SPECTRAL PROPERTIES OF THE GENERALISED SPIN-FERMION MODELS

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In order to account for competition and interplay of localized and itinerant magnetic behaviour in correlated many body systems with complex spectra the various types of spin-fermion models have been considered in the context of the Irreducible Green's Functions (IGF) approach. Examples are generalised d–f model and Kondo–Heisenberg model. The calculations of the quasiparticle excitation spectra with damping for these models 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 Generalised Mean Fields (elastic scattering corrections) and self-energy (inelastic scattering) in terms of the Dyson equation has been generalised in order to include the presence of the two interacting subsystems of localised spins and itinerant electrons. A general procedure is given to obtain the quasiparticle damping in a self-consistent way. This approach gives the complete and compact description of quasiparticles and show the flexibility and richness of the generalised spin-fermion model concept.

1. Introduction

The existence and properties of localised and itinerant magnetism in metals, oxides and alloys and their interplay is an interesting and not yet fully understood problem of quantum theory of magnetism. The behaviour and the true nature of the electronic and spin states and their quasiparticle dynamics are of central importance to the understanding of the physics of correlated systems such as magnetism and Mott–Hubbard metal-insulator transition in metal and oxides, magnetism and heavy fermions (HF) in rare-earths compounds, high-temperature superconductivity (HTSC) in cuprates and anomalous transport properties in perovskite manganites. This class of systems are characterized by the complex, many-branch spectra of elementary excitations and, moreover, the correlations effects are essential.

Recently there has been considerable interest in identyfying the microscopic origin of quasiparticle states in such systems and a number of model approaches

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have been proposed. A principle importance of these studies is concerned with a fundamental problem of electronic solid state theory, namely with the tendency of $3d$ electrons in transition metal compounds and $4f$ electrons in rare-earth metal compounds to exhibit both localized and delocalized behaviour. The interesting electronic and magnetic properties of these substances are intimately related to this dual behaviour of electrons. In spite of experimental and theoretical achievements still it remains much to be understood concerning such systems.

Many magnetic and electronic properties of these materials may be interpreted in terms of combined spin-fermion models (SFM), which include the interacting spin and charge subsystems. This add the richness to physical behaviour and brings in significant and interesting physics, e.g. the bound states and magnetic polarons, HF and collosal negative magnetoresistance.

The problem of the adequate description of quasiparticle many-body dynamics of generalised spin-fermion models has been studied intensively during the last decades, especially in the context of magnetic and transport properies of rare-earth and transition metals and their compounds,[1−4] magnetic semiconductors,[5,6] interplay of magnetism and HF,[7,8] HTSC[9−14] and magnetic and transport properties of perovskite manganites.[4,15,16] Variety of metal–insulator transitions and correlated metals phenomena in $d(f)$-electron systems as well as the relevant models have been comprehensively discussed recently in Ref. 4.

The basic theory of the physical behaviour of SFMs has been studied mainly within mean field approximation. However many experimental investigations call for a better understanding of the nature of solutions (especially magnetic) to the spin-fermion and related correlated models, such as t–J, Kondo–Heisenberg model, etc.[4,12]

In the previous papers we set up the formalism of the method of the Irreducible Green's Functions (IGF).[17−25] This IGF method allows one to describe the quasiparticle spectra with damping for the systems with compex spectra and strong correlation in a very general and natural way. This scheme differs from the traditional method of decoupling of the infinite chain of the equations[26] and permits to construct the relevant dynamical solutions in a self-consistent way on the level of the Dyson equation without decoupling the chain of the equation of motion for the GFs.

In this paper we apply the formalism to consider the quasiparticle spectra for the complex systems, consisting of a few interacting subsystems. It is the purpose of this paper to explore more fully the notion of Generalized Mean Fields (GMF)[12] which may arise in the system of interacting localized spins and lattice fermions to justify and understand the "nature" of relevant mean-fields and damping effects.

It is worthy to emphasize that in order to understand quantitatively the electrical, thermal and superconducting properties of metals and their alloys one needs a proper description an electron–lattice interaction too.[27−29] A systematic, self-consistent simultaneous treatment of the electron–electron and electron–phonon interaction plays an important role in recent studies of strongly correlated systems.[24]

The natural approach for the description of electron-lattice effects in such type of compounds is the Modified Tight-Binding Approximation (MTBA).[28,29] We shall consider here the effects of electron-lattice interaction within the spin-fermion model approach.

The purpose of this paper is to extend the general analysis to obtain the quasi-particle spectra and their damping of the concrete model systems consisting of two or more interacting subsystems within various types of spin-fermion models to extend their applicability and show the effectiveness of IGF method.

2. Irreducible Green's Functions Method

In this paper we will use the IGF 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 system with complex spectra and strong interaction is related closely with the field theoretical approach and use the advantage of the Green's functions language and the Dyson equation. It is possible to say that our method tend to emphasize the fundamental and central role of the Dyson equation for the single-particle dynamics of the many-body systems at finite temperatures.

In this Section, we will discuss briefly this novel nonperturbative approach for the description of the many-body dynamics of many branch and strongly correlated systems. 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 a helpful reformulation of the two-time GFs method[26] which is especially adjusted[17] for the correlated fermion systems on a lattice and systems with complex spectra.[5,6] The similar method has been proposed in Ref. 30 for Bose systems (anharmonic phonons and spin dynamics of pure Heisenberg ferromagnet). 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 complex spectra and do not reduce to the functional of the mean densities of the electrons or spins, when we calculate excitations spectra at finite temperatures.

To clarify the foregoing, let us consider the retarded GF of the form[26]

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

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.[20] It is based on the notion of the *"IRRE-DUCIBLE"* parts of GFs (or the irreducible parts of the operators, out of which the GF is constructed) in term of which it is possible, without recourse to a truncation

of the hierarchy of equations for the GFs, to write down the exact Dyson equation and to obtain an exact analytical representation for the self-energy operator. By definition we introduce the irreducible part **(ir)** of the GF

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

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

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

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, irreducible GF are defined so that they 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 extract all relevant (for the problem under consideration) mean field contributions and puts them into the generalized mean-field GF, which here are defined as

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

To calculate the IGF $^{\text{ir}}\langle[A,H]_-(t),\, A^+(t')\rangle$ 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 a 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

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

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

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

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

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

which has a well known formal solution of the form

$$G = [(G^0)^{-1} - M]^{-1}; \qquad M = G_0^{-1} - G^{-1}. \tag{11}$$

Thus, by introducing irreducible parts of GF (or the irreducible parts of the operators, out of which the GF is constructed) the equation of motion (2) for the GF can be exactly (but using constraint (4)) transformed into Dyson equation for the two-time thermal GF. This is very remarkable result, which deserves underlining, because of the traditional form of the GF method did not include this point. The projection operator technique has essentially the same philosophy, but with using the constraint (4) in our approach we emphasize the fundamental and central role of the Dyson equation for the calculation of the single-particle properties of the many-body systems. It is important to note, that for the retarded and advanced GFs the notion of the proper part is symbolic in nature.[20] 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 analogue 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. 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 the adequate introduction of mean fields and internal symmetries of the Hamiltonian. In many-body interacting systems, the symmetry is important in classifying of the different phases and in understanding of the phase transitions between them. The problem of finding of the ferromagnetic and antiferromagnetic "symmetry broken" solutions of the correlated lattice fermion models within IGF method has been investigated in Ref. 25. A unified scheme for the construction of Generalised Mean Fields (elastic scattering corrections) and self-energy (inelastic scattering) in terms of the Dyson equation has been generalised in order to include the presence of the "source fields". The "symmetry broken" dynamical solutions of the Hubbard model, which correspond to various types of itinerant antiferromagnetism has been discussed. This approach complements previous studies of microscopic theory of Heisenberg antiferromagnet[19] and clarifies the nature of the concepts of Neel sublattices for

localized and itinerant antiferromagnetism and "spin-aligning fields" of correlated lattice fermions.

3. Quasiparticle Dynamics of the *d–f* Model

3.1. *Generalised d–f model*

The concept of the $s(d)$–f model play an important role in the quantum theory of magnetism.[1,27] In this section we consider the generalised d–f model, which describe the localized $4f(5f)$-spins interacting with d-like tight-binding itinerant electrons and take into consideration the electron–electron and electron–phonon interaction in the framework of MTBA.[28,29]

The total Hamiltonian of the model is given by

$$H = H_d + H_{d-f} + H_{d-\mathrm{ph}} + H_{\mathrm{ph}}\,. \tag{12}$$

The Hamiltonian of tight-binding electrons is given by

$$H_d = \sum_{ij}\sum_{\sigma} t_{ij} a_{i\sigma}^+ a_{j\sigma} + \frac{1}{2}\sum_{i\sigma} U n_{i\sigma} n_{i-\sigma}\,. \tag{13}$$

This is the Hubbard model.[31] The band energy of Bloch electrons $\epsilon(\mathbf{k})$ is defined as follows

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

where N is the number of the lattice sites. For the tight-binding electrons in cubic lattice we use the standard expression for the dispersion

$$\epsilon(\mathbf{k}) = 2\sum_{\alpha} t(\mathbf{a}_\alpha)\cos(\mathbf{k}\cdot\mathbf{a}_\alpha)\,, \tag{14}$$

where $\mathbf{a}_\alpha$ denotes the lattice vectors in a simple lattice with inversion centre.

The term H_{d-f} describes the interaction of the total $4f(5f)$-spins with the spin density of the itinerant electrons

$$H_{d-f} = \sum_i J\boldsymbol{\sigma}_i \cdot \mathbf{S}_i = -JN^{-1/2}\sum_{kq}\sum_{\sigma}[S_{-q}^{-\sigma} a_{k\sigma}^+ a_{k+q-\sigma} + z_\sigma S_{-q}^z a_{k\sigma}^+ a_{k+q\sigma}]\,, \tag{15}$$

where sign factor z_σ is given by

$$z_\sigma = (+\,\mathrm{or}-) \quad \mathrm{for} \quad \sigma = (\uparrow\,\mathrm{or}\downarrow)$$

and

$$S_{-q}^{-\sigma} = \begin{cases} S_{-q}^- & \text{if } \sigma = + \\ S_{-q}^+ & \text{if } \sigma = - \end{cases}\,.$$

In general the indirect exchange integral J strongly depends on the wave vectors $J(\mathbf{k};\mathbf{k}+\mathbf{q})$ having its maximum value at $k = q = 0$. We omit this dependence for the sake of brevity of notations only.

For the electron–phonon interaction we use the following Hamiltonian[28]

$$H_{d-\mathrm{ph}} = \sum_{\nu\sigma} \sum_{\mathbf{kq}} V^\nu(\mathbf{k}, \mathbf{k}+\mathbf{q}) Q_{\mathbf{q}\nu} a^+_{\mathbf{k}+\mathbf{q}\sigma} a_{\mathbf{k}\sigma} \,, \tag{16}$$

where

$$V^\nu(\mathbf{k}, \mathbf{k}+\mathbf{q}) = \frac{2iq_0}{(NM)^{1/2}} \sum_\alpha t(\mathbf{a}_\alpha) e^\alpha_\nu(\mathbf{q}) [\sin \mathbf{a}_\alpha \cdot \mathbf{k} - \sin \mathbf{a}_\alpha \cdot (\mathbf{k}-\mathbf{q})] \,, \tag{17}$$

here q_0 is the Slater coefficient[28] originated in the exponential decrease of the wave functions of d-electrons, N is the number of unit cells in the crystal and M is the ion mass. The $\mathbf{e}_\nu(\mathbf{q})$ are the polarization vectors of the phonon modes.

For the ion subsystem we have

$$H_{\mathrm{ph}} = \frac{1}{2} \sum_{\mathbf{q}\nu} (P^+_{\mathbf{q}\nu} P_{\mathbf{q}\nu} + \omega^2(\mathbf{q}\nu) Q^+_{\mathbf{q}\nu} Q_{\mathbf{q}\nu}) \,, \tag{18}$$

where $P_{\mathbf{q}\nu}$ and $Q_{\mathbf{q}\nu}$ are the normal coordinates and $\omega(q\nu)$ are the acoustical phonon frequencies. Thus, as in Hubbard model,[31] the d- and $s(p)$-bands are replaced by one effective band in our d–f model. However, the s-electrons give rise to screening effects and are taken into effects by choosing proper values of U and J and the acoustical phonon frequencies.

