,$$

then the quasiparticle spectra are given by

$$\det|\hat{E}_{11}| = 0, \quad \det|\hat{E}_{22}| = 0\,.$$

For the multiorbital Hubbard model (5) we find

$$G_{011}^\alpha(\omega) = \left[\omega - \varepsilon_\alpha(k) - UN_\downarrow^\alpha - V\sum_\nu (1-\delta_{\alpha\nu})(N_\downarrow^\nu + N_\uparrow^\nu) + I\sum_\nu (1-\delta_{\alpha\nu})N_\uparrow^\nu\right]^{-1}. \tag{51}$$

Finally, we turn to the calculation of the damping. In the general case to find the damping of the electronic states, one needs to find the matrix elements of self-energy in (43). Thus, we have

$$\begin{pmatrix} \hat{G}_{11} & \hat{G}_{12} \\ \hat{G}_{21} & \hat{G}_{22} \end{pmatrix} = \left[\begin{pmatrix} \hat{G}_{011} & \hat{G}_{012} \\ \hat{G}_{021} & \hat{G}_{022} \end{pmatrix}^{-1} - \begin{pmatrix} \widehat{M}_{11} & \widehat{M}_{12} \\ \widehat{M}_{21} & \widehat{M}_{22} \end{pmatrix}\right]^{-1}. \tag{52}$$

From this matrix equation we have

$$\hat{G}_{11} = (\hat{G}_{011}^{-1} - \hat{\Sigma}_{11})^{-1}, \quad \hat{G}_{21} = (\hat{G}_{021}^{-1} - \hat{\Sigma}_{21})^{-1}\,,$$
$$\hat{G}_{12} = (\hat{G}_{012}^{-1} - \hat{\Sigma}_{12})^{-1} \quad \hat{G}_{22} = (\hat{G}_{022}^{-1} - \hat{\Sigma}_{22})^{-1}\,, \tag{53}$$

where true self-energy has the form

$$\hat{\Sigma}_{11} = \widehat{M}_{11} - \hat{E}_{12}\hat{E}_{22}^{-1}\widehat{M}_{21} + [\widehat{M}_{12}\hat{E}_{22}^{-1} + (\widehat{M}_{12} - \hat{E}_{12})\hat{E}_{22}^{-1}\widehat{M}_{22}(\hat{E}_{22} - \widehat{M}_{22})^{-1}](\widehat{M}_{21} - \hat{E}_{21})\,. \tag{54}$$

The elements of the mass operator matrix $\widehat{M}$ are proportional to the higher-order GF of the following form:

$$({}^{(ir)}\langle\langle a_{k+p\alpha\sigma_1} a^{+}_{p+q\nu\sigma_2} a_{q\nu\sigma_2} | a^{+}_{k+s\beta\sigma_3} a^{+}_{r\mu\sigma_4} a_{r+s\mu\sigma_4}\rangle\rangle^{(ir),p})\,.$$

For the explicit approximate calculation of the elements of the self-energy it is convenient to write down the GFs in (54) in terms of correlation functions by using the well-known spectral theorem [54]:

$$\begin{aligned}
&({}^{(ir)}\langle\langle a_{k+p\alpha\sigma_1} a^{+}_{p+q\nu\sigma_2} a_{q\nu\sigma_2} | a^{+}_{k+s\beta\sigma_3} a^{+}_{r\mu\sigma_4} a_{r+s\mu\sigma_4}\rangle\rangle^{(ir),p}) \\
&= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{d\omega'}{\omega - \omega'}(\exp(\beta\omega') + 1)\int_{-\infty}^{+\infty} \exp(-i\omega' t)\,dt \\
&\times \langle a^{+}_{k+s\beta\sigma_3}(t) a^{+}_{r\mu\sigma_4}(t) a_{r+s\mu\sigma_4}(t) | a_{k+p\alpha\sigma_1} a^{+}_{p+q\nu\sigma_2} a_{q\nu\sigma_2}\rangle^{(ir),p})\,.
\end{aligned} \tag{55}$$

