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Physica B 355 (2005) 318–340
PHYSICA B
www.elsevier.com/locate/physb

Role of correlation and exchange for quasiparticle spectra of magnetic and diluted magnetic semiconductors

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Received 16 September 2004; received in revised form 3 November 2004; accepted 4 November 2004

Abstract

Theoretical foundation and applications of the generalized spin-fermion (sp–d) exchange lattice model to various magnetic systems, e.g., rare-earth metals and compounds, and magnetic semiconductors are discussed. The capabilities of the model to describe spin quasiparticle spectra are investigated. The main emphasis is put on the dynamic behavior of two interacting subsystems, the localized spins and spin density of itinerant carriers. A nonperturbative many-body approach is used to describe the quasiparticle dynamics. Scattering states are investigated and three branches of magnetic excitations are calculated in the regime characteristic of a magnetic semiconductor. For a simplified version of the model (Kondo lattice model) we study the spectra of quasiparticle excitations with special attention given to diluted magnetic semiconductors in a simple approximation to demonstrate the role of disorder effects. For this, to include the effects of disorder, a modified mean field is determined self-consistently. The approach permits to investigate and clarify the role of various interactions and disorder effects in unified and coherent fashion.

PACS: 71.10.−w; 75.10.−b; 75.30.Ds; 75.50.Pp

Keywords: Quantum theory of magnetism; Spin-fermion model; Quasiparticle spectra; Spin waves

1. Introduction

The existence and properties of localized and itinerant magnetism in metals, oxides, and alloys, and their interplay is an interesting but not yet fully understood problem of quantum theory of magnetism [1–6]. The behavior and the true nature of the electronic and spin states, and their quasiparticle dynamics are of central importance to the understanding of physics of correlated systems such as magnetism and

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doi:10.1016/j.physb.2004.11.071

Mott–Hubbard metal–insulator transition in metals and oxides, magnetism and heavy fermions in rare-earth compounds, and anomalous transport properties in perovskite manganites [7,8]. This class of systems is characterized by complex, many-branch spectra of elementary excitations. Moreover, the correlation effects (competition and interplay of Coulomb correlation, direct or indirect exchange, sp–d hybridization, electron-phonon interaction, disorder, etc.) are essential [9]. These materials are systems of great interest both intrinsically and as a possible source of understanding the magnetism of matter generally [6]. Beginning with Zener [10–14], Ruderman and Kittel [15] de Gennes [16], and others [17–19], various formulations of spin-fermion model for interacting spin and charge subsystems have been studied. There has been considerable interest in identifying the microscopic origin of quasiparticle states [20] in these systems and a few model approaches have been proposed. Many magnetic and electronic properties of rare-earth metals and compounds [1,17], and magnetic semiconductors [20–23] and related materials may reasonably be interpreted in terms of combined spin-fermion models (SFM) which include interacting spin and charge subsystems [2,3,5,19,20]. This approach permits one to describe significant and interesting physics, e.g., bound states and magnetic polarons [24], anomalous transport properties, etc.

The problem of adequate physical description within various types of spin-fermion model [25–28] has intensively been studied during the last decades, especially in the context of magnetic and transport properties of rare-earth and transition metals and their compounds and magnetic semiconductors [20,29,30]. Substances which we refer to as magnetic semiconductors, occupy an intermediate position between magnetic metals and magnetic dielectrics. Magnetic semiconductors are characterized by the existence of two well defined subsystems, the system of magnetic moments which are localized at lattice sites, and a band of itinerant or conduction carriers (conduction electrons or holes). Typical examples are the Eu-chalcogenides, where the local moments arise from 4f electrons of the Eu ion, and the spinell chalcogenides containing Cr^{3+} as a magnetic ion. There is experimental evidence of a substantial mutual influence of spin and charge subsystems in these compounds. This is possible due to the sp–d(f) exchange interaction of the localized spins and itinerant charge carriers [21,31]. More recent efforts have been directed to the study of the properties of diluted magnetic semiconductors (DMS) [32–38]. Further attempts have been made to study and exploit carriers which are exchange-coupled to the localized spins. The effect of carriers on the magnetic ordering temperature is found to be very strong in DMS. DMS are mixed crystals in which magnetic ions (usually Mn^{++}) are incorporated in a substitutional position of the host (typically a II–VI or III–V) crystal lattice. DMS offer a unique possibility for a gradual change of the magnitude and sign of exchange interaction by means of technological control of carrier concentration and band parameters. This field is very active and there are many aspects to the problem. A lot of materials were synthesized and tested [39–41]. The new material design approach to fabrication of new functional DMS resulted in producing a variety of compounds. The presence of the spin degree of freedom in DMS may lead to a new semiconductor spin electronics which will combine the advantages of the semiconducting devices with the new features due to the possibilities of controlling the magnetic state. However, the coexistence of ferromagnetism and semiconducting properties in these compounds require a suitable theoretical model which would describe well both the magnetic cooperative behavior and the semiconducting properties as well as a rich field of interplay between them. The majority of theoretical papers on DMS studied their properties mainly within the mean-field approximation and continuous media terms. In a picture like this the disorder effects, which play an essential role[42–46], can be taken into account roughly only. Moreover, there are different opinions on the intrinsic origin and the nature of disorder in DMS [47–49]. Recently, there were made a lot of efforts to go beyond the simplest level of approximation, the virtual crystal approximation (VCA) and many effective schemes for a better treatment of disorder effects were elaborated [42,46,44,50–53]. Thus, many experimental and theoretical investigations call for a better understanding of the relevant physics and the nature of solutions (especially magnetic) within the lattice spin-fermion model [5,20,31]. In this paper, we concentrate on the description of the magnetic excitation spectra and treat the disorder effects in the simplest VCA to emphasize the chief purpose of this paper, the need for a suitable