3.2. *Spin dynamics of the d–f model*

In this section, to make the discussion more concrete and to illustrate the nature of spin excitations in the d–f model we consider the double-time thermal GF of localized spins,[26] which is defined as

$$G^{+-}(k; t-t') = \langle\langle S^+_k(t), S^-_{-k}(t') \rangle\rangle = -i\theta(t-t') \langle [S^+_k(t), S^-_{-k}(t')]_- \rangle$$

$$= 1/2\pi \int_{-\infty}^{+\infty} d\omega \exp(-i\omega t) G^{+-}(k; \omega) \,. \tag{19}$$

The next step is to write down the equation of motion for the GF. Our attention will be focused on spin dynamics of the model. To describe self-consistently the spin dynamics of the d–f model one should take into account the full algebra of relevant operators of the suitable "spin modes", which are appropriate when the goal is to describe self-consistently the quasiparticle spectra of two interacting subsystems. This relevant algebra should be described by the "spinor" $\binom{\mathbf{S}_i}{\boldsymbol{\sigma}_i}$ ("relevant degrees of freedom"), according to IGF strategy of Sec. 2.

Once this has been done, we must introduce the generalized matrix GF of the form

$$\begin{pmatrix} \langle\langle S^+_k | S^-_{-k} \rangle\rangle & \langle\langle S^+_k | \sigma^-_{-k} \rangle\rangle \\ \langle\langle \sigma^+_k | S^-_{-k} \rangle\rangle & \langle\langle \sigma^+_k | \sigma^-_{-k} \rangle\rangle \end{pmatrix} = \hat{G}(k; \omega) \,. \tag{20}$$

Here

$$\sigma^+_k = \sum_q a^+_{k\uparrow} a_{k+q\downarrow} \,, \qquad \sigma^-_k = \sum_q a^+_{k\downarrow} a_{k+q\uparrow}$$

To explore the advantages of the IGF in the most full form, we shall do the calculations in the matrix form.

To demonstrate the utility of the IGF method we consider the following steps in a more detail form. Differentiating the GF $\langle S_k^+(t)|B(t')\rangle$ with respect to the first time, t, we find

$$\omega\langle\langle S_k^+|B\rangle\rangle_\omega = \left\{\begin{array}{c} 2N^{-1/2}\langle S_0^z\rangle \\ 0 \end{array}\right\}$$
$$+ \frac{J}{N}\sum_{pq}\langle\langle 2S_{k-q}^z a_{p\uparrow}^+ a_{p+q\downarrow} - S_{k-q}^+(a_{p\uparrow}^+ a_{p+q\uparrow} - a_{p\downarrow}^+ a_{p+q\downarrow})|B\rangle\rangle_\omega\,,$$

$$(21)$$

where

$$B = \left\{\begin{array}{c} S_{-k}^- \\ \sigma_{-k}^- \end{array}\right\}\,.$$

Let us introduce by definition irreducible (ir) operators as

$$(S_{k-q}^z)^{\text{ir}} = S_{k-q}^z - \langle S_0^z\rangle\delta_{k,q}$$
$$(a_{p\uparrow}^+ a_{p+q\uparrow})^{\text{ir}} = a_{p\uparrow}^+ a_{p+q\uparrow} - \langle a_{p\uparrow}^+ a_{p\uparrow}\rangle\delta_{q,0}\,.$$

$$(22)$$

Using the definition of the irreducible parts the equation of motion (21) can be exactly transformed to the following form

$$[\omega - JN^{-1}(n_\uparrow - n_\downarrow)]\langle\langle S_k^+|B\rangle\rangle_\omega + 2JN^{-1}\langle S_0^z\rangle\langle\langle\sigma_k^+|S_{-k}^-\rangle\rangle_\omega$$

$$= \left\{\begin{array}{c} 2N^{-1/2}\langle S_0^z\rangle \\ 0 \end{array}\right\} \mp \frac{J}{N}\sum_{pq}$$

$$\times\langle\langle 2(S_{k-q}^z)^{\text{ir}} a_{p\uparrow}^+ a_{p+q\downarrow} - S_{k-q}^+(a_{p\uparrow}^+ a_{p+q\uparrow} - a_{p\downarrow}^+ a_{p+q\downarrow})^{\text{ir}}|B\rangle\rangle_\omega\,,\qquad(23)$$

where

$$n_\sigma = \sum_q\langle a_{q\sigma}^+ a_{q\sigma}\rangle = \sum_q f_{q\sigma} = \sum_q(e^{\beta\epsilon(q\sigma)}+1)^{-1}\,.$$

To write down the equation of motion for the Fourier transform of the GF $\langle\langle\sigma_k^+(t),B(t')\rangle\rangle$ we need the following auxiliary equation of motion

$$(\omega + \epsilon(p) - \epsilon(p-k) - 2JN^{-1/2}\langle S_0^z\rangle - UN^{-1}(n_\uparrow - n_\downarrow))\langle\langle a_{p\uparrow}^+ a_{p+k\downarrow}|B\rangle\rangle_\omega$$

$$+ UN^{-1}(f_{p\uparrow} - f_{p+k\downarrow})\langle\sigma_k^+|B\rangle_\omega + JN^{-1/2}(f_{p\uparrow} - f_{p+k\downarrow})\langle\langle S_k^+|B\rangle\rangle_\omega$$

$$= \left\{\begin{array}{c} 0 \\ (f_{p\uparrow} - f_{p+k\downarrow}) \end{array}\right\} - JN^{-1/2}\sum_{qr}\langle\langle S_{-r}^+(a_{p\uparrow}^+ a_{q+r\uparrow}\delta_{p+k,q} - a_{q\downarrow}^+ a_{p+k\downarrow}\delta_{p,q+r})^{\text{ir}}|B\rangle\rangle_\omega$$

$$- JN^{-1/2}\sum_{qr}\langle\langle(S_{-r}^z)^{\text{ir}}(a_{q\uparrow}^+ a_{p+k\downarrow}\delta_{p,q+r} + a_{p\uparrow}^+ a_{q+r\downarrow}\delta_{p+k,q})|B\rangle\rangle_\omega$$

$$+ UN^{-1} \sum_{qr} \langle\langle (a_{p\uparrow}^+ a_{q+r\uparrow}^+ a_{q\uparrow} a_{p+r+k\downarrow} - a_{p+r\uparrow}^+ a_{q-r\downarrow}^+ a_{q\downarrow} a_{p+k\downarrow})^{\text{ir}} | B \rangle\rangle_\omega$$

$$+ \sum_{\nu q} \langle\langle (V^\nu(q, k+p-q) a_{p\uparrow}^+ a_{k+p-q\downarrow} - V^\nu(q,p) a_{p+q\uparrow}^+ a_{k+p\downarrow}) Q_{q\nu} | B \rangle\rangle_\omega \,. \qquad (24)$$

Let us use now the following notations:

$$A = \frac{J}{N} \sum_{pq} [2(S_{k-q}^z)^{\text{ir}} a_{p\uparrow}^+ a_{p+q\downarrow} - S_{k-q}^+ (a_{p\uparrow}^+ a_{p+q\uparrow} - a_{p\downarrow}^+ a_{p+q\downarrow})^{\text{ir}}] \,,$$

$$B_p = J N^{-1/2} \sum_{qr} [S_{-r}^+ (a_{p\uparrow}^+ a_{q+r\uparrow} \delta_{p+k,q} - a_{q\downarrow}^+ a_{p+k\downarrow} \delta_{p,q+r})^{\text{ir}}$$

$$- (S_{-r}^z)^{\text{ir}} (a_{q\uparrow}^+ a_{p+k\downarrow} \delta_{p,q+r} + a_{p\uparrow}^+ a_{q+r\downarrow} \delta_{p+k,q})]$$

$$+ UN^{-1} \sum_{qr} (a_{p\uparrow}^+ a_{q+r\uparrow}^+ a_{q\uparrow} a_{p+r+k\downarrow} - a_{p+r\uparrow}^+ a_{q-r\downarrow}^+ a_{q\downarrow} a_{p+k\downarrow})^{\text{ir}}$$

$$+ \sum_{\nu q} (V^\nu(q, k+p-q) a_{p\uparrow}^+ a_{k+p-q\downarrow} - V^\nu(q,p) a_{p+q\uparrow}^+ a_{k+p\downarrow}) \,, \qquad (25)$$

$$\Omega_1 = \omega - J N^{-1}(n_\uparrow - n_\downarrow) \,; \qquad \Omega_2 = 2J N^{-1} \langle S_0^z \rangle \,,$$

$$\omega_{p,k} = (\omega + \epsilon(p) - \epsilon(p+k) - \Delta) \,,$$

$$\Delta = 2J N^{-1/2} \langle S_0^z \rangle - U N^{-1}(n_\uparrow - n_\downarrow) \,,$$

$$\chi_0^{df}(k, \omega) = N^{-1} \sum_p \frac{(f_{p+k\downarrow} - f_{p\uparrow})}{\omega_{p,k}} \,.$$

In the matrix notations the full equation of motion can be summarized now in the following form

$$\hat\Omega \hat{G}(k; \omega) = \hat{I} + \sum_p \hat\Phi(p) \begin{pmatrix} \langle\langle A | S_{-k}^- \rangle\rangle & \langle\langle A | \sigma_{-k}^- \rangle\rangle \\ \langle\langle B_p | S_{-k}^- \rangle\rangle & \langle\langle B_p | \sigma_{-k}^- \rangle\rangle \end{pmatrix} \qquad (26)$$

where

$$\hat\Omega = \begin{pmatrix} \Omega_1 & \Omega_2 \\ -J N^{-1/2} \chi_0^{df} & (1 - U \chi_0^{df}) \end{pmatrix} \,; \qquad \hat{I} = \begin{pmatrix} J^{-1} N^{1/2} \Omega_2 & 0 \\ 0 & -N \chi_0^{df} \end{pmatrix} \,;$$

$$\hat\Phi(p) = \begin{pmatrix} N^{-1} & 0 \\ 0 & \omega_{p,k}^{-1} \end{pmatrix} \,. \qquad (27)$$

To calculate the higher-order GFs in (26), 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

$$\hat\Omega \hat{G}(k; \omega) = \hat{I} + \sum_{pq} \hat\Phi(p) \hat{P}(p, q) \hat\Phi(q)(\hat\Omega^+)^{-1} \,. \qquad (28)$$

This equation can be identically transformed to the standard form (7)

$$\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{P} \hat{G}_0 \,. \tag{29}$$

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

$$\hat{G}_0 = \hat{\Omega}^{-1} \hat{I} \,. \tag{30}$$

The scattering operator P has the form

$$\hat{P} = \hat{I}^{-1} \sum_{pq} \hat{\Phi}(p) \hat{P}(p, q) \hat{\Phi}(q) \hat{I}^{-1} \,. \tag{31}$$

Here we have used the obvious notation

$$\hat{P}(k, q; \omega) = \begin{pmatrix} \langle\langle A^{\mathrm{ir}} | \tilde{A}^{\mathrm{ir}} \rangle\rangle & \langle\langle A^{\mathrm{ir}} | \tilde{B}_q^{\mathrm{ir}} \rangle\rangle \\ \langle\langle B_p^{\mathrm{ir}} | \tilde{A}^{\mathrm{ir}} \rangle\rangle & \langle\langle B_p^{\mathrm{ir}} | \tilde{B}_q^{\mathrm{ir}} \rangle\rangle \end{pmatrix} \,. \tag{32}$$

The operators $\tilde{A}$ and $\tilde{B}_q$ follow from A and B_q by interchange $\uparrow \to \downarrow$, $\mathbf{k} \to -\mathbf{k}$ and $S^+ \to -S^-$.

As shown in Sec. 2, Eq. (29) can be transformed exactly into a Dyson Eq. (10) by means of the definition (9). Hence, the determination of the full GF $\hat{G}$ has been reduced to the determination of $\hat{G}_0$ and $\hat{M}$.