Further insight is gained if we select the suitable relevant "trial" approximation for the correlation function on the r.h.s. of (55). In this paper we show that the earlier formulations, based on the decoupling or/and diagrammatic methods can arrive at from our technique but in a self-consistent way. Clearly that the choice of the relevant trial approximation for correlation function in (55) can be done in a few ways. For example, the reasonable and workable one may be the following "pair approximation" [3], which is especially suitable for the low density of the quasiparticles:

$$\begin{aligned}
&\langle a^{+}_{k+s\beta\sigma}(t) a^{+}_{r\mu-\sigma}(t) a_{r+s\mu-\sigma}(t) a_{k+p\alpha\sigma} a^{+}_{p+q\nu-\sigma} a_{q\nu-\sigma}\rangle^{ir} \\
&\approx \langle a^{+}_{k+s\beta\sigma}(t) a_{k+p\alpha\sigma}\rangle\langle a^{+}_{r\mu-\sigma}(t) a_{q\nu-\sigma}\rangle\langle a_{r+s\mu-\sigma}(t) a^{+}_{p+q\nu-\sigma}\rangle \\
&+ \langle a^{+}_{k+s\beta\sigma}(t) a_{q\nu-\sigma}\rangle\langle a^{+}_{r\mu-\sigma}(t) a_{k+p\alpha\sigma}\rangle\langle a_{r+s\mu-\sigma}(t) a^{+}_{p+q\nu-\sigma}\rangle\,.
\end{aligned} \tag{56}$$

Using (56) in (55) 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):

$$\begin{aligned}
M_{11}^{\alpha\beta}(k,\omega) = \frac{1}{N^2\pi^3}\sum_{pq\mu\nu}\Bigg(B_1^{\alpha\nu}B_1^{\mu\beta}\int \frac{d\omega_1\, d\omega_2\, d\omega_3}{\omega + \omega_1 - \omega_2 - \omega_3} \\
\times N(\omega_1,\omega_2,\omega_3)[g^{\mu\nu}_{p+q\uparrow\uparrow}(\omega_1) g^{\nu\mu}_{q\uparrow\uparrow}(\omega_2) g^{\alpha\beta}_{k+p\uparrow\uparrow}(\omega_3) \\
+ g^{\alpha\mu}_{k+p\uparrow\uparrow}(\omega_3) g^{\nu\beta}_{q\uparrow\uparrow}(\omega_2) g^{\mu\nu}_{p+q\uparrow\uparrow}(\omega_1)]
\end{aligned}$$

$$+B_1^{\alpha\nu}B_2^{\mu\beta}\int\frac{d\omega_1\,d\omega_2\,d\omega_3}{\omega+\omega_1-\omega_2-\omega_3}N(\omega_1,\omega_2,\omega_3)[(\downarrow\uparrow)(\uparrow\downarrow)(\uparrow\uparrow)$$

$$+(\uparrow\downarrow)(\downarrow\uparrow)(\uparrow\uparrow)]+B_2^{\alpha\nu}B_1^{\mu\beta}\int\frac{d\omega_1\,d\omega_2\,d\omega_3}{\omega+\omega_1-\omega_2-\omega_3}$$

$$\times N(\omega_1,\omega_2,\omega_3)[(\uparrow\downarrow)(\downarrow\uparrow)(\uparrow\uparrow)+(\uparrow\uparrow)(\uparrow\downarrow)(\downarrow\uparrow)]$$

$$+B_2^{\alpha\nu}B_2^{\mu\beta}\int\frac{d\omega_1\,d\omega_2\,d\omega_3}{\omega+\omega_1-\omega_2-\omega_3}N(\omega_1,\omega_2,\omega_3)[(\downarrow\downarrow)(\downarrow\downarrow)(\uparrow\uparrow)$$

$$\left.+(\uparrow\downarrow)(\downarrow\downarrow)(\downarrow\uparrow)]\right), \tag{57}$$

where we have used the notations

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

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

Here we present for brevity the explicit expression for a part of Hamiltonian only without last term. Eqs. (43) and(57) 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, one may use on the r.h.s. of (57) any workable first iteration-step forms of the GFs and find a solution by repeated iterations. It is most convenient to choose as the first iteration step of the following simple one-pole approximation:

$$g_{k\sigma}(\omega)\approx\delta(\omega-\varepsilon(k\sigma)). \tag{58}$$

Then, using (58) in (57), one can get for the self-energy an explicit expression. However, the actual explicit calculations will be much more transparent if we confine ourselves of the single-orbital Hubbard model to discuss more explicitly the reliability of the present approach.