definition of the relevant generalized mean fields (GMF) and for internal self-consistency in the description of the spin quasiparticle many-body dynamics.

In the previous papers, we set up the formalism of the method of Irreducible Green Functions (IGF) [9]. This IGF method allows one to describe quasiparticle spectra with damping for many-particle systems on a lattice with complex spectra and a strong correlation in a very general and natural way. This scheme differs from the traditional method of decoupling of an infinite chain of equations [54] and permits a construction of the relevant dynamic solutions in a self-consistent way at the level of the Dyson equation without decoupling the chain of equations of motion for the GFs.

In this paper, we apply the IGF formalism to consider quasiparticle spectra for the lattice spin-fermion model consisting of two interacting subsystems. It is the purpose of this paper to explore more fully the notion of GMF [9] which may arise in the system of interacting localized spins (including effects of disorder) and lattice fermions to justify and understand the nature of the relevant mean fields. Background and applications of the generalized spin-fermion (sp–d) exchange model to magnetic and DMS are discussed in some detail. The capabilities of the model to describe quasiparticle spectra are investigated. The key problem of most of this work is the formation of spin excitation spectra under various conditions on the parameters of the model. The intention is to investigate the quasiparticle spectra and GMF of the magnetic semiconductors consisting of two interacting charge and spin subsystems within the lattice spin-fermion model in a unified and coherent fashion to analyze the role and influence of the Coulomb correlation and exchange. An added motivation for performing new consideration and a careful analysis of the magnetic excitation spectra arise from the circumstance that the various new materials were fabricated and tested, and a lot of new experimental facts were accumulated. The chief purpose of this paper has been to call attention to the need for internal self-consistency in the description of spin quasiparticle dynamics of interacting spin and charge subsystems.

2. The spin-fermion model

The concept of the sp–d (or d–f) model plays an important role in the quantum theory of magnetism [1,2,5,14,20,31]. In this section, we describe the sp–d model which describes the localized 3d(4f)-spins interacting with s(p)-like conduction (itinerant) electrons (or holes) and takes into consideration the electron–electron interaction.

The total Hamiltonian of the model is given by

$$H = H_{\mathrm{s}} + H_{\mathrm{s-d}} + H_{\mathrm{d}}. \tag{1}$$

The Hamiltonian of band electrons (or holes) is given by

$$H_{\mathrm{s}} = \sum_{ij} \sum_{\sigma} t_{ij} a^{\dagger}_{i\sigma} a_{j\sigma} + \frac{1}{2} \sum_{i\sigma} U n_{i\sigma} n_{i-\sigma}. \tag{2}$$

This is the Hubbard model. We adopt the notation

$$a_{i\sigma} = N^{-1/2} \sum_{\vec{k}} a_{k\sigma} \exp(\mathrm{i}\vec{k}\vec{R}_i) \quad a^{\dagger}_{i\sigma} = N^{-1/2} \sum_{\vec{k}} a^{\dagger}_{k\sigma} \exp(-\mathrm{i}\vec{k}\vec{R}_i).$$

In the case of a pure semiconductor, at low temperatures the conduction electron band is empty and the Coulomb term U is therefore not so important. A partial occupation of the band leads to an increase in the role of the Coulomb correlation. It is clear that we treat conduction electrons as s-electrons in the Wannier representation. In doped DMS the carrier system is the valence band p-holes.

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

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

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

$$\varepsilon(\vec{k}) = 2 \sum_{\alpha} t(\vec{a}_\alpha) \cos(\vec{k}\vec{a}_\alpha), \tag{3}$$

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

The term $H_{\mathrm{s-d}}$ describes the interaction of the total 3d(4f)-spin with the spin density of the itinerant carriers [31]

$$H_{\mathrm{s-d}} = -2 \sum_{i} I\vec{\sigma}_i\vec{S}_i = -IN^{-1/2} \sum_{kq} \sum_{\sigma} [S^{-\sigma}_{-q} a^{\dagger}_{k\sigma} a_{k+q-\sigma} + z_\sigma S^{z}_{-q} a^{\dagger}_{k\sigma} a_{k+q\sigma}], \tag{4}$$

where sign factor z_σ is given by

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

and

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

In DMS the local exchange coupling resulted from the p–d hybridization between the Mn d levels and the p valence band $I \sim V^2_{\mathrm{p-d}}$. For the subsystem of localized spins we have

$$H_{\mathrm{d}} = -\frac{1}{2} \sum_{ij} J_{ij}\vec{S}_i\vec{S}_j = -\frac{1}{2} \sum_{q} J_q \vec{S}_q \vec{S}_{-q}. \tag{5}$$