3.3. *Generalized mean-field GF*

From the definition (30) the GF matrix in generalized mean-field approximation reads

$$\hat{G}_0 = R^{-1} \begin{pmatrix} (1 - U\chi_0^{df}) J^{-1} N^{1/2} \Omega_2 & \Omega_2 N \chi_0^{df} \\ \Omega_2 N \chi_0^{df} & -\Omega_1 N \chi_0^{df} \end{pmatrix} \tag{33}$$

where

$$R = (1 - U\chi_0^{df})\Omega_1 + \Omega_2 J N^{1/2} \chi_0^{df} \,.$$

The spectrum of quasiparticle excitations without damping follows from the poles of the generalized mean-field GF (33).

Let us write down explicitly the first matrix element G_0^{11}

$$\langle\langle S_k^+ | S_{-k}^- \rangle\rangle^0 = \frac{2JN^{-1/2}\langle S_0^z \rangle}{\omega - JN^{-1}(n_\uparrow - n_\downarrow) + 2J^2 N^{-1/2}\langle S_0^z \rangle(1 - U\chi_0^{df})^{-1}\chi_0^{df}} \,. \tag{34}$$

This result can be considered as reasonable approximation for description of the dynamics of localized spins in heavy rare-earth metals like Gd. (c.f. Refs. 1 and 27).

The magnetic excitation spectrum following from the GF (34) consists of three branches — the acoustical spin wave, the optical spin wave and the Stoner continuum.[27] In the hydrodynamic limit, $k \to 0$, $\omega \to 0$ the GF (34) can be written as

$$\langle\langle S_k^+ | S_{-k}^- \rangle\rangle^0 = \frac{2N^{-1/2}\langle \tilde{S}_0^z \rangle}{\omega - E(k)} \,, \tag{35}$$

where the acoustical spin wave energies are given by

$$E(k) = Dk^2 = \frac{1/2 \sum_q (f_{q\uparrow} + f_{q\downarrow})(\mathbf{k}\frac{\partial}{\partial \mathbf{q}})^2 \epsilon(\mathbf{q}) + (2\Delta)^{-1} \sum_q (f_{q\uparrow} - f_{q\downarrow})(\mathbf{k}\frac{\partial}{\partial \mathbf{q}} \epsilon(\mathbf{q}))^2}{2N^{1/2}\langle S_0^z \rangle + (n_\uparrow - n_\downarrow)}$$

(36)

and

$$\langle \tilde{S}_0^z \rangle = \langle S_0^z \rangle \left[1 + \frac{(n_\uparrow - n_\downarrow)}{2N^{3/2}\langle S_0^z \rangle} \right]^{-1}$$

(37)

For s.c. lattice the spin wave dispersion relation (36) becomes

$$E(k) = (2N^{1/2}\langle S_0^z \rangle + (n_\uparrow - n_\downarrow))^{-1}$$

$$\times \left[\frac{2t^2 a^2}{\Delta} \sum_q (f_{q\uparrow} - f_{q\downarrow})(k_x \sin(q_x a) + k_y \sin(q_y a) + k_z \sin(q_z a))^2 \right.$$

$$\left. - ta^2 \sum_q (f_{q\uparrow} + f_{q\downarrow})(k_x^2 \cos(q_x a) + k_y^2 \cos(q_y a) + k_z^2 \cos(q_z a)) \right].$$

(38)

In GMF approximation the density of itinerant electrons (and the band splitting Δ) can be evaluated by solving the equation

$$n_\sigma = \sum_k \langle a_{k\sigma}^+ a_{k\sigma} \rangle$$

$$= \sum_k \{\exp[\beta(\epsilon(k) + UN^{-1}n_{-\sigma} - JN^{-1/2}\langle S_0^z \rangle - \epsilon_{\mathrm{F}})] + 1\}^{-1}.$$

(39)

Hence, the stiffness constant D can be expressed by the parameters of the Hamiltonian (12).

The spectrum of the Stoner excitations is given by[27]

$$\omega_k = \epsilon(k + q) - \epsilon(q) + \Delta.$$

(40)

If we consider the optical spin wave branch then by direct calculation one can easily show that

$$E_{\mathrm{opt}}(k) = E_{\mathrm{opt}}^0 + D\left(\frac{UE_{\mathrm{opt}}}{J\Delta - 1}\right)k^2,$$

$$E_{\mathrm{opt}}^0 = J(n_\uparrow - n_\downarrow) + 2J\langle S_0^z \rangle.$$

(41)

From the Eq. (33) one also finds the GF of itinerant spin density in the generalized mean-field approximation

$$\langle\langle \sigma_k^+ | \sigma_{-k}^- \rangle\rangle_\omega^0 = \frac{\chi_0^{df}(k,\omega)}{1 - [U - 2J^2\langle S_0^z \rangle/[\omega - J(n_\uparrow - n_\downarrow)]]\chi_0^{df}(k,\omega)}.$$

(42)

3.4. *Dyson equation for d–f model*

The Dyson Eq. (10) for the generalized d–f model has the following form

$$\hat{G}(k;\omega) = \hat{G}_0(k;\omega) + \sum_{pq} \hat{G}_0(p;\omega)\hat{M}(pq;\omega)\hat{G}(q;\omega)\,. \qquad (43)$$

The mass operator

$$\hat{M}(pq;\omega) = \hat{P}^{(p)}(pq;\omega)$$

describes the inelastic (retarded) part of the electron–phonon, electron–spin and electron–electron interactions. To obtain workable expressions for matrix elements of the mass operator one should use the spectral theorem, inverse Fourier transformation and make relevant approximation in the time correlation functions. The elements of the mass operator matrix $\hat{M}$ are proportional to the higher-order GF of the following (conditional) form

$$\left(^{(\mathrm{ir})}\langle\langle (S^+)a_{k+p\sigma_1}a^+_{p+q\sigma_2}a_{q\sigma_2}|(S^-)a^+_{k+s\sigma_3}a^+_{r\sigma_4}a_{r+s\sigma_4}\rangle\rangle^{(\mathrm{ir}),p}\right)\,.$$

For the explicit approximate calculation of the elements of the mass operator it is convenient to write down the GFs in (44) in terms of correlation functions by using the well-known spectral theorem[26]:

$$\left(^{(\mathrm{ir})}\langle\langle (S^+)a_{k+p\sigma_1}a^+_{p+q\sigma_2}a_{q\sigma_2}|(S^-)a^+_{k+s\sigma_3}a^+_{r\sigma_4}a_{r+s\sigma_4}\rangle\rangle^{(\mathrm{ir}),p}\right)$$

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

$$\times \left(\langle\langle (S^-(t))a^+_{k+s\sigma_3}(t)a^+_{r\sigma_4}(t)a_{r+s\sigma_4}(t)|(S^+)a_{k+p\sigma_1}a^+_{p+q\sigma_2}a_{q\sigma_2}\rangle^{(\mathrm{ir}),p}\right)\,. \quad (44)$$

Let us first consider the GF $\langle\langle A|\tilde{A}\rangle\rangle$ appearing in M_{11}. Further insight is gained if we select the suitable relevant "trial" approximation for the correlation function on the r.h.s. of (44). In this paper we show that the earlier formulations, based on the decoupling or/and on diagrammatic methods can be arrived at from our technique but in a self-consistent way. Clearly the choice of the relevant trial approximation for the correlation function in (44) can be done in a few ways. The suitable or relevant approximations follow from the concrete physical conditions of the problem under consideration. We consider here for illustration the contributions from charge and spin degrees of freedom by neglecting higher order contributions between the magnetic excitations and charge density fluctuations as we did in the theory of ferromagnetic[5] and antiferromagnetic[32,33] semiconductors. For example, a reasonable and workable one may be the following approximation of two interacting modes[3]

$$\langle\langle A|\tilde{A}\rangle\rangle^{\mathrm{ir},p} \approx \frac{J^2}{N^2\pi^2} \sum_{kk_1k_2k_3k_4\sigma} \int \frac{d\omega_1 d\omega_2}{\omega - \omega_1 - \omega_2} F(\omega_1, \omega_2,) \qquad (45)$$

$$\mathrm{Im}\langle\langle S^+_{k-k_4}|S^-_{-k-k_2}\rangle\rangle_{\omega_1} \mathrm{Im}\langle\langle a^+_{k_3\sigma}a_{k_3+k_4\sigma}|a^+_{k_1\sigma}a_{k_1+k_2\sigma}\rangle\rangle_{\omega_2} ;$$

$$F(\omega_1, \omega_2,) = \frac{(\exp(\beta(\omega_1+\omega_2))) + 1}{(\exp(\beta\omega_1) - 1)(\exp(\beta\omega_2) - 1)} .$$

On the diagrammatic language this approximate expression results from the neglecting of the vertex corrections.

The system of Eqs. (43) and (45) form a closed self-consistent system of equations. In principle, one may use on the r.h.s. of (45) 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 the following approximations:

$$\mathrm{Im}\langle\langle S^+_{k-k_4}|S^-_{-k-k_2}\rangle\rangle_{\omega_1} \approx 2\pi N^{-1/2}\langle S^z_0\rangle\delta(\omega_1 - E(k+k_2))\delta_{k_4,-k_2} ; \qquad (46)$$

$$\mathrm{Im}\langle\langle a^+_{k_3\sigma}a_{k_3+k_4\sigma}|a^+_{k_1\sigma}a_{k_1+k_2\sigma}\rangle\rangle_{\omega_2}$$

$$\approx \pi(f_{k_3\sigma} - f_{k_1\sigma})\delta(\omega_2 + \epsilon(k_3\sigma) - \epsilon(k_3+k_4\sigma))\delta_{k_3,k_1+k_2}\delta_{k_1,k_3+k_4} .$$

Then, using (46) in (45), one can get an explicit expression for the M_{11}

$$\langle\langle A|\tilde{A}\rangle\rangle^{\mathrm{ir},p}$$

$$\approx \frac{2J^2}{N^2} \sum_{pq\sigma} \frac{[1 + N(E(k+q)) - f_{p\sigma}]f_{p+q\sigma} + N(E(k+q))f_{p\sigma}(1 - 2f_{p+q\sigma})}{\omega - E(k+q) - \epsilon(p\sigma) + \epsilon(p+q\sigma)} , \quad (47)$$

where

$$\epsilon(k\sigma) = \epsilon(k) + U\langle n_{-\sigma}\rangle ; \qquad N(E(k)) = [\exp(\beta E(k)) - 1]^{-1} . \qquad (48)$$

The calculations of the matrix elements M_{12}, M_{21} and M_{22} can be done in the same manner, but with additional initial approximation for phonon GF

$$\langle\langle Q_{k\nu}|Q^+_{k\nu}\rangle\rangle \approx (\omega^2 - \omega^2(k\nu))^{-1} . \qquad (49)$$

It is transparent that the construction of the GF $\langle\langle B_p|\tilde{B}_q\rangle\rangle$ will consist of contributions of the electron–phonon, electron–magnon and electron–electron inelastic scattering.

$$\langle\langle B_p|\tilde{B}_q\rangle\rangle = \langle\langle B_p|\tilde{B}_q\rangle\rangle^{\mathrm{ph-e}} + \langle\langle B_p|\tilde{B}_q\rangle\rangle^{\mathrm{m-e}} + \langle\langle B_p|\tilde{B}_q\rangle\rangle^{\mathrm{e-e}} .$$

As a result we find the explicit expressions for the GFs in mass operator

$$\langle\langle B_p|\tilde{B}_q\rangle\rangle^{\mathrm{ph-e}} = \frac{1}{2}\sum_{r\nu}\sum_{\alpha=\pm}\omega^{-1}(r\nu)$$

$$\times \left\{ \frac{[1 + N(\alpha\omega(r\nu)) - f_{p+q+r\downarrow}]f_{p\uparrow} + N(\alpha\omega(r\nu))f_{p+q+r\downarrow}(1 - 2f_{p\uparrow})}{\omega - [\alpha\omega(r\nu) - \epsilon(p\uparrow) + \epsilon(p+k+r\downarrow)]} \right.$$

$$\times [(V^\nu(r,p+k))^2 \delta_{q,p+k} - V^\nu(r,p)V^\nu(r,p+k)\delta_{q,p+k+r}]$$

$$+ \frac{[1+N(\alpha\omega(r\nu)) - f_{p+k\downarrow}]f_{p+r\uparrow} + N(\alpha\omega(r\nu))f_{p+k\downarrow}(1-2f_{p+r\uparrow})}{\omega - [\alpha\omega(r\nu) - \epsilon(p+r\uparrow) + \epsilon(p+k\downarrow)]}$$

$$\times [(V^\nu(r,p))^2 \delta_{q,p+k} - V^\nu(r,p)V^\nu(r,p+k)\delta_{q,p+k+r}] \Bigg\} . \tag{50}$$