8. Antiferromagnetic single-particle states

The technique for obtaining of the antiferromagnetic solutions to the correlated fermions on a lattice is presented in this section for single-orbital Hubbard model (10). In general, it can be easily applied for multiorbital extended Hubbard model.

As discussed above, the self-consistent approach to calculation of the one-particle properties requires the calculation of the following GF:

$$\begin{pmatrix}\langle\langle a_{i\sigma}|a_{j\sigma}^{+}\rangle\rangle & \langle\langle a_{i\sigma}|a_{j-\sigma}^{+}\rangle\rangle\\ \langle\langle a_{i-\sigma}|a_{j\sigma}^{+}\rangle\rangle & \langle\langle a_{i-\sigma}|a_{j-\sigma}^{+}\rangle\rangle\end{pmatrix}=\hat{G}(ij;\omega). \tag{59}$$

The equation of motion for the Fourier transform of the GF has the form

$$\sum_m\hat{A}(im)\hat{G}(mj;\omega)=\delta_{ij}\delta_{\sigma\sigma'}+U\langle\langle a_{i\sigma}n_{i-\sigma}|a_{j\sigma'}^{+}\rangle\rangle, \tag{60}$$

where

$$\hat{A}(im) = \begin{pmatrix} (\omega\delta_{mi} - t_{im}) & 0 \\ 0 & (\omega\delta_{mi} - t_{im}) \end{pmatrix} . \tag{61}$$

Using the definition of the irreducible parts (26) the equation of motion can be exactly transformed to the following form:

$$\sum_m \hat{A}_1(im)\hat{G}(mj;\omega) = \delta_{ij}\delta_{\sigma\sigma'} + U\hat{D}^{ir}(ij;\omega) , \tag{62}$$

where

$$\hat{A}_1(im) = \begin{pmatrix} (\omega\delta_{mi} - t_{im} - U\langle n_{i-\sigma}\rangle) & -U\langle a_{i\sigma}a^{+}_{i-\sigma}\rangle \\ -U\langle a_{i-\sigma}a^{+}_{i\sigma}\rangle & (\omega\delta_{mi} - t_{im} - U\langle n_{i\sigma}\rangle) \end{pmatrix} . \tag{63}$$

To calculate the irreducible higher-order GF D^{ir} we have to write the equation of motion for it. After introducing the irreducible parts for the right-hand-side operators we find

$$\sum_n \hat{D}^{ir}(in;\omega)\hat{A}_2(nj) = U^2\hat{D}_1(ij;\omega) , \tag{64}$$

where

$$\hat{D}_1(ij;\omega) = \begin{pmatrix} {}^{(ir)}\langle\langle a_{i\sigma}n_{i-\sigma}|a^{+}_{j\sigma}n_{j-\sigma}\rangle\rangle^{(ir)} & {}^{(ir)}\langle\langle a_{i\sigma}n_{i-\sigma}|a^{+}_{j-\sigma}n_{j\sigma}\rangle\rangle^{(ir)} \\ {}^{(ir)}\langle\langle a_{i-\sigma}n_{i\sigma}|a^{+}_{j\sigma}n_{j-\sigma}\rangle\rangle^{(ir)} & {}^{(ir)}\langle\langle a_{i-\sigma}n_{i\sigma}|a^{+}_{j-\sigma}n_{j\sigma}\rangle\rangle^{(ir)} \end{pmatrix} . \tag{65}$$