Here we use the notation

$$S^{\alpha}_{i} = N^{-1/2} \sum_{\vec{k}} S^{\alpha}_{k} \exp(\mathrm{i}\vec{k}\vec{R}_i), \quad S^{\alpha}_{k} = N^{-1/2} \sum_{\vec{i}} S^{\alpha}_{i} \exp(-\mathrm{i}\vec{k}\vec{R}_i), \quad [S^{\pm}_{k}, S^{z}_{q}] = \frac{1}{N^{1/2}} \mp S^{\pm}_{k+q} \quad [S^{+}_{k}, S^{-}_{q}] = \frac{2}{N^{1/2}} S^{z}_{k+q},$$

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

This term describes a direct exchange interaction [4] between the localized 3d (4f) magnetic moments at the lattice sites i and j. In the DMS system this interaction is rather small. The ferromagnetic interaction between the local Mn moments is mediated by the real itinerant carriers in the valence band of the host semiconductor material. The carrier polarization produces the RKKY exchange interaction of Mn local moments

$$H_{\mathrm{RKKY}} = -\sum_{i \neq j} K_{ij}\vec{S}_i\vec{S}_j. \tag{6}$$

We emphasize that $K_{ij} \sim |I^2| \sim V^4_{\mathrm{p-d}}$. To explain this, let us remind that the microscopic model [31], which contains basic physics, is the Anderson–Kondo model

$$H = \sum_{ij} \sum_{\sigma} t_{ij} a^{\dagger}_{i\sigma} a_{j\sigma} - V \sum_{ij} \sum_{\sigma} (a^{+}_{i\sigma} d_{j\sigma} + \mathrm{h.c.}) - E_{\mathrm{d}} \sum_{i} \sum_{\sigma} n^{d}_{i\sigma} + \frac{1}{2} \sum_{i\sigma} U n^{d}_{i\sigma} n^{d}_{i-\sigma}. \tag{7}$$

For the symmetric case $U = 2E_d$ and for $U \gg V$ Eq. (7) can be mapped onto the Kondo lattice model (KLM)

$$H = \sum_{ij} \sum_{\sigma} t_{ij} a^{\dagger}_{i\sigma} a_{j\sigma} - \sum_{i} 2I\vec{\sigma}_i \vec{S}_i \tag{8}$$

Here $I \sim 4V^2/E_d$. The KLM may be viewed as the low-energy sector of the initial model Eq. (7).

We follow the previous treatments and take as our model Hamiltonian expression (1). As stated above, the model will represent an assembly of itinerant charge carriers in a periodic atomic lattice. The carriers are represented by quantized Fermi operators. The lattice sites are occupied by the localized spins. Thus, this model can really be called the spin-fermion model.

3. Outline of the IGF method

In this section, we discuss the main ideas of the IGF approach that allows one to describe completely quasiparticle spectra with damping in a very natural way.

We reformulated the two-time GF method [9] to the form which is especially adjusted to correlated fermion systems on a lattice and systems with complex spectra. A very important concept of the whole method is the *Generalized Mean Fields* (GMF), as it was formulated in [9]. These GMF have a complicated structure for the strongly correlated case and complex spectra, and are not reduced to the functional of mean densities of the electrons or spins when one calculates excitation spectra at finite temperatures. A practical way of determining the GMF is to calculate a corresponding GF as it will be described below.

To clarify the foregoing, let us consider a retarded GF of the form [54]

$$G = \langle\langle A(t), A^{\dagger}(t')\rangle\rangle = -\mathrm{i}\theta(t-t')\langle[A(t)A^{\dagger}(t')]_{\eta}\rangle, \ \eta = \pm. \tag{9}$$

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

$$\omega G(\omega) = \langle[A, A^{\dagger}]_{\eta}\rangle + \langle\langle[A, H]_{-} \mid A^{\dagger}\rangle\rangle_{\omega}. \tag{10}$$

Here we use the notation $\langle\langle A(t), A^{\dagger}(t')\rangle\rangle$ for the time-dependent GF and $\langle\langle A \mid A^{\dagger}\rangle\rangle_{\omega}$ for its Fourier transform [54]. The notation $[A, B]_{\eta}$ refers to commutation and anticommutation depending on the value of $\eta = \pm$.