The contribution from inelastic electron–magnon scattering is given by

$$\langle\langle B_p | \tilde{B}_q \rangle\rangle^{\mathrm{m-e}} = -\frac{2J^2}{N^2}\langle S_0^z \rangle \sum_r$$

$$\times \Bigg\{ \frac{[1+N(E(r)) - f_{p+k+r\uparrow}]f_{p\uparrow} + N(E(r))f_{p+k+r\uparrow}(1-2f_{p\uparrow})}{\omega - [E(r) - \epsilon(p\uparrow) + \epsilon(p+k+r\uparrow)]}$$

$$+ \frac{[1+N(E(r)) - f_{p+k\downarrow}]f_{p+r\downarrow} + N(E(r))f_{p+k\downarrow}(1-2f_{p+k\downarrow})}{\omega - [E(r) - \epsilon(p+r\downarrow) + \epsilon(p+k\downarrow)]} \Bigg\} \delta_{q,p+k} . \tag{51}$$

The term due to the electron–electron inelastic scattering processes becomes

$$\langle\langle B_p | \tilde{B}_q \rangle\rangle^{\mathrm{e-e}} = \frac{U^2}{N^2}$$

$$\times \Bigg\{ \sum_{rs} \Bigg[\frac{(1-f_{p+k\downarrow})(1-f_{r+s\downarrow})f_{r\downarrow}f_{p+k\uparrow} + f_{p+k\downarrow}f_{r+s\downarrow}(1-f_{r\downarrow})(1-f_{p+s\uparrow})}{\omega - [\epsilon(p+k\downarrow) - \epsilon(p+s\uparrow) + \epsilon(r+s\downarrow) - \epsilon(r\downarrow)]}$$

$$+ \frac{(1-f_{p+k+s\downarrow})(1-f_{r-s\uparrow})f_{r\uparrow}f_{p\uparrow} + f_{p+k+s\downarrow}f_{r-s\uparrow}(1-f_{r\uparrow})(1-f_{p\uparrow})}{\omega - [\epsilon(p+k+n\downarrow) - \epsilon(p\uparrow) + \epsilon(r-s\uparrow) - \epsilon(r\uparrow)]} \Bigg]$$

$$- \sum_r \Bigg\{ \frac{(1-f_{q\downarrow})(1-f_{p+k\downarrow})f_{r\downarrow}f_{p+q-r\uparrow} + f_{q\downarrow}f_{p+k\downarrow}(1-f_{r\downarrow})(1-f_{p+q-m\uparrow})}{\omega - [\epsilon(p+k\downarrow) + \epsilon(q\downarrow) - \epsilon(r\downarrow) - \epsilon(p+q-r\uparrow)]} \Bigg\}$$

$$+ \frac{(1-f_{q+r\downarrow})(1-f_{p-r\uparrow})f_{p\uparrow}f_{q-k\uparrow} + f_{q+r\downarrow}f_{p-r\uparrow}(1-f_{p\uparrow})(1-f_{q-k\uparrow})}{\omega - [\epsilon(q+r\downarrow) + \epsilon(p-r\uparrow) - \epsilon(p\uparrow) - \epsilon(q-k\uparrow)]} \Bigg] \Bigg\} \delta_{q,p+k} . \tag{52}$$

In the same way for off-diagonal contributions we find

$$\langle\langle A | \tilde{B}_q \rangle\rangle = -\frac{2J^2}{N^2}\langle S_0^z \rangle \sum_r$$

$$\times \Bigg\{ \frac{[1+N(E(r)) - f_{q+r\uparrow}]f_{q-k\uparrow} + N(E(r))f_{q+r\uparrow}(1-2f_{q-k\uparrow})}{\omega - (E(r) + \epsilon(q+r\uparrow) - \epsilon(q-k\uparrow))}$$

$$+ \frac{[1+N(E(r)) - f_{q\downarrow}]f_{q+r-k\downarrow} + N(E(r))f_{q\downarrow}(1-2f_{q+r-k\downarrow})}{\omega - (E(r) - \epsilon(q+r-k\downarrow) + \epsilon(q\downarrow))} \Bigg\} . \tag{53}$$

And we have $\langle\langle B_p|\tilde{A}\rangle\rangle = \langle\langle A|\tilde{B}_{p+k}\rangle\rangle$.

3.5. *Self-energy and damping*

Finally we turn to the calculation of the damping. To find the damping of the quasiparticle states in the general case, one needs to find the matrix elements of the mass-operator in (43). Thus we have

$$\begin{pmatrix} \hat{G}_{11} & \hat{G}_{12} \\ \hat{G}_{21} & \hat{G}_{22} \end{pmatrix} = \left[\begin{pmatrix} \hat{G}_{011} & \hat{G}_{012} \\ \hat{G}_{021} & \hat{G}_{022} \end{pmatrix}^{-1} - \begin{pmatrix} \hat{M}_{11} & \hat{M}_{12} \\ \hat{M}_{21} & \hat{M}_{22} \end{pmatrix} \right]^{-1} . \tag{54}$$

From this matrix equation we have

$$M_{11} = \frac{J^2}{N\Omega_2^2}\langle\langle A|\tilde{A}\rangle\rangle \, ;$$

$$M_{21} = \frac{J}{\Omega_2 N^{3/2}\chi_0^{df}} \sum_p (\omega_{p,k})^{-1}\langle\langle B_p|\tilde{A}\rangle\rangle \, ;$$

$$\tag{55}$$

$$M_{12} = \frac{J}{\Omega_2 N^{3/2}\chi_0^{df}} \sum_q (\omega_{q,p})^{-1}\langle\langle A|\tilde{B}_q\rangle\rangle \, ;$$

$$M_{22} = \frac{1}{N^2(\chi_0^{df})^2} \sum_{pq} (\omega_{p,k}\omega_{q,k})^{-1}\langle\langle B_p|\tilde{B}_q\rangle\rangle \, .$$

With (54) and (55) the GF $\hat{G}$ becomes

$$\hat{G} = \frac{1}{\det(\hat{G}_0^{-1} - \hat{M})} \begin{pmatrix} -[(1-U\chi_0^{df})/N\chi_0^{df}] - M_{22} & -[(J/N^{1/2}) - M_{12}] \\ -[(J/N^{1/2}) - M_{21}] & [(J/N^{1/2})(\Omega_1/\Omega_2) - M_{11}] \end{pmatrix} . \tag{56}$$

Let us estimate the damping of magnetic excitations. From (56) we find

$$\langle S_k^+|S_{-k}^-\rangle_\omega = \frac{1}{(G_0^{11})^{-1} - \Sigma(k,\omega)} . \tag{57}$$

Here the self-energy Σ is given by

$$\Sigma(k,\omega) = M_{11} + \frac{J^2\chi_0^{df}}{1 - U\chi_0^{df}}$$

$$- (JN^{-1/2} - M_{12})(JN^{-1/2} - M_{21})N\chi_0^{df}((1 - U\chi_0^{df}) + M_{22}N\chi_0^{df})^{-1} . \tag{58}$$

Let us consider the damping of the acoustical magnons. Considering only the linear terms in the matrix elements of the mass operator in (58), we find for small **k** and ω

$$\langle\langle S_k^+|S_{-k}^-\rangle\rangle_\omega \approx \frac{2N^{-1/2}\langle\tilde{S}_0^z\rangle}{\omega - E(k) - 2N^{-1/2}\langle\tilde{S}_0^z\rangle\Sigma(k,\omega)} , \tag{59}$$

where

$$\Sigma(k,\omega) \approx M_{11} + (M_{12} + M_{21})\frac{JN^{1/2}\chi_0^{df}}{1 - U\chi_0^{df}} + \frac{J^2 N(\chi_0^{df})^2}{(1 - U\chi_0^{df})^2} M_{22}. \quad (60)$$

Then the spectral density of the spin-wave excitations will be given as

$$-\frac{1}{\pi}\text{Im}\, G^{11}(k,\omega + i\varepsilon) = -\frac{1}{\pi}\text{Im}\langle\langle S_k^+ | S_{-k}^-\rangle\rangle_\omega$$

$$= \frac{2N^{-1/2}\langle\tilde{S}_0^z\rangle\Gamma(k,\omega)}{(\omega - E(k) - \Delta(k,\omega))^2 + \Gamma^2(k,\omega)} \quad (61)$$

where

$$\Delta(k,\omega) = 2N^{-1/2}\langle\tilde{S}_0^z\rangle\,\text{Re}\,\Sigma(k,\omega)$$

$$\Gamma(k,\omega) = 2N^{-1/2}\langle\tilde{S}_0^z\rangle\,\text{Im}\,\Sigma(k,\omega + i\varepsilon) \quad (62)$$

describes the shift and the damping of the magnons, respectively.

Finally we estimate the temperature dependence of $\Gamma(k,\omega)$ due to the mass operator terms in (58). Considering the first contribution in (58) we get

$$\text{Im}\, M_{11} = \text{Im}\langle\langle A|\tilde{A}\rangle\rangle_\omega$$

$$\approx J^2\langle S_0^z\rangle\sum_{pq\sigma}((1 + N(E(k+q)) - f_{p\sigma})f_{p+q\sigma}$$

$$+ N(E(k+q))f_{p\sigma}(1 - 2f_{p+q\sigma}))\delta(\omega - E(k+p) + \epsilon(p+q) - \epsilon(p)). \quad (63)$$

Using the standard relations

$$\sum_{pq} \to \frac{V^2}{(2\pi)^6}\int d^3p \int d^3q N(E(q))|_{q\to 0} = (\exp(\beta Dq^2) - 1)^{-1} \quad (64)$$

we find

$$\text{Im}\, M_{11} \sim J^2\langle S_0^z\rangle\frac{V^2}{(2\pi)^6}2\pi\int d^3p \int_0^{q_{\max}} q^2 dq \int d(\cos\Theta)$$

$$\times \tilde{F}(f_{p\sigma}, N(E(k+p)))\frac{\delta(\cos\Theta - \cos\Theta_0)}{|\partial\epsilon/\partial p|q}$$

$$\sim \frac{1}{2\beta D}\int_0^{\beta E_{\max}} dx\frac{1}{e^x - 1} \sim T. \quad (65)$$

The other contributions to $\Gamma(k,\omega)$ can be treated in the same way, where M_{12}, M_{21} and electron–magnon contribution to M_{22} are proportional to T, too. For the electron–phonon contribution to M_{22} we find

$$\text{Im}\, M_{22}^{\text{ph}} = \text{Im}\langle\langle B_p|\tilde{B}_q\rangle\rangle_\omega^{\text{ph}} \sim \frac{1}{\beta^3}\int x^2 dx\frac{1}{e^x - 1} \sim T^3. \quad (66)$$

Hence, the damping of the acoustical magnons at low temperatures can be written as

$$\Gamma(k,\omega)|_{k,\omega\to 0} \sim \Gamma_1 + \Gamma_2 T + \Gamma_3 T^3 \,, \tag{67}$$

where the coefficients Γ_i, $(i = 1, 2, 3)$ vanish for $k = \omega = 0$ and furthermore for $J = 0$.