Then equation of motion for the GF can be exactly transformed into the following scattering equation:

$$G(ij;\omega) = G_0(ij;\omega) + \sum_{mn} G_0(im;\omega)P(mn;\omega)G_0(nj;\omega) , \tag{66}$$

where the generalized mean-field GF G_0 reads

$$\sum_m A_1(im)G_0(mj;\omega) = \delta_{ij} \tag{67}$$

and the scattering operator P have the form

$$\hat{P}(ij;\omega) = U^2 \begin{pmatrix} {}^{(ir)}\langle\langle a_{i\sigma}n_{i-\sigma}|a^{+}_{j\sigma}n_{j-\sigma}\rangle\rangle^{(ir)} & {}^{(ir)}\langle\langle a_{i\sigma}n_{i-\sigma}|a^{+}_{j-\sigma}n_{j\sigma}\rangle\rangle^{(ir)} \\ {}^{(ir)}\langle\langle a_{i-\sigma}n_{i\sigma}|a^{+}_{j\sigma}n_{j-\sigma}\rangle\rangle^{(ir)} & {}^{(ir)}\langle\langle a_{i-\sigma}n_{i\sigma}|a^{+}_{j-\sigma}n_{j\sigma}\rangle\rangle^{(ir)} \end{pmatrix} . \tag{68}$$

The Dyson equation (41) then will be reduced for the single-band Hubbard model to the following form:

$$G(ij;\omega) = G_0(ij;\omega) + \sum_{mn} G_0(im;\omega)M(mn;\omega)G(nj;\omega) . \tag{69}$$

The mass operator $M(mn;\omega) = U^2P^{(p)}(mn;\omega)$ describes the inelastic (retarded) part of the electron–electron interaction. For purposes of analogy with the theory of superconductivity [19] let us write the Hartree–Fock (elastic) part of the Coulomb mass operator (not included in (68)):

$$\widehat{M}^{HF}(im) = U \begin{pmatrix} \langle n_{i-\sigma}\rangle & \langle a_{i\sigma}a^{+}_{i-\sigma}\rangle \\ \langle a_{i-\sigma}a^{+}_{i\sigma}\rangle & \langle n_{i\sigma}\rangle \end{pmatrix} \delta_{im} . \tag{70}$$

To obtain workable expressions for various parts of the mass operator we use the spectral theorem, inverse Fourier transformation and make relevant approximation in the time-correlation functions. In analogy with the theory of superconductivity the suitable approximation which describe the interaction between the charge and spin collective excitations can be written as

$$\begin{aligned}
&\langle a^+_{n\sigma}(t)a^+_{n-\sigma}(t)a_{n-\sigma}(t)a_{m\sigma}a^+_{m-\sigma}a_{m-\sigma}\rangle^{ir} \\
&\quad\approx \langle a^+_{n\sigma}(t)a_{m\sigma}\rangle\langle n_{n-\sigma}(t)n_{m-\sigma}\rangle \\
&\qquad+\langle a^+_{n-\sigma}(t)a_{m-\sigma}\rangle\langle a^+_{n\sigma}(t)a_{n-\sigma}(t)a_{m\sigma}a^+_{m-\sigma}\rangle \\
&\qquad+\langle a_{n-\sigma}(t)a^+_{m-\sigma}\rangle\langle a^+_{n\sigma}(t)a^+_{n-\sigma}(t)a_{m\sigma}a_{m-\sigma}\rangle \\
&\qquad+\langle a^+_{n\sigma}(t)a_{m-\sigma}\rangle\langle a^+_{n-\sigma}(t)a_{n-\sigma}(t)a_{m\sigma}a^+_{m-\sigma}\rangle \\
&\qquad+\langle a^+_{n-\sigma}(t)a_{m\sigma}\rangle\langle a^+_{n\sigma}(t)a_{n-\sigma}(t)a^+_{m-\sigma}a_{m-\sigma}\rangle \\
&\qquad+\langle a_{m-\sigma}(t)a_{m\sigma}\rangle\langle a^+_{n\sigma}(t)a^+_{n-\sigma}(t)a^+_{m-\sigma}a_{m-\sigma}\rangle\,.
\end{aligned} \tag{71}$$