The essence of the method is as follows [9]:

It is based on the notion of the "*IRREDUCIBLE*" parts of GFs (or the irreducible parts of the operators, A and $A^{\dagger}$, 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 analytic representation for the self-energy operator. By definition, we introduce the irreducible part (ir) of the GF

$$^{(\mathrm{ir})}\langle\langle[A, H]_{-}|A^{\dagger}\rangle\rangle = \langle\langle[A, H]_{-} - zA|A^{\dagger}\rangle\rangle. \tag{11}$$

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

$$\langle[^{(\mathrm{ir})}[A, H]_{-}, A^{\dagger}]_{\eta}\rangle = 0 \tag{12}$$

which is an analogue of the orthogonality condition in the Mori formalism. Let us emphasize that due to the complete equivalence of the definition of the irreducible parts for the GFs ($^{(\mathrm{ir})}\langle\langle[A, H]_{-}|A^{\dagger}\rangle\rangle$) and operators $(^{(\mathrm{ir})}[A, H]_{-}) \equiv ([A, H]_{-})^{(\mathrm{ir})}$ we will use both the notation freely ($^{(\mathrm{ir})}\langle\langle A|B\rangle\rangle$ is the same as $\langle\langle(A)^{(\mathrm{ir})}|B\rangle\rangle$). A choice one notation over another is determined by the brevity and clarity of notation only.

From condition (12) one can find

$$z = \frac{\langle [[A, H]_-, A^\dagger]_\eta \rangle}{\langle [A, A^\dagger]_\eta \rangle} = \frac{M_1}{M_0}. \tag{13}$$

Here M_0 and M_1 are the zeroth and first-order moments of the spectral density. Therefore, the irreducible GFs are defined so that they cannot be reduced to the lower-order ones by any kind of decoupling. It is worth noting that the term "*irreducible*" in a group theory means a representation of a symmetry operation that cannot be expressed in terms of lower dimensional representations. Irreducible (or connected) correlation functions are known in statistical mechanics. In the diagrammatic approach, the irreducible vertices are defined as graphs that do not contain inner parts connected by the G^0-line. With the aid of definition (11) these concepts are expressed in terms of retarded and advanced GFs. The procedure extracts all relevant (for the problem under consideration) mean-field contributions and puts them into the generalized mean-field GF which is defined here as

$$G^0(\omega) = \frac{\langle [A, A^\dagger]_\eta \rangle}{(\omega - z)}. \tag{14}$$

To calculate the IGF ${}^{(\mathrm{ir})}\langle\langle [A, H]_-(t), A^\dagger(t')\rangle\rangle$ in (10), we have to write the equation of motion for it after differentiation with respect to the second time variable t'. The condition of orthogonality (12) removes the inhomogeneous term from this equation and is a very crucial point of the whole approach. If one introduces the irreducible part for the right-hand side operator, as discussed above for the "left" operator, the equation of motion (10) can be exactly rewritten in the following form:

$$G = G^0 + G^0 P G^0 \tag{15}$$

The scattering operator P is given by

$$P = (M_0)^{-1}(\langle\langle ([A, H]_-)^{(\mathrm{ir})} | ([A^\dagger, H]_-)^{(\mathrm{ir})}\rangle\rangle)(M_0)^{-1}. \tag{16}$$

The structure of Eq. (16) enables us to determine the self-energy operator M by analogy with the diagram technique

$$P = M + MG^0 P. \tag{17}$$

We use here the notation M for self-energy (mass operator in quantum field theory). From definition (17) it follows that the self-energy operator M is defined as a proper (in the diagrammatic language, "connected") part of the scattering operator $M = (P)^p$. As a result, we obtain the exact Dyson equation for the thermodynamic double-time Green functions

$$G = G^0 + G^0 M G. \tag{18}$$

The difference between P and M can be regarded as two different solutions of two integral Eqs. (15) and (18). However, from the Dyson equation (18) only the full GF is seen to be expressed as a formal solution of the form

$$G = [(G^0)^{-1} - M]^{-1}. \tag{19}$$

Eq. (19) can be regarded as an alternative form of Dyson equation (18) and the *definition* of M provides that the generalized mean-field GF G^0 is specified. On the contrary, for the scattering operator P, instead of the property $G^0 G^{-1} + G^0 M = 1$, one has the property

$$(G^0)^{-1} - G^{-1} = P G^0 G^{-1}.$$

Thus, the *very functional form* of the formal solution (19) precisely determines the difference between P and M.

Thus, by introducing irreducible parts of GF (or irreducible parts of the operators, out of which the GF is constructed) the equation of motion (10) for the GF can exactly be (but using the orthogonality constraint (12)) transformed into the Dyson equation for the double-time thermal GF (18). This result is very remarkable because the traditional form of the GF method does not include this point. Note that all quantities thus considered are exact. Approximations can be generated not by truncating the set of coupled equations of motion but by a specific approximation of the functional form of the mass operator M within a self-consistent scheme expressing M in terms of the initial GF $M \approx F[G]$. Different approximations are relevant to different physical situations.

The projection operator technique has essentially the same philosophy. But with using constraint (12) in our approach we emphasize the fundamental and central role of the Dyson equation for calculation of single-particle properties of many-body systems. The problem of reducing the whole hierarchy of equations involving higher-order GFs by a coupled nonlinear set of integro-differential equations connecting the single-particle GF to the self-energy operator is rather nontrivial. A characteristic feature of these equations is that besides the single-particle GF they involve also higher-order GF. The irreducible counterparts of the GFs, vertex functions, serve to identify correctly the self-energy as

$$M = G_0^{-1} - G^{-1}.$$

The integral form of Dyson equation (18) gives M the physical meaning of a nonlocal and energy-dependent effective single-particle potential. This meaning can be verified for the exact self-energy using the diagrammatic expansion for the causal GF.