3.6. *Charge dynamics of d–f model*

To describe the quasiparticle charge dynamics or dynamics of carriers of the d–f model (12) we should consider the equation of motion for the GF of the form

$$G_{k\sigma} = \langle\langle a_{k\sigma} | a_{k\sigma}^+ \rangle\rangle \,. \tag{68}$$

Performing the first time differentiation of (68) we find

$$
(\omega - \epsilon(k))G_{k\sigma} = 1 + \frac{U}{N}\sum_{pq}\langle\langle a_{p+q-\sigma}^+ a_{p-\sigma} a_{k+q\sigma} | a_{k\sigma}^+\rangle\rangle
$$
$$
- \frac{J}{N^{1/2}}\sum_q (\langle\langle S_{-q}^{-\sigma} a_{k+q-\sigma} | a_{k\sigma}^+\rangle\rangle + z_\sigma\langle\langle S_{-q}^z a_{k+q\sigma} | a_{k\sigma}^+\rangle\rangle)
$$
$$
+ \sum_{q\nu\alpha} V^\alpha(k-q,k)\langle\langle a_{k-q\sigma} Q_{q\nu} | a_{k\sigma}^+\rangle\rangle \,. \tag{69}
$$

Following the previous consideration we should introduce the irreducible GFs and perform the differentiation of the higher-order GFs on second time. Using this approach the the equation of motion (69) can be exactly transformed into the Dyson equation

$$G_{k\sigma}(\omega) = G_{k\sigma}^0(\omega) + G_{k\sigma}^0(\omega) M_{k\sigma}(\omega) G_{k\sigma}(\omega) \tag{70}$$

where

$$
G_{k\sigma}^0 = (\omega - \epsilon^0(k\sigma))^{-1} \,,
$$
$$
\epsilon^0(k\sigma) = \epsilon(k) - z_\sigma\frac{1}{N^{1/2}}\langle S_0^z\rangle + \frac{U}{N}n_{-\sigma} \,. \tag{71}
$$

Here the mass operator has the following exact representation

$$M_{k\sigma}(\omega) = M_{k\sigma}^{\mathrm{e-e}}(\omega) + M_{k\sigma}^{\mathrm{e-m}}(\omega) + M_{k\sigma}^{\mathrm{e-ph}}(\omega) \tag{72}$$

where

$$M_{k\sigma}^{\mathrm{e-e}}(\omega) = \frac{U^2}{N^2}\sum_{pqrs}{}^{(\mathrm{ir})}\langle a_{p+q-\sigma}^+ a_{p-\sigma} a_{p+q\sigma} | a_{r+s-\sigma}^+ a_{r-\sigma} a_{k-s\sigma}^+\rangle^{(\mathrm{ir}),p}) \tag{73}$$

$$M_{k\sigma}^{\mathrm{e-m}}(\omega) = \frac{J^2}{N} \sum_{qs} [(^{(\mathrm{ir})}\langle\langle S_{-q}^{-\sigma} a_{k+q-\sigma} | S_s^{\sigma} a_{k+s-\sigma}^+ \rangle\rangle^{(\mathrm{ir}),p})$$

$$+ (^{(\mathrm{ir})}\langle\langle S_{-q}^z a_{k+q\sigma} | S_s^z a_{k+s\sigma}^+ \rangle\rangle^{(\mathrm{ir}),p})] \qquad (74)$$

$$M_{k\sigma}^{\mathrm{e-ph}}(\omega) = \sum_{q\nu\alpha} \sum_{s\mu\alpha'} V_{q\nu}^{\alpha}(p-q,p) V_{s\mu}^{\alpha'}(p,p+q)(^{(\mathrm{ir})}\langle\langle Q_{q\nu} a_{p-q\sigma} | Q_{s\mu}^+ a_{p+q\sigma}^+ \rangle\rangle^{(\mathrm{ir}),p}).$$

$$(75)$$

As previously, we express the GF in terms of the correlation functions. In order to calculate the mass operator self-consistently we shall use the "pair" approximation[17,22] for the $M^{\mathrm{e-e}}$ and approximation of two interacting modes for $M^{\mathrm{e-m}}$ and $M^{\mathrm{e-ph}}$.[5,28] Then the corresponding expressions can be written as

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

$$\times g_{p+q,-\sigma}(\omega_1) g_{k+p,\sigma}(\omega_2) g_{p,-\sigma}(\omega_3), \qquad (76)$$

where

$$g_{k\sigma}(\omega) = -\frac{1}{\pi}\mathrm{Im}\langle\langle a_{k\sigma} | a_{k\sigma}^+ \rangle\rangle_{\omega+\varepsilon}$$

and

$$F^{\mathrm{e-e}}(\omega_1, \omega_2, \omega_3) = [f(\omega_1)(1 - f(\omega_2) - f(\omega_3) + f(\omega_2)f(\omega_3))].$$

Let us consider now the spin-electron inelastic scattering. As previously, we shall neglect of the vertex corrections, i.e. correlation between the propagations of the charge and spin excitations. Then we obtain from (74)

$$M_{k\sigma}^{\mathrm{e-m}}(\omega) = \frac{J^2}{N} \sum_{q} \int \frac{d\omega_1 d\omega_2}{\omega - \omega_1 - \omega_2} F^{\mathrm{e-m}}(\omega_1, \omega_2)$$

$$\times \left(g_{k+p,-\sigma}(\omega_2) \left(-\frac{1}{\pi}\mathrm{Im}\langle\langle S_{-q}^{\sigma} | S_q^{-\sigma} \rangle\rangle_{\omega_1} \right) \right.$$

$$\left. + g_{k+p,\sigma}(\omega_2) \left(-\frac{1}{\pi}\mathrm{Im}\langle\langle S_q^z | S_{-q}^z \rangle\rangle_{\omega_1} \right) \right) \qquad (77)$$

where

$$F^{\mathrm{e-m}}(\omega_1, \omega_2) = (1 + N(\omega_1) - f(\omega_2)).$$

And finally we shall find the similar expression for electron–phonon inelastic scattering contribution (75)

$$M_{k\sigma}^{\text{e-ph}}(\omega) = \sum_{q\nu} |V_\nu(\mathbf{p} - \mathbf{q}, \mathbf{p})^2 \int \frac{d\omega_1 d\omega_2}{\omega - \omega_1 - \omega_2} F^{\text{e-ph}}(\omega_1, \omega_2)$$

$$\times \, g_{p-q,\sigma}(\omega_1) \left(-\frac{1}{\pi} \text{Im} \langle\langle Q_{q\nu} | Q_{q\nu}^+ \rangle\rangle_{\omega_2} \right), \tag{78}$$

where

$$F^{\text{e-ph}}(\omega_1, \omega_2) = 1 + N(\omega_2) - f(\omega_1). $$

Equations (70) and (76)–(78) form a closed self-consistent system of equations for one-fermion GF of the carriers for a generalized spin-fermion model. To find explicit expressions for the mass operator (72) we choose for the first iteration step in (76)–(78) the following trial approximation

$$g_{k\sigma}(\omega) = \delta(\omega - \epsilon^0(k\sigma)). \tag{79}$$

Then we find

$$M_{k\sigma}^{\text{e-e}}(\omega) = \frac{U^2}{N^2} \sum_{pq} \frac{f_{p+q\sigma}(1 - f_{k+p\sigma} - f_{q-\sigma}) + f_{k+p\sigma} f_{q-\sigma}}{\omega + \epsilon^0(q, -\sigma) - \epsilon^0(p+q, \sigma) - \epsilon^0(k+p\sigma)}. \tag{80}$$

For the initial trial approximation for the spin GF we take the expression (46) in the following form

$$-\frac{1}{\pi} \text{Im} \langle\langle S_q^\sigma | S_{-q}^{-\sigma} \rangle\rangle \approx z_\sigma (2N^{-1/2} \langle S_0^z \rangle) \delta(\omega - z_\sigma E(q)). \tag{81}$$

We obtain[5]

$$M_{k\uparrow}^{\text{e-m}}(\omega) = \frac{2J^2 \langle S_0^z \rangle}{N^{3/2}} \sum_q \frac{f_{k+q,\downarrow} + N(E(q))}{\omega - \epsilon^0(k+q, \downarrow) - E(q)};$$

$$\tag{82}$$

$$M_{k\downarrow}^{\text{e-m}}(\omega) = \frac{2J^2 \langle S_0^z \rangle}{N^{3/2}} \sum_q \frac{1 - f_{k-q,\uparrow} + N(E(q))}{\omega - \epsilon^0(k-q, \uparrow) - E(q)}. $$

This result is written for the low temperature region, when one can drop the contributions from the dymamics of longitudinal (zz) GF which is essential at high temperatures and in some special cases.

In order to calculate the electron–phonon term (78) we need to take as initial approximation the expressions (49) and (79). We then get

$$M_{k\sigma}^{\text{e-ph}}(\omega) = \sum_{q\nu} \frac{|V_\nu(\mathbf{p} - \mathbf{q}, \mathbf{p})|^2}{2\omega(q\nu)} \left(\frac{1 - f_{k-q,\sigma} + N(\omega(q\nu))}{\omega - \epsilon^0(k-q, \uparrow) - \omega(q\nu)} \right.$$

$$\left. + \frac{f_{k-q,\sigma} + N(\omega(q\nu))}{\omega - \epsilon^0(k-q, \uparrow) + \omega(q\nu)} \right) \tag{83}$$

where

$$|V_\nu(\mathbf{p} - \mathbf{q}, \mathbf{p})|^2 = \sum_\alpha \frac{4q^0 t^2}{NM} (\sin \mathbf{a}_\alpha \cdot \mathbf{p} - \sin \mathbf{a}_\alpha \cdot (\mathbf{p} - \mathbf{q}))^2 |e_\nu^\alpha(\mathbf{q})|^2. \tag{84}$$

Then analysis of the electron–phonon term can be done as in Ref. 28.

For the fully self-consistent solution of the problem the phonon GF can be easily calculated too. The final result is

$$\langle\langle Q_{k\nu}|Q_{k\nu}^{+}\rangle\rangle = (\omega^2 - \omega^2(k\nu) - \Pi_{k\nu}(\omega))^{-1}\,, \tag{85}$$

where the polarization operator Π has the form

$$\Pi_{k\nu}(\omega) = \sum_{q\sigma} |V_\nu(\mathbf{q}-\mathbf{k},\mathbf{q})|^2 \frac{f_{q-k,\sigma} - f_{q\sigma}}{\omega + \epsilon^0(q-k,\sigma) - \epsilon^0(q\sigma)}\,. \tag{86}$$

The above expressions were derived in the self-consistent way for the generalized spin-fermion model and for finite temperatures.

It is important to note that to investigate the spin and charge dynamics in doped manganite perovskites the scheme described above should be modified to take into account the strong Hund rule coupling in these systems but it deserve of separate consideration. In the present paper to show clearly the advantage of the IGF approach we shall consider another interesting example, the dynamics of carriers for the Kondo–Heisenberg model.

4. Dynamics of Carriers in the Spin-Fermion Model

4.1. *Hole dynamics in cuprates*

To show the specific behaviour of the carriers in the framework of spin-fermion model we shall consider a dynamics of holes in HTSC cuprates. A vast amount of theoretical searches for the relevant mechanism of high temperature superconductivity deals with the strongly correlated electron models.[12] Much attention has been devoted to the formulation of successful theory of the electrons (or holes) propagation in the CuO_2 planes in copper oxides. In particular, much efforts have been done to describe self-consistently the hole propagation in the doped two-dimensional quantum antiferromagnet.[34–47] The understanding of the true nature of the electronic states in HTSC are one of the central topics of the current experimental and theoretical efforts in the field.[12,40] Theoretical description of strongly correlated fermions on two-dimensional lattices and the hole propagation in the antiferromagnetic background still remains controversial. The role of quantum spin fluctuations was found to be quite crucial for the hole propagation. The essence of the problem is in the inherent interaction (and coexistence) between charge and spin degrees of freedom which are coupled in a self-consistent way. The propagating hole perturbs the antiferromagnetic background and move then together with the distorted underlying region. There were many attempts to describe adequately this motion. However, a definite proof of the fully adequate mechanism for the coherent propagation of the hole is still lacking. In this paper we will analyse the physics of the doped systems and the true nature of carriers in the two-dimensional antiferromagnetic background from the many-body theory point of view. The dynamics of the charge degrees of freedom for the CuO_2 planes in copper oxides will be described in the

framework of the spin-fermion (Kondo–Heisenberg) model,[9,38] using the approach described in Sec. 3.