The suitable or relevant approximations follows from the concrete physical conditions of the problem under consideration. We consider here for illustration the contributions from charge and spin collective degrees of freedom. We get

$$\begin{aligned}
M(ij;\omega) &= \frac{U^2}{2\pi^2}\int_{-\infty}^{+\infty} \mathrm{d}\omega_1\,\mathrm{d}\omega_2 \frac{ctg\beta\omega_1/2 + tg\beta\omega_2/2}{\omega-\omega_1-\omega_2} \\
&\times\left(\begin{pmatrix} \mathrm{Im}\,\langle\langle n_{i-\sigma}|n_{j-\sigma}\rangle\rangle_{\omega_1}\mathrm{Im}\,\langle\langle a_{i\sigma}|a^+_{j\sigma}\rangle\rangle_{\omega_2} & \mathrm{Im}\,\langle\langle n_{i-\sigma}|n_{j\sigma}\rangle\rangle_{\omega_1}\mathrm{Im}\,\langle\langle a_{i\sigma}|a^+_{j-\sigma}\rangle\rangle_{\omega_2} \\ \mathrm{Im}\,\langle\langle n_{i\sigma}|n_{j-\sigma}\rangle\rangle_{\omega_1}\mathrm{Im}\,\langle\langle a_{i-\sigma}|a^+_{j\sigma}\rangle\rangle_{\omega_2} & \mathrm{Im}\,\langle\langle n_{i\sigma}|n_{j\sigma}\rangle\rangle_{\omega_1}\mathrm{Im}\,\langle\langle a_{i-\sigma}|a^+_{j-\sigma}\rangle\rangle_{\omega_2} \end{pmatrix}\right. \\
&+\left.\begin{pmatrix} \mathrm{Im}\,\langle\langle S^{-\sigma}_i|S^{\sigma}_j\rangle\rangle_{\omega_1}\mathrm{Im}\,\langle\langle a_{i-\sigma}|a^+_{j-\sigma}\rangle\rangle_{\omega_2} & \mathrm{Im}\,\langle\langle S^{-\sigma}_i|S^{-\sigma}_j\rangle\rangle_{\omega_1}\mathrm{Im}\,\langle\langle a_{i-\sigma}|a^+_{j\sigma}\rangle\rangle_{\omega_2} \\ \mathrm{Im}\,\langle\langle S^{\sigma}_i|S^{\sigma}_j\rangle\rangle_{\omega_1}\mathrm{Im}\,\langle\langle a_{i\sigma}|a^+_{j-\sigma}\rangle\rangle_{\omega_2} & \mathrm{Im}\,\langle\langle S^{\sigma}_i|S^{-\sigma}_j\rangle\rangle_{\omega_1}\mathrm{Im}\,\langle\langle a_{i\sigma}|a^+_{j\sigma}\rangle\rangle_{\omega_2} \end{pmatrix}\right)\,.
\end{aligned} \tag{72}$$

It shows that it is possible to do all calculations in the localized Wannier basis as we did while deriving the equations for the strong coupling superconductivity in transition metals [19]. This has the great advantage for consideration of disordered transition metal alloys.

As for the translationally invariant crystal with broken symmetry the following special Fourier transform should be performed for the generalized mean-field GF $G_0(ij;\omega)$ (67):

$$\begin{aligned}
G^{11}_0(ij;\omega) &= \sum_k \exp[ik(R_i-R_j)]G^{11}_0(k;\omega)\,, \\
G^{12}_0(ij;\omega) &= \sum_k \exp[ikR_i - i(k+Q)R_j]G^{12}_0(k;\omega)\,, \\
G^{21}_0(ij;\omega) &= \sum_k \exp[i(k+Q)R_i - ikR_j]G^{21}_0(k;\omega)\,, \\
G^{22}_0(ij;\omega) &= \sum_k \exp[i(k+Q)(R_i-R_j)]G^{22}_0(k;\omega)\,.
\end{aligned} \tag{73}$$

The result of this transformation is then

$$G_0 = \begin{pmatrix} G_0^{11} & G_0^{12} \\ G_0^{21} & G_0^{22} \end{pmatrix} = \frac{\begin{pmatrix} \omega - E_{\downarrow}^{HF}(k+Q) & \Delta_{\uparrow\downarrow}(k) \\ \Delta_{\downarrow\uparrow}(k) & \omega - E_{\uparrow}^{HF}(k) \end{pmatrix}}{(\omega - E_1^{MF}(k))(\omega - E_2^{MF}(k))} , \tag{74}$$

where

$$\begin{aligned} E_{\sigma}^{HF} &= \varepsilon(k) + U\langle n_{\sigma}\rangle , \\ \Delta_{\sigma-\sigma}(k) &= U \sum i\exp(ikR_i)\langle a_{i\sigma}a_{i-\sigma}^{+}\rangle , \\ E_{1,2}^{MF} & \\ &= \left(\frac{E_{\uparrow}^{HF}(k) + E_{\downarrow}^{HF}(k+Q)}{2} \pm \sqrt{\left(\frac{E_{\uparrow}^{HF}(k) - E_{\downarrow}^{HF}(k+Q)}{2}\right)^2 + \Delta_{\uparrow\downarrow}(k)\Delta_{\downarrow\uparrow}(k)}\right) . \end{aligned} \tag{75}$$