Here a sketchy form of the IGF method was presented. We demonstrated in Ref. [9] that the IGF method is a powerful tool for describing the quasiparticle excitation spectra, allowing a deeper understanding of elastic and inelastic quasiparticle scattering effects and the corresponding aspects of damping and finite lifetimes. In the present context, it provides an efficient tool for analysis of the mean fields and GMF of the complicated many-body models. Thus, in this article we will confine ourselves by calculation of the generalized mean-field GF G^0.

4. Quasiparticle dynamics of the (sp–d) model

To describe self-consistently the spin dynamics of the extended sp–d 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 quasiparticle spectra of two interacting subsystem.

We have two kinds of spin variables

$$S_k^+, \quad S_{-k}^- = (S_k^+)^\dagger, \quad \sigma_k^+ = \sum_q a_{q\uparrow}^+ a_{k+q\downarrow}, \quad \sigma_{-k}^- = (\sigma_k^+)^\dagger = \sum_q a_{k+q\downarrow}^+ a_{q\uparrow}.$$

Let us consider the equations of motion

$$[S_k^+, H_{\mathrm{s-d}}]_- = -IN^{-1} \sum_{pq} [2S_{k-q}^z a_{p\uparrow}^\dagger a_{p+q\downarrow} - S_{k-q}^+ (a_{p\uparrow}^\dagger a_{p+q\uparrow} - a_{p\downarrow}^\dagger a_{p+q\downarrow})], \tag{20}$$

$$[S_{-k}^-, H_{\mathrm{s-d}}]_- = -IN^{-1} \sum_{pq} [2S_{k-q}^z a_{p\downarrow}^\dagger a_{p+q\uparrow} - S_{k-q}^- (a_{p\uparrow}^\dagger a_{p+q\uparrow} - a_{p\downarrow}^\dagger a_{p+q\downarrow})], \tag{21}$$

$$[S_k^z, H_{\mathrm{s-d}}]_- = -IN^{-1} \sum_{pq} (S_{k-q}^+ a_{p\downarrow}^\dagger a_{p+q\uparrow} - S_{k-q}^- a_{p\uparrow}^\dagger a_{p+q\downarrow}), \tag{22}$$

$$[S_k^+, H_{\rm d}]_- = N^{-1/2}\sum_q J_q(S_q^z S_{k-q}^+ - S_{k-q}^z S_q^+), \tag{23}$$

$$[S_{-k}^-, H_{\rm d}]_- = N^{-1/2}\sum_q J_q(S_{-(k+q)}^z S_q^- - S_q^z S_{-(k+q)}^-), \tag{24}$$

$$[a_{q\uparrow}^\dagger a_{q+k\downarrow}, H_{\rm s}]_- = (\varepsilon(q+k)-\varepsilon(q))a_{q\uparrow}^\dagger a_{q+k\downarrow} + UN^{-1}\sum_{pp'}(a_{q\uparrow}^\dagger a_{p+p'\uparrow}^\dagger a_{p\uparrow}a_{q+p'+k\downarrow} - a_{q+p'\uparrow}^\dagger a_{p-p'\downarrow}^\dagger a_{p\downarrow}a_{q+k\downarrow}), \tag{25}$$

$$[a_{q\uparrow}^\dagger a_{q+k\downarrow}, H_{\rm s-d}]_- = IN^{-1/2}\sum_{pp'}[S_{-p'}^+(a_{q\uparrow}^\dagger a_{p+p'\uparrow}\delta_{p,q+k} - a_{p\downarrow}^\dagger a_{q+k\downarrow}\delta_{q,p+p'}) - S_{-p'}^z(a_{q\uparrow}^\dagger a_{p+p'\downarrow}\delta_{p,q+k} + a_{p\uparrow}^\dagger a_{q+k\downarrow}\delta_{q,p+p'})]. \tag{26}$$

From Eqs. (20)–(26) it follows that the localized and itinerant spin variables are coupled. Suitable algebra of relevant operators should be described by the "spinor" $\begin{pmatrix}\vec{S}_i\\ \vec{\sigma}_i\end{pmatrix}$ ("relevant degrees of freedom"), according to the IGF strategy. In principle, the complete algebra of the relevant "spin modes" should include the longitudinal components σ_k^z and S_k^z. However, the correlations of the longitudinal spin components are rather small at low temperatures and becomes essential with approaching the Curie temperature. The calculation of the Green function for the longitudinal spin components is a special nontrivial task [55]. Since we are interested here in the low-energy spin-wave type of excitations, we will consider the transversal components only.