4.2. *Hubbard model and t–J model*

Before investigating the Kondo–Heisenberg model it is instructive to consider the t–J model very briefly. The t–J model is a special development of the spin-fermion model approach which reflect the specific of strongly correlated systems. To remind this let us consider first the Hubbard model.[31]

The model Hamiltonian which is usually refered as to Hubbard Hamiltonian is given by

$$H = \sum_{ij\sigma} t_{ij} a_{i\sigma}^+ a_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} \,. \tag{87}$$

For the strong coupling limit, when Coulomb integral $U \rangle W$, where W is the effective bandwidth, the Hubbard Hamiltonian is reduced in the low-energy sector to t–J model Hamiltonian of the form

$$H = \sum_{ij\sigma} (t_{ij}(1 - n_{i-\sigma}) a_{i\sigma}^+ a_{j\sigma}(1 - n_{j-\sigma}) + \text{H.c.}) + J \sum_{ij} S_i S_j \,. \tag{88}$$

This Hamiltonian play an important role in the theory of HTSC. Let us consider the carrier motion. The hopping at half-filling is impossible and this model describe the planar Heisenberg antiferromagnet. The most interesting problem is the behaviour of this system when the doped holes are added. In the t–J model ($U \to \infty$) doped holes can move only in the projected space, without producing doubly occupied configurations ($\langle n_\uparrow \rangle + \langle n_\downarrow \rangle \leq 1$). There is then a strong competition between the kinetic energy of the doped carriers and the magnetic order present in the system. According to Ref. 37, it is possible to rewrite first term in (88) in the following form

$$H_t = t \sum_{\langle ij \rangle} (a_{i\uparrow}^+ S_i^- S_j^+ a_{j\uparrow} + a_{i\downarrow}^+ S_i^+ S_j^- a_{j\downarrow} + \text{H.c.}) \,. \tag{89}$$

This form show clearly the nature hole-spin correlated motion over antiferromagnetic background. It is follows from (89) that to describe in a self-consistent way a correlated motion of a carrier one need to consider the following matrix GF:

$$G(i,j) = \begin{pmatrix} \langle\langle a_{i\uparrow} | a_{i\uparrow}^+ \rangle\rangle & \langle\langle a_{i\uparrow} | a_{j\downarrow}^+ \rangle\rangle & \langle\langle a_{i\uparrow} | S_j^+ \rangle\rangle & \langle\langle a_{i\uparrow} | S_j^- \rangle\rangle \\ \langle\langle a_{i\downarrow} | a_{j\uparrow}^+ \rangle\rangle & \langle\langle a_{i\downarrow} | a_{j\downarrow}^+ \rangle\rangle & \langle\langle a_{i\downarrow} | S_j^+ \rangle\rangle & \langle\langle a_{i\downarrow} | S_j^- \rangle\rangle \\ \langle\langle S_i^- | a_{j\uparrow}^+ \rangle\rangle & \langle\langle S_i^- | a_{j\downarrow}^+ \rangle\rangle & \langle\langle S_i^- | S_j^+ \rangle\rangle & \langle\langle S_i^- | S_j^- \rangle\rangle \\ \langle\langle S_i^+ | a_{j\uparrow}^+ \rangle\rangle & \langle\langle S_i^+ | a_{j\downarrow}^+ \rangle\rangle & \langle\langle S_i^+ | S_j^+ \rangle\rangle & \langle\langle S_i^+ | S_j^- \rangle\rangle \end{pmatrix} \,. \tag{90}$$

It may be shown after straightforward but tediuos manipulations by using IGF method of Sec. 2 that the equation of motion (2) for the GF (90) can be rewritten as a Dyson Eq. (10)

$$G(i,j;\omega) = G_0(i,j;\omega) + \sum_{mn} G_0(i,m;\omega)M(m,n;\omega)G(n,j;\omega)\,. \tag{91}$$

The algebraic structure of the full GF in (91) which follows from (11) is rather complicated. For clarity, we illustrate some features by means of simplified problem.

4.3. *Hole spectrum of t–J model*

It is well known[40,47] how to write down the special ansatz for fermionic operator as a composite operator of dressed hole operator and spin operator for the case $J\rangle t$. The hole operator h_i corresponding to fermion operator $a_{i\sigma}^+$ on the spin-up sublattice using the ansatz $a_{i\uparrow}^+ = h_i S_i^-$ and similarly for spin-down sublattice have been introduced (for a recent discussion see e.g. Ref. 47). Then the Hamiltonian (89) obtain the form

$$H_t = t \sum_{ij} I_{ij} h_j^+ h_i (b_i^+ + b_j)\,. \tag{92}$$

Here b_i and b_j^+ are the boson operators, which results from the Holstein–Primakoff transformation of spins into bosons. Equation (92) is not convenient form because of its non-diagonal structure. Caution should be exercised because the new vacuum is a distorted Neel vacuum.

The equation of motion (2) and (3) for the hole GF can be written in the following form

$$\omega\langle\langle h_j|h_k^+\rangle\rangle - t\sum_n I_{jn}\langle B_{nj}\rangle\langle\langle h_n|h_k^+\rangle\rangle = \delta_{jk} + t\sum_n I_{jn}(^{\mathrm{ir}}\langle\langle h_n B_{nj}|h_k^+\rangle\rangle)\,. \tag{93}$$

Here $B_{nj} = (b_n^+ + b_j)$. The "mean-field" GF (6) is defined by

$$\sum_i (\omega\delta_{ij} - tI_{ij}\langle B_{ji}\rangle)G_0(i,k;\omega) = \delta_{jk}\,. \tag{94}$$

Note, that "spin distortion" $\langle B_{mn}\rangle$ does not depend on $(R_m - R_n)$. Then the Dyson Eq. (91) becomes

$$G(g,k) = G_0(g,k) + \sum_{jl} G_0(g,j)M(j,l)G(l,k)\,, \tag{95}$$

where self-energy operator is given by

$$M(j,l) = t^2 \sum_{mn} I_{jn}(^{\mathrm{ir}}\langle\langle h_n B_{nj}|h_m^+ B_{lm}\rangle\rangle^{\mathrm{ir}})I_{ml}\,. \tag{96}$$

The standard IGF-method's prescriptions for the approximate calculation of the self-energy (c.f. Sec. 3.4), can be written in the form

$$M(j, l; \omega) = t^2 \sum_{mn} I_{jn} I_{ml} \int_{-\infty}^{+\infty} d\omega_1 d\omega_2 \frac{1 + N(\omega_1) - f(\omega_2)}{\omega - \omega_1 - \omega_2}$$

$$\times \left(\frac{1}{\pi} \mathrm{Im} \langle\langle B_{nj} | B_{lm} \rangle\rangle_{\omega_1} \right) \left(\frac{1}{\pi} \mathrm{Im}\, G(n, m; \omega_2) \right) . \tag{97}$$

It is worthy to note that the "mass" operator (97) is proportional to t^2. The standard iterative self-consistent procedure of IGF approach for the calculation of mass operator encounter the need of choosing as a first iteration "trial" solution the non-diagonal initial spectral function Im G_0; in another words, there are no reasonable "zero-order" approximation for dynamical behaviour. The initial hole GF in paper[36] was defined as

$$G_0(j, k; \omega) = \frac{\delta_{jk}}{\omega + i\epsilon} , \tag{98}$$

which corresponds to static hole, without dispersion. In contrast, the approximation for the magnon GF yield the momentum distribution of a free magnon gas. After integration in (97), the mass operator is given by an expression quite similar to the one encountered in Ref. 35 where the Bogolubov-de Gennes equations has been derived. It can be checked that the present set of Eqs. (95)–(97) gives the finite temperature generalisation of the results.[36] As we just mentioned, one of its main merits is that it enables one to see clearly the "composite" nature of the hole states in an antiferromagnetic background, but in the quasi-static limit. The recent analysis[45,47] show that the difficulties of the consistent description of the coherent hole motion within t–J model are rather intrinsic properties of the model and of the very complicated many-body effects. From this point of view it will be instructive to reanalyse the less complicated model Hamiltonian, in spite of the fact that its applicability has been determined as the less reliable.

4.4. *Kondo–Heisenberg Model*

As far as the CuO_2-planes in the copper oxides are concerned, it was argued[9,38] that a relatively reasonable workable model with which one can discuss the dynamical properties of charge and spin subsystems is the spin-fermion (or Kondo–Heisenberg) model.[9] This model allows for motion of doped holes and results from d–p model Hamiltonian. We consider the interacting hole-spin model for a copper-oxide planar system described by the Hamiltonian

$$H = H_t + H_K + H_J , \tag{99}$$

where H_t is the doped hole Hamiltonian

$$H_t = - \sum_{\langle ij \rangle \sigma} (t a_{i\sigma}^+ a_{j\sigma} + \mathrm{H.c.}) = \sum_{k\sigma} \epsilon(k) a_{k\sigma}^+ a_{k\sigma} \tag{100}$$

where $a_{i\sigma}^+$ and $a_{i\sigma}$ are the creation and annihilation second quantized fermion operators, respectively for itinerant carriers with energy spectrum

$$\epsilon(q) = -4t \cos\left(\frac{1}{2q_x}\right) \cos\left(\frac{1}{2q_y}\right) = t\gamma_1(q) \,. \tag{101}$$

The term H_J in (99) denotes Heisenberg superexchange Hamiltonian

$$H_J = \sum_{\langle mn \rangle} J \mathbf{S}_m \cdot \mathbf{S}_n = \frac{1}{2N} \sum_q J(q) \mathbf{S}_q \cdot \mathbf{S}_{-q} \,. \tag{102}$$

Here $\mathbf{S}_n$ is the operator for a spin at copper site $\mathbf{r}_n$ and J is the n.n. superexchange interaction

$$J(q) = 2J[\cos(q_x) + \cos(q_y)] = J\gamma_2(q) \,. \tag{103}$$

Finally, the hole-spin (Kondo type) interaction H_K may be written as (for one doped hole)

$$H_K = \sum_i K \boldsymbol{\sigma}_i \cdot \mathbf{S}_i = N^{-1/2} \sum_{kq} \sum_\sigma K(q)[S_{-q}^{-\sigma} a_{k\sigma}^+ a_{k+q-\sigma} + z_\sigma S_{-q}^z a_{k\sigma}^+ a_{k+q\sigma}] \,. \tag{104}$$

This part of the Hamiltonian was written as the sum of a dynamic (or spin-flip) part and a static one. Here K is hole-spin interaction energy

$$K(q) = K\left[\cos\left(\frac{1}{2}q_x\right) + \cos\left(\frac{1}{2}q_y\right)\right] = K\gamma_3(q) \,. \tag{105}$$

We start in this paper with the one doped hole model (99), which is considered to have captured the essential physics of the multi-band strongly correlated Hubbard model in the most interesting parameters regime $t > J, |K|$. We apply the IGF method to this two-dimensional variant of the spin-fermion model. It will be shown that we are able to give a much more detailed and self-consistent description of the fermion and spin excitation spectra than in papers Refs. 10 and 11, including the damping effects and finite lifetimes.

For a recent discussion of the one-dimensional Kondo–Heisenberg model and the classification of the ground-state phases of this model in the context of a fixed-point strategy see Ref. 48.

4.5. *Hole dynamics in the Kondo–Heisenberg model*

The two-time thermodynamic GFs to be studied here are given by

$$G(k\sigma, t - t') = \langle a_{k\sigma}(t), a_{k\sigma}^+(t') \rangle = -i\theta(t - t')\langle [a_{k\sigma}(t), a_{k\sigma}^+(t')]_+ \rangle \,, \tag{106}$$

$$\chi^{+-}(mn, t - t') = \langle S_m^+(t), S_n^-(t') \rangle = -i\theta(t - t')\langle [S_m^+(t), S_n^-(t')]_- \rangle \,. \tag{107}$$

In order to evaluate the GFs (106) and (107) we need to use the suitable information about a ground state of the system. For the two-dimensional spin-1/2 quantum antiferromagnet in a square lattice the calculation of the exact ground state is a very

difficult problem. In this paper we assume the two-sublattice Neel ground state. To justify this choice one can suppose that there are well developed short-range order (c.f. Ref. 49) or there are weak interlayer exchange interaction which stabilize this antiferromagnetic order. According to Neel model, the spin Hamiltonian (102) may be expressed as[19,32]

$$H_J = \sum_{\langle mn \rangle} \sum_{\alpha, \beta} J^{\alpha\beta} \mathbf{S}_{m\alpha} \cdot \mathbf{S}_{n\beta} \,. \tag{108}$$

Here $(\alpha, \beta) = (a, b)$ are the sublattice indices.