It is evident that one can define the Overhauser's angle θ_k

$$\cos^2\theta_k = \frac{\Delta_{\uparrow\downarrow}(k)\Delta_{\downarrow\uparrow}(k)}{(\omega - E_{\uparrow}^{HF}(k))^2 + \Delta_{\uparrow\downarrow}(k)\Delta_{\downarrow\uparrow}(k)} . \tag{76}$$

In Overhauser's notations $\Delta_{\uparrow\downarrow}(k) = \Delta_{\downarrow\uparrow}(k) = \Delta$. The self-consistent set of equations for determining of the SDW (or "gap") order parameter Δ, chemical potential μ and averaged moment $\langle s^z\rangle$ is

$$\begin{aligned} \Delta &= U/N \sum_k \langle a_{k+Q\downarrow}^{+} a_{k\uparrow}\rangle , \\ \langle s^z\rangle &= U/N \sum_k \langle a_{k\uparrow}^{+} a_{k\uparrow} - a_{k\downarrow}^{+} a_{k\downarrow}\rangle , \\ n &= N^{-1} \sum_k (n(E_1^{MF}(k)) + n(E_2^{MF}(k))) . \end{aligned} \tag{77}$$

The above expressions were derived for correlated itinerant fermions on a lattice within Hubbard model and for finite temperatures. These equations were also deduced in previous papers in the course of their analysis. Here we deduced it by using more sophisticated arguments of the IGFs method in complete analogy with our description of the Heisenberg antiferromagnet at finite temperatures [53]. However, the self-consistent system of equations (69) and (72) for determining the quasiparticle spectra with damping is not as obvious generalization as Eqs. (77). This is intrinsically the many-body manifestation of the correlation effects of itinerant fermions on a lattice and show clearly the advantage of the present approach.

To confirm this, the explicit calculations of the damping should be performed. The natural way to tackle this program would then to look at the calculations of the collective GFs or generalized spin (and charge) susceptibilities in (72) but it deserves of separate consideration. Again this problem bears close similarity to paramagnetic Hubbard model and antiferromagnetic Heisenberg model and it can be argued that this effect of interference of single particle and collective modes of excitations should be considered carefully.

9. Discussion

We have been concerned in this paper with establishing what is the essence of single-particle excitations of correlated lattice fermions, rather with their detailed properties. We have considered the single- and multiband Hubbard model but the calculational details were mainly presented for single-band Hubbard model where the appropriate concepts are easier to demonstrate. We have considered a general family of symmetry broken solutions for itinerant lattice fermions, identifing the type of ordered states and then derived explicitly the functional of generalized mean fields and self-consistent set of equations which describe the quasiparticle spectra and their damping in the most general way. While such generality is not so obvious in all applications, it is highly desirable in treatments of such complicated problems as the competition and interplay of antiferromagnetism and superconductivity, heavy fermions and antiferromagnetism, etc., because of the non-trivial character of coupled equations which occur there. Both of these problems are subjects of current but independent research.

Another development of the present approach is the consideration of the itinerant antiferromagnetism of highly correlated lattice fermions when U is very big but finite. Like the weak-coupled case described in this paper, the symmetry broken approach will work, but matters are complicated by the necessity of constructing of the more extended algebra of relevant operators [3]. This idea has been carried out for the paramagnetic solution of the single-band Hubbard model [10]. It would be interesting to understand on a deeper level the relationship between Mott–Hubbard metal–insulator transition and various ordered magnetic states within the Hubbard model.

In conclusion, we have demonstrated that irreducible Green's functions approach is a workable and efficient scheme for the consistent description of the correlated fermions on a lattice at finite temperatures and can be generalized naturally to include the symmetry broken concept.

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