The model Hamiltonian $H = H_{\rm s} + H_{\rm s-d} + H_{\rm d}$ was used in Refs. [56,57] for calculations of the spin-wave spectra and was called the modified Zener model. In this model, as applied to transition metals, the itinerant electrons are described by a Hubbard Hamiltonian and the itinerant electron couples the localized spin (Hund's rule coupling) by a term $H_{\rm s-d}$. Because of the inequivalent spin systems, localized and itinerant, a consequence of the model is the existence of acoustic and optic branches of the quasiparticle spectrum of spin excitations. In DMS the local antiferromagnetic interaction $H_{\rm s-d}$ produces the coupling between the carriers (which are holes in GaMnAs) and the Mn magnetic moments ($s = \frac{5}{2}$), which leads to ferromagnetic ordering of Mn spins in a certain range of concentration. The Kondo physics is irrelevant in this case, but the fully determined and consistent microscopic mechanism of the ferromagnetic ordering is still under debates [33,34]. An important question in this context is the self-consistent picture of the quasiparticle many-body dynamics which takes into account the complex structure of the spectra.

To calculate the spectrum of spin excitations in the sp–d model we shall use the double-time thermal GF of localized spins [54] which is defined as

$$G^{+-}(k;t-t') = \langle\langle S_k^+(t), S_{-k}^-(t')\rangle\rangle = -{\rm i}\theta(t-t')\langle[S_k^+(t), S_{-k}^-(t')]_-\rangle = 1/2\pi\int_{-\infty}^{+\infty}{\rm d}\omega\exp(-{\rm i}\omega t)G^{+-}(k;\omega). \tag{27}$$

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 sp–d 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. We introduce the generalized matrix GF of the form

$$\begin{pmatrix}\langle\langle S_k^+|S_{-k}^-\rangle\rangle & \langle\langle S_k^+|\sigma_{-k}^-\rangle\rangle\\ \langle\langle \sigma_k^+|S_{-k}^-\rangle\rangle & \langle\langle \sigma_k^+|\sigma_{-k}^-\rangle\rangle\end{pmatrix} = \hat{G}(k;\omega). \tag{28}$$

Here

$$\sigma_k^+ = \sum_q a_{k\uparrow}^\dagger a_{k+q\downarrow}; \quad \sigma_k^- = \sum_q a_{k\downarrow}^\dagger a_{k+q\uparrow}.$$

Equivalently, we can do the calculations with the matrix of the form

$$\begin{pmatrix} \langle\langle S_k^+ | S_{-k}^- \rangle\rangle & \langle\langle S_k^+ | a_{k+q\downarrow}^\dagger a_{q\uparrow} \rangle\rangle \\ \langle\langle a_{q\uparrow}^\dagger a_{q+k\downarrow} | S_{-k}^- \rangle\rangle & \langle\langle a_{q\uparrow}^\dagger a_{q+k\downarrow} | a_{k+q\downarrow}^\dagger a_{q\uparrow} \rangle\rangle \end{pmatrix} = \hat{G}'(k;\omega), \tag{29}$$

but the form of Eq. (28) is slightly more convenient.

The equation of motion for the GF $\hat{G}(k;\omega)$ can be exactly transformed to Dyson equation (18) by applying the formalism of Section 3 (for details see Appendix A)

$$\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{M} \hat{G}_0 \tag{30}$$

with the self-energy operator M given as

$$\hat{M} = (\hat{P})^p. \tag{31}$$

Hence, the determination of the full GF $\hat{G}$ has been reduced to that of $\hat{G}_0$ and $\hat{M}$.

5. Generalized mean-field GF

We now proceed to give an explicit expression for the generalized mean-field GF. From the definition (A.25), the GF matrix in the generalized mean-field approximation reads

$$\hat{G}_0 = R^{-1} \begin{pmatrix} (1 - U\chi_0^s) I^{-1} N^{1/2} \Omega_2 & \Omega_2 N \chi_0^s \\ \Omega_2 N \chi_0^s & -\Omega_1 N \chi_0^s \end{pmatrix}, \tag{32}$$

where

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

Let us write down explicitly the diagonal matrix elements G_0^{11} and G_0^{22}

$$\langle\langle S_k^+ | S_{-k}^- \rangle\rangle^0 = \frac{2S_z}{\Omega_1 + 2I^2 S_z \chi^s(k,\omega)} \tag{33}$$

$$\langle\langle \sigma_k^+ | \sigma_{-k}^- \rangle\rangle^0 = \frac{\Omega_1 \chi^s(k,\omega)}{\Omega_1 + 2I^2 S_z \chi^s(k,\omega)} \tag{34}$$

where

$$\chi^s(k,\omega) = \chi_0^s(k,\omega)(1 - U\chi_0^s(k,\omega))^{-1} \quad S_z = N^{-1/2}\langle S_0^z \rangle \tag{35}$$

To clarify the functional structure of the generalized mean-field GFs (33) and (34), let us consider a few limiting cases.