To calculate the electronic states induced by hole-doping in the spin-fermion model approach we need to calculate the energies of a hole introduced in the Neel antiferromagnet. To be consistent with (108) and (90) we define the single-particle fermion GF as

$$G(k\sigma, \omega) = \begin{pmatrix} \langle\langle a_a(k\sigma)|a_a^+(k\sigma)\rangle\rangle & \langle\langle a_a(k\sigma)|a_b^+(k\sigma)\rangle\rangle \\ \langle\langle a_b(k\sigma)|a_a^+(k\sigma)\rangle\rangle & \langle\langle a_b(k\sigma)|a_b^+(k\sigma)\rangle\rangle \end{pmatrix} \,. \tag{109}$$

Note, that the same fermion operators $a_\alpha(i\sigma)$, annihilates a fermion with spin σ on the (α)-sublattice in the ith unit cell has been used in paper Ref. 10. The equation of motion for the elements of GF (109) are written as

$$\sum_\gamma (\omega \delta_{\alpha\gamma} - \epsilon^{\alpha\beta}(k)) \langle\langle a_\gamma(k\sigma)|a_\beta^+(k\sigma)\rangle\rangle = \delta_{\alpha\beta} - \langle\langle A(k\sigma, \alpha)|a_\beta^+\rangle\rangle \,, \tag{110}$$

where

$$A(k\sigma, \alpha) = N^{-1/2} \sum_p K(p)(S_{-p\alpha}^{-\sigma} a_\alpha(k + p - \sigma) + z_\sigma S_{-p\alpha}^z a_\alpha(k + p\sigma)) \,. \tag{111}$$

We make use of the IGF approach (see Sec. 2) to threat the equation of motion (110). It may be shown that Eq. (110) can be rewritten as the Dyson Eq. (10)

$$G(k\sigma, \omega) = G_0(k\sigma, \omega) + G_0(k\sigma, \omega)M(k\sigma, \omega)G(k\sigma, \omega) \,. \tag{112}$$

Here $G_0(k\sigma, \omega) = \Omega^{-1}$ describes the behaviour of the electronic subsystem in the Generalized Mean-Field (GMF) approximation. The Ω matrix have the form

$$\Omega(k\sigma, \omega) = \begin{pmatrix} \omega - \epsilon_a(k\sigma) & -\epsilon^{ab}(k) \\ -\epsilon^{ba}(k) & \omega - \epsilon_b(k\sigma) \end{pmatrix} \,, \tag{113}$$

where

$$\epsilon_\alpha(k\sigma) = \epsilon^{\alpha\alpha}(k) - z_\sigma N^{-1/2} \sum_p K(p)\langle S_{p\alpha}^z \rangle \delta_{p,0} = \epsilon^{\alpha\alpha}(k) - z_\sigma K S_z \,,$$

$$S_z = N^{-1/2}\langle S_{0\alpha}^z \rangle \,, \tag{114}$$

is the renormalized band energy of the holes.

The elements of the matrix GF $G_0(k\sigma, \omega)$ are found to be

$$G_0^{aa}(k\sigma, \omega) = \frac{u^2(k\sigma)}{\omega - \epsilon_+(k\sigma)} + \frac{v^2(k\sigma)}{\omega - \epsilon_-(k\sigma)}, \tag{115}$$

$$G_0^{ab}(k\sigma, \omega) = \frac{u(k\sigma)v(k\sigma)}{\omega - \epsilon_+(k\sigma)} - \frac{u(k\sigma)v(k\sigma)}{\omega - \epsilon_-(k\sigma)} = G_0^{ba}(k\sigma, \omega), \tag{116}$$

$$G_0^{bb}(k\sigma, \omega) = \frac{v^2(k\sigma)}{\omega - \epsilon_+(k\sigma)} + \frac{u^2(k\sigma)}{\omega - \epsilon_-(k\sigma)}, \tag{117}$$

where

$$u^2(k\sigma) = \frac{1}{2}\left[1 - z_\sigma \frac{KS_z}{R(k)}\right]; \qquad v^2(k\sigma) = \frac{1}{2}\left[1 + z_\sigma \frac{KS_z}{R(k)}\right]; \tag{118}$$

$$\epsilon_\pm(k\sigma) = \pm R(k) = (\epsilon^{ab}(k)^2 + K^2 S_z^2)^{1/2}, \tag{119}$$

the simplest assumption is that each sublattice is s.c. and $\epsilon^{\alpha\alpha}(k) = 0(\alpha = a, b)$. In spite that we have worked in the GFs formalism, our expressions (115)–(117) are in accordance with the results of the Bogolubov (u, v)-transformation for fermions, but, of course, the present derivation is more general.

The mass operator M in Dyson Eq. (112), which describes hole-magnon scattering processes, is given by as a "proper" part of the irreducible matrix GF of higher order

$$M(k\sigma, \omega)$$
$$= \begin{pmatrix} {}^{(ir)}\langle\langle A(k\sigma, a)|A^+(k\sigma, a)\rangle\rangle^{(ir)} & {}^{(ir)}\langle\langle A(k\sigma, a)|A^+(k\sigma, b)\rangle\rangle^{(ir)} \\ {}^{(ir)}\langle\langle A(k\sigma, b)|A^+(k\sigma, a)\rangle\rangle^{(ir)} & {}^{(ir)}\langle\langle A(k\sigma, b)|A^+(k\sigma, b)\rangle\rangle^{(ir)} \end{pmatrix}. \tag{120}$$

To find the renormalization of the spectra $\epsilon_\pm(k\sigma)$ and the damping of the quasiparticles it is necessary to determine the self-energy for each type of excitations. From the formal solution (11) one immediately obtain

$$G_\pm(k\sigma) = (\omega - \epsilon_\pm(k\sigma) - \Sigma^\pm(k\sigma, \omega))^{-1}. \tag{121}$$

Here the self-energy operator is given by

$$\Sigma^\pm(k\sigma, \omega) = A^\pm M^{aa} \pm A_1(M^{ab} + M^{ba}) + A^\mp M^{bb}, \tag{122}$$

where

$$A^\pm = \begin{pmatrix} u^2(k\sigma) \\ v^2(k\sigma) \end{pmatrix},$$

$$A_1 = u(k\sigma)v(k\sigma).$$

Equations (121) determines the quasiparticle spectrum with damping ($\omega = E - i\Gamma$) for the hole in the AFM background. Contrary to the calculations of the hole GF

in Sec. 4.3, the self-energy (122) is proportional to K^2 but not t^2 (c.f. Eq. (97))

$$M^{\alpha\beta}(k\sigma, \omega) = N^{-1}K^2 \sum_q \int_{-\infty}^{+\infty} d\omega_1 d\omega_2 \frac{1 + N(\omega_1) - f(\omega_2)}{\omega - \omega_1 - \omega_2}$$

$$\times (F_{\alpha\beta}^{\sigma, -\sigma}(q, \omega_1) g_{\alpha\beta}(k + q - \sigma, \omega_2) + F_{\alpha\beta}^{zz}(q, \omega_1) g_{\alpha\beta}(k + q, \omega_2)).$$

$$(123)$$

Here functions $N(\omega)$ and $f(\omega)$ are Bose and Fermi distributions, respectively and the following notations have been used for spectral intensities

$$F_{\alpha\beta}^{ij}(q, \omega) = -\frac{1}{\pi} \text{Im} \langle\langle S_{q\alpha}^i | S_{-q\beta}^j \rangle\rangle_\omega$$

$$g_{\alpha\beta}(k\sigma, \omega) = -\frac{1}{\pi} \text{Im} \langle\langle a_\alpha(k\sigma) | a_\beta^+(k\sigma) \rangle\rangle_\omega \, ; \qquad i, j = (+, -, z) \, .$$

$$(124)$$

The Eqs. (123) and (112) forms the self-consistent set of equations for the determining of the GF (109). Coupled Eqs. (123) and (112) can be solved analytically by suitable iteration procedure. In principle, we can use, in the right-hand side of (123) any workable first iteration step for of the relevant GFs and find a solution by repeated iteration.

4.6. *Dynamics of spin subsystem*

It will be useful to discuss briefly the dynamics of spin subsystem of the Kondo–Heisenberg model. When calculating the spin wave spectrum of this model we shall use the approach of Ref. 19 where the quasiparticle dynamics of the two-sublattice Heisenberg antiferromagnet has been studied within IGF method. The contribution of the conduction electrons to the energy and damping of the acoustic magnons in the antiferromagnetic semiconductors within IGF scheme have been considered in Refs. 32 and 33. The main advantage of the approach of paper[19] was the using of concept of "anomalous averages" (c.f. Ref. 25) fixing the relevant (Neel) vacuum and providing a possibility to determine properly the generalized mean fields. The functional structure of required GF has the following matrix form

$$\begin{pmatrix} \langle\langle S_{ka}^+ | S_{-ka}^- \rangle\rangle & \langle\langle S_{ka}^+ | S_{-kb}^- \rangle\rangle \\ \langle\langle S_{kb}^+ | S_{-ka}^- \rangle\rangle & \langle\langle S_{kb}^+ | S_{-kb}^- \rangle\rangle \end{pmatrix} = \hat{\chi}(k; \omega) \, . \qquad (125)$$

Here the spin operators $S_{ka(b)}^\pm$ refer to the two sublattices (a, b).

The equation of motion for GF (125) after introducing the irreducible parts has the form[33]

$$\sum_\gamma ((\omega + \omega_0^\alpha)\delta_{\alpha\gamma} - \omega_k^{\gamma\alpha}(1 - \delta_{\alpha\gamma}))\langle\langle S_{k\gamma}^+ | B \rangle\rangle_\omega$$

$$+ \frac{K}{N^{1/2}} \langle S_\alpha^z \rangle \langle\langle \sigma_k^+ | B \rangle\rangle_\omega = \langle [S_{k\alpha}^+, B] \rangle + \langle\langle C_{k\alpha}^{\text{ir}} | B \rangle\rangle_\omega \, , \qquad (126)$$

where the following notations have been used

$$B = \begin{Bmatrix} S^-_{-ka} \\ S^-_{-kb} \end{Bmatrix}, \qquad \alpha = (a, b),$$

$$\omega^a_0 = 2\left(\langle S^z_b \rangle J_0 + N^{-1/2} \sum_q J_q A^{ab}_q \right) = -\omega^b_0;$$

$$\omega^{ba}_k = 2\left(\langle S^z_b \rangle J_k + N^{-1/2} \sum_q J_{k-q} A^{ba}_q \right) = -\omega^{ab}_k;$$

$$A^{ab}_q = \frac{2\langle (S^z_{-qa})^{\mathrm{ir}} (S^z_{qb})^{\mathrm{ir}} \rangle}{2N^{1/2} \langle S^z_a \rangle}.$$

(127)

The construction of the irreducible GF $\langle\langle C^{\mathrm{ir}}_{k\alpha} | B \rangle\rangle$ is related with the operators

$$C^{\mathrm{ir}}_{k\alpha} = A^{\mathrm{ir}}_{k\alpha} + B^{\mathrm{ir}}_{k\alpha},$$

$$A^{\mathrm{ir}}_{ka} = \frac{2}{N^{1/2}} \sum_q J_q [S^+_{qb}(S^z_{k-qa})^{\mathrm{ir}} - S^+_{k-qa}(S^z_{qb})^{\mathrm{ir}}]^{\mathrm{ir}},$$

(128)

$$B^{\mathrm{ir}}_{ka} = -\frac{K}{N^{1/2}} \sum_{pq} (S^z_{k-qa})^{\mathrm{ir}} a^+_{p\uparrow} a_{p+q\downarrow} + \frac{K}{2N} \sum_{pq\sigma} z_\sigma S^+_{k-qa} (a^+_{p\sigma} a_{p+q\sigma})^{\mathrm{ir}}.$$