5.1. Uncoupled subsystems

To clarify the calculation of quasiparticle spectra of coupled localized and itinerant subsystems, it is instructive to consider an artificial limit of uncoupled subsystems. We then assume that the local exchange

parameter $I = 0$. In this limiting case we have

$$\langle\langle S_k^+ | S_{-k}^- \rangle\rangle^0 = \frac{2S_z}{\omega - S_z(J_0 - J_k) - \dfrac{1}{2NS_z}\sum_q (J_q - J_{q-k})(2K_q^{zz} + K_q^{-+})} \tag{36}$$

$$\langle\langle \sigma_k^+ | \sigma_{-k}^- \rangle\rangle^0 = \chi^s(k, \omega). \tag{37}$$

The spectrum of quasiparticle excitations of localized spins without damping follows from the poles of the generalized mean-field GF (36)

$$\omega(k) = S_z(J_0 - J_k) + \frac{1}{2NS_z}\sum_q (J_q - J_{q-k})(2K_q^{zz} + K_q^{-+}). \tag{38}$$

It is seen that due to the correct definition of generalized mean fields we get the result for the localized spin Heisenberg subsystem which includes both the simplest spin-wave result and the result of Tyablikov decoupling as limiting cases. In the hydrodynamic limit $k \to 0$, $\omega \to 0$ it leads to the dispersion law $\omega(k) = Dk^2$.

The exchange integral J_k can be written in the following way:

$$J_k = \sum_i \exp(-\mathrm{i}\vec{k}\vec{R}_i) J(|\vec{R}_i|). \tag{39}$$

The expansion in small $\vec{k}$ gives

$$J_k = \sum_i J(|\vec{R}_i|) - \frac{1}{2}\sum_i (\vec{k}\vec{R}_i)^2 J(|\vec{R}_i|) = J_0 - \frac{k^2}{2}\sum_i (\vec{n}\vec{R}_i)^2 J(|\vec{R}_i|). \tag{40}$$

Here $\vec{n} = \vec{k}/k$ is the unit vector. The values J_{k-q} can be evaluated in a similar way

$$J_{k-q} = J_q - (\vec{k}\nabla_q)J_q + \frac{1}{2}(\vec{k}\nabla_q)^2 J_q + \cdots,$$

$$(\vec{k}\nabla_q)J_q = -\mathrm{i}\sum_i (\vec{k}\vec{R}_i) J(|\vec{R}_i|)\exp(-\mathrm{i}\vec{q}\vec{R}_i),$$

$$(\vec{k}\nabla_q)^2 J_q = -\frac{1}{2}\sum_i (\vec{k}\vec{R}_i)^2 J(|\vec{R}_i|)\exp(-\mathrm{i}\vec{q}\vec{R}_i). \tag{41}$$

Combining Eqs. (41), (40), and (38) we get

$$\langle\langle S_k^+ | S_{-k}^- \rangle\rangle^0 = \frac{2S_z}{\omega - \omega(k)}$$

$$\omega(k \to 0) = (S_z(J_0 - J_k) + \frac{1}{2NS_z}\sum_q (J_q - J_{q-k})(2K_q^{zz} + K_q^{-+})) \simeq D_1 k^2$$

$$= \left(\frac{S_z}{2}\psi_0 + \frac{N}{2S_z^2}\sum_q \psi_q (2K_q^{zz} + K_q^{-+})\right)k^2,$$

$$\psi_q = \sum_i (\vec{k}\vec{R}_i)^2 J(|\vec{R}_i|)\exp(-\mathrm{i}\vec{q}\vec{R}_i). \tag{42}$$

Let us now consider the spin susceptibility of itinerant carriers, Eq. (37), in the hydrodynamic limit $k \to 0$, $\omega \to 0$. It is convenient to consider the static limit of Eq. (37)

$$\langle\langle \sigma_k^+ | \sigma_{-k}^- \rangle\rangle^0|_{\omega=0} = \frac{\chi_0^s(k,0)}{1 - U\chi_0^s(k,0)},$$

$$\chi_0^s(k,0) = \frac{1}{N}\sum_q \frac{f_{q+k\downarrow} - f_{q\uparrow}}{\varepsilon(q) - \varepsilon(q+k) - \Delta_U}, \quad \Delta_U = U(n_\uparrow - n_\downarrow) = Um. \tag{43}$$

To proceed, we make a small-k expansion of the form

$$\varepsilon(q+k) - \varepsilon(q) = (\vec{k}\nabla_q)\varepsilon(q) + \frac{1}{2}(\vec{k}\nabla_q)^2\varepsilon(q) + \cdots,$$

$$\chi_0^s(k,0) = \frac{1}{N\Delta_U}\sum_q (f_{q\uparrow} - f_{q\downarrow}) - \frac{1}{N\Delta_U^2}\sum_q (f_{q\uparrow} + f_{q\downarrow})\frac{1}{2}(\vec{k}\nabla_q)^2\varepsilon(q) + \frac{1}{N\Delta_U^3}\sum_q (f_{q\uparrow} - f_{q\downarrow})(\vec{k}\nabla_q\varepsilon(q))^2 + \cdots. \tag{44}$$