With the aid of (24) and (25) the equation of motion for the mixed GF can be written as

$$\langle\langle \sigma^+_k | B \rangle\rangle = \frac{K N^{1/2}}{2} \chi^{df}_0(k, \omega) \sum_\gamma \langle\langle S^+_{k\gamma} | B \rangle\rangle + \frac{K}{2N^{1/2}} \sum_p \frac{1}{\omega_{p,k}} \langle\langle (D^\gamma_{pk})^{\mathrm{ir}} | B \rangle\rangle. \quad (129)$$

Combining the equations of motion (126) and (129) we find

$$\hat{\Omega}_s \hat{\chi}(k\omega) = \hat{I} + \hat{D}_1, \tag{130}$$

where

$$\hat{\Omega}_s = \begin{pmatrix} \omega + \omega_0 + (K^2 S_z/2)\chi^{df}_0 & \gamma_2(k)\omega_0 + (K^2 S_z/2)\chi^{df}_0 \\ -(\gamma_2(k)\omega_0 + (K^2 S_z/2\chi^{df}_0) & \omega - \omega_0 - (K^2 S_z/2)\chi^{df}_0) \end{pmatrix},$$

$$\hat{I} = \begin{pmatrix} 2S_z & 0 \\ 0 & -2S_z \end{pmatrix}.$$

(131)

Then Eq. (130) can be transformed exactly into the Dyson equation for the spin subsystem

$$\hat{\chi}(k\omega) = \hat{\chi}^0(k\omega) + \hat{\chi}^0(k\omega)\hat{M}^s(k\omega)\hat{\chi}(k\omega). \tag{132}$$

Here

$$\hat{\chi}^0(k\omega) = \hat{\Omega}^{-1}_s \hat{I}. \tag{133}$$

The mass operator of the spin excitations is given by the expression

$$\hat{M}^{\mathrm{s}}(k\omega) = \frac{1}{4S_z^2} \begin{pmatrix} \langle\langle C_{ka}^{\mathrm{ir}} | (C_{ka}^{+})^{\mathrm{ir}} \rangle\rangle & \langle\langle C_{ka}^{\mathrm{ir}} | (C_{kb}^{+})^{\mathrm{ir}} \rangle\rangle \\ \langle\langle C_{kb}^{\mathrm{ir}} | (C_{ka}^{+})^{\mathrm{ir}} \rangle\rangle & \langle\langle C_{kb}^{\mathrm{ir}} | (C_{kb}^{+})^{\mathrm{ir}} \rangle\rangle \end{pmatrix} . \tag{134}$$

We are interesting here in the calculation of the spin excitation spectrum in the generalized mean field approximation. This spectrum is given by the poles of the GF $\hat{\chi}^0$

$$\det \Omega_s(k\omega) = 0 . \tag{135}$$

Depending of the interrelation of the parameters this spectra have different forms. For the standard condition $2t\rangle KS_z$ we obtain for the magnon energy[33]

$$\omega_k^{\pm} = \pm\omega_k = \pm \left[\omega_0 \sqrt{1 - \gamma_2(k)^2} \mp \frac{K^2 S_z}{2} \chi_0^{df}(k, \omega_k) \sqrt{\frac{1 - \gamma_2(k)}{1 + \gamma_2(k)}} \right] . \tag{136}$$

The acoustic magnon dispersion law for the $k \to 0$ is given by

$$\omega_{\mathbf{k}}^{\pm} = \pm\tilde{D}(T)|\mathbf{k}| , \tag{137}$$

where the stiffness constant[33]

$$\tilde{D}(T) = zJS_z \left[1 - \frac{1}{\sqrt{N}S_z} \sum_q \gamma_2(\mathbf{q}) A_q^{ab} \right] - \frac{K^2 S_z}{4N} \lim_{k \to 0} \chi_0^{df}(k, \omega_k) . \tag{138}$$

The detailed consideration of the spin quasiparticle damping will be done in separate publication. Here we now proceed with calculating the damping of the hole quasiparticles.

4.7. *Damping of hole quasiparticles*

It is most convenient to choose as the first iteration step in (123) the simplest two-pole expressions, corresponding to the GF structure for a mean field, in the following form

$$g_{\alpha\beta}(k\sigma, \omega) = Z_+ \delta(\omega - t_+(k\sigma)) + Z_- \delta(\omega - t_-(k\sigma)) , \tag{139}$$

where $Z_{\pm}$ are the certain coefficients depending on $u(k\sigma)$ and $v(k\sigma)$. The magnetic excitation spectrum corresponds to the frequency poles of the GFs (107). Using the results of Sec. 4.5 on spin dynamics of the present model, we shall content ourselves here with the simplest initial approximation for the spin GF occuring in (123)

$$\frac{1}{2z_\sigma S_z} F_{\alpha\beta}^{\sigma-\sigma}(q, \omega) = L_+ \delta(\omega - z_\sigma \omega_q) - L_- \delta(\omega + z_\sigma \omega_q) . \tag{140}$$

Here ω_q is the energy of the antiferromagnetic magnons (136) and $L_{\pm}$ are the certain coefficients (see Ref. 19). We are now in a position to find an explicit solution of coupled equations obtained so far. This is achieved by using (139) and (140) in the

right- hand-side of (123). Then the hole self-energy in two-dimensional quantum antiferromagnet for the low-energy quasiparticle band $t_-(k\sigma)$ is

$$\Sigma^-(k\sigma, \omega)$$

$$= \frac{K^2 S_z}{2N} \sum_q Y_1^2 \left[\frac{1 + N(\omega_q) - f(t_-(k-q))}{\omega - \omega_q - t_-(k-q)} + \frac{N(\omega) + f(t_-(k+q))}{\omega + \omega_q - t_-(k+q)} \right]$$

$$+ \frac{2K^2 S_z^2}{N} \sum_{qp} Y_2^2 \frac{N(\omega_{q+p})[1 + N(\omega_q)] + f(t_-(k+p))[N(\omega_q) - N(\omega_{q+p})]}{\omega + \omega_{q+p} - \omega_q - t_-(k+p)} \,.$$

$$(141)$$

Here we have used the notations

$$Y_1^2 = (U_q + V_q)^2 \,; \qquad Y_2^2 = (U_q U_{q+p} - V_q V_{q+p})^2 \,,$$

where the coefficients U_q and V_q appears as a results of explicit calculation of the mean-field magnon GF.[19,33]

A remarkable feature of this result is that our expression (141) accounts for the hole-magnon inelastic scattering processes with the participation of one or two magnons.

The self-energy representation in a self-consistent form (123) provide a possibility to model the relevant spin dynamics by selecting spin-diagonal or spin-off-diagonal coupling as a dominating or having different characteristic frequency scales. As a workable pattern, we consider now the static trial approximation for the correlation functions of the magnon subsystem[19] in the expression (123). Then the following expression is readily obtained

$$M_{\alpha\beta}^{\rm s}(k\sigma, \omega) = \frac{K^2}{N} \sum_q \int_{-\infty}^{+\infty} \frac{d\omega'}{\omega - \omega'} [\langle S_{-q\beta}^{-\sigma} S_{q\alpha}^{\sigma} \rangle g_{\alpha\beta}(k + q - \sigma, \omega')$$

$$+ \langle (S_{-q\beta}^z)^{\rm ir} (S_{q\alpha}^z)^{\rm ir} \rangle g_{\alpha\beta}(k + q\sigma, \omega')] \,. \qquad (142)$$

Taking into account (141) we find the following approximative form

$$\Sigma^-(k\sigma, \omega) \approx \frac{K^2}{2N} \sum_q \frac{\chi^{-+}(q) + \chi^{z,z}(q)}{\omega - t_-(k+q)} (1 - \gamma_3(q)) \,. \qquad (143)$$

It should be noted, however, that in order to make this kind of study valuable as one of the directions to studying the mechanism of HTSC the binding of quasiparticles must be taking into account. This very important problem deserves the separate consideration. In spite of formal analogy of the our model (99) with that of a Kondo lattice, the physics are different. There is a dense system of spins interacting with a smaller concentration of holes. This question is in close relation with the right definition of the magnon vacuum for the case when $K \neq 0$.

In this Section we has considered the simplest possibility, assuming that dispersion relation $\epsilon^{\alpha\alpha}(k) = 0$ ($\alpha = a, b$). In paper Ref. 41 a model of hole carriers in

an antiferromagnetic background has been discussed, which explains many specific properties of cuprates. The effect of strong correlations is contained in the dispersion relation of the holes. The main assumption is that the influence of antiferromagnetism and strong correlations is contained in the special dispersion relation, $\epsilon(k)$, which was obtained using a numerical method. The best fit corresponds to[41]

$$\epsilon(k) = -1.255 + 0.34 \cos k_x \cos k_y + 0.13(\cos 2k_x + \cos 2k_y). \qquad (144)$$

As a result, the main effective contribution to $\epsilon(k)$ arises from hole hopping between sites belonging to the same sublattice, to avoid distorting the antiferromagnetic background.

Our IGF method is essentially self-consistent, i.e. do not depends on the special initial form for the hole propagator. For the self-consistent calculation by iteration of the self-energy (123) we can take as the fist iteration step the expression (139) with the dispersion relation (144) or another suitable form. This must be done for the calculation mean-field GF (113) and dispersion relation (119) too.

To summarize, in Sec. 4 we have presented calculations for normal phase of HTSC, which are describable in terms of the spin-fermion model. We have characterized the true quasiparticle nature of the carriers and the role of magnetic correlations. It was shown that the physics of spin-fermion model can be understood in terms of competition between antiferromagnetic order on the CuO_2-plane preferred by superexchange J and the itinerant motion of carriers. In the light of this situation it is clearly of interest to explore in details how the hole motion influence the antiferromagnetic background. Considering that the carrier-doping results in the HTSC for the realistic parameters range $t \rangle J$, K, corresponding the situation in oxide superconductors, the careful examination of the collective behaviour of the carriers for a moderately doped system must be performed. It seems that this behaviour can be very different from that of single hole case. The problem of the coexistence of the suitable Fermi-surface of mobile fermions and the antiferromagnetic long range or short range order has to be clarified.

5. Conclusions

We have been concerned in this paper with establishing the essence of quasiparticle excitations of charge and spin degrees of freedom within a generalized spin-fermion model, rather than with their detailed properties. We have considered the generalized d–f model and Kondo–Heisenberg model as the most typical examples but the similar calculation can be performed for other analogous models. To summarize, we therefore reanalyzed within IGF approach the quasiparticle many body dynamics of the generalized spin-fermion model in a way which provides us with an effective and workable scheme for consideration of the quasiparticle spectra and their damping for the correlated systems with complex spectra. The calculated temperature behaviour of the damping of acoustical magnons (67) can be useful for analysis of the experimental results for heavy rare-earth metals like Gd.[1] The

present analysis of the two-dimensional Kondo–Heisenberg model complements the previous analytical[13] and numerical[38] studies, showing clearly the important role of the damping effects.

We have considered from a general point of view the family of solutions for itinerant lattice fermions and localized spins on a lattice, identifing the type of ordered states and then derived explicitly the functional of generalized mean fields and the 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 nontrivial character of coupled equations which occur there. The problem of the coexistence of HF and magnetism is extremely nontrivial[7,8] many-body problem and have no appropriate solution in spite that there are many experimental evidences of the competition and interplay of HF and antiferromagnetism.[8] Both these problems are subject of current but independent research.

Another development of the present approach is the consideration of the competition and interplay of itinerant and localized magnetism and antiferromagnetism of the doped manganite perovskites where the interrelation between parameters of the spin-fermion model is quite different and the new scheme of approximation should be invented. Especially, the situation, when Hund rule interaction is very large but finite should be carefully analysed. It would be interesting to understand on a deeper level the relationship between different possible phase states in manganites and various ordered magnetic states within the generalized spin-fermion model.

In conclusion, we have demonstrated that the Irreducible Green's Functions approach is a workable and efficient scheme for the consistent description of the quasiparticle dynamics of compicated many body models.

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