The poles of the spin susceptibility of itinerant carriers are determined by the equation

$$1 - U\chi_0^s(k,\omega) = 0. \tag{45}$$

In another form this reads in detail

$$1 = \frac{U}{N}\sum_q \frac{f_{q\uparrow} - f_{q+k\downarrow}}{\varepsilon(k+q) - \varepsilon(q) + \Delta_U - \omega}.$$

If we set $\omega = E(k)$ and then put $k = 0$, we get the equation for the excitation energy $E(k=0)$

$$1 = \frac{U}{N}\sum_q \frac{f_{q\uparrow} - f_{q\downarrow}}{\Delta_U - E(k=0)} = \frac{U}{\Delta_U - E(k=0)}\frac{\Delta_U}{U},$$

which is satisfied if $E(k=0) = 0$. Thus, a solution of Eq. (45) exists which has the property $\lim_{k\to 0} E(k) = 0$ and this solution corresponds to an acoustic spin-wave branch of excitations

$$E(k) = D_2k^2 = -\frac{U}{2N\Delta_U}\sum_q (f_{q\uparrow} + f_{q\downarrow})(\vec{k}\nabla_q)^2\varepsilon(\vec{q}) + \frac{U}{N\Delta_U^2}\sum_q (f_{q\uparrow} - f_{q\downarrow})(\vec{k}\nabla_q\varepsilon(\vec{q}))^2,$$

$$\omega = \varepsilon(k+q) - \varepsilon(q) + \Delta_U. \tag{46}$$

It is seen that the stiffness constant D_2 can be interpreted as expanded in $1/\Delta_U$. For the tight-binding electrons in s.c. lattice the spin wave dispersion relation D_2k^2 becomes

$$\begin{aligned} D_2k^2 &= (3(n_\uparrow - n_\downarrow))^{-1}\sum_q \left[\frac{(f_{q\uparrow} - f_{q\downarrow})}{\Delta_U}|\nabla_q\varepsilon(\vec{q})|^2 - \frac{(f_{q\uparrow} + f_{q\downarrow})}{2}\nabla_q^2\varepsilon(\vec{q})\right] \\ &= (3(n_\uparrow - n_\downarrow))^{-1}\left(\frac{2t^2a^2}{\Delta_U}\sum_q (f_{q\uparrow} - f_{q\downarrow})(k_x\sin(q_xa) + k_y\sin(q_ya) + k_z\sin(q_za))^2\right. \\ &\quad \left. - ta^2\sum_q (f_{q\uparrow} + f_{q\downarrow})(k_x^2\cos q_xa + k_y^2\cos q_ya + k_z^2\cos q_za)\right). \end{aligned} \tag{47}$$

5.2. Coupled subsystems

The next stage in the analysis of the quasiparticle spectra of the (sp–d) model is the introduction of the nonzero coupling I. The full generalized mean-field GFs can be rewritten as

$$\langle\langle S_k^+|S_{-k}^-\rangle\rangle^0 = \frac{2S_z}{\omega - Im - S_z(J_0 - J_k) - \dfrac{1}{2NS_z}\sum_q (J_q - J_{q-k})(2K_q^{zz} + K_q^{-+}) + 2I^2 S_z \chi^s(k,\omega)}, \tag{48}$$

$$\langle\langle \sigma_k^+|\sigma_{-k}^-\rangle\rangle^0 = \frac{\chi_0^s(k,\omega)}{1 - U_{\text{eff}}(\omega)\chi_0^s(k,\omega)}. \tag{49}$$

Here the notation is used

$$U_{\text{eff}} = U - \frac{2I^2 S_z}{\omega - Im}; \quad m = (n_\uparrow - n_\downarrow).$$

The expression, Eq. (49), coincides with that for the itinerant spin susceptibility, as calculated in Ref. [2]. It is instructive to consider separately the four different cases,

(i) $I \neq 0,\ J = 0,\ U = 0,$
(ii) $I \neq 0,\ J \neq 0,\ U = 0,$
(iii) $I \neq 0,\ J = 0,\ U \neq 0,$
(iv) $I \neq 0,\ J \neq 0,\ U \neq 0.$

5.2.1. Kondo lattice model

The first case $I \neq 0,\ J = 0,\ U = 0$ corresponds to a model which is commonly called the Kondo lattice model. It can be seen that GFs (48) and (49) are then equal to

$$\langle\langle S_k^+|S_{-k}^-\rangle\rangle^0 = \frac{2S_z}{\omega - Im + 2I^2 S_z \chi_0^s(k,\omega)}, \tag{50}$$

$$\langle\langle \sigma_k^+|\sigma_{-k}^-\rangle\rangle^0 = \frac{\chi_0^s(k,\omega)}{\omega + \dfrac{2I^2 S_z}{\omega - Im}\chi_0^s(k,\omega)}. \tag{51}$$

In order to calculate the acoustic pole of the GF (50), we make use of the small (k,ω) expansion. Hence, we get

$$\langle\langle S_k^+|S_{-k}^-\rangle\rangle^0 \approx \frac{2S_z(1 + m/2S_z)^{-1}}{\omega - (1 + m/2S_z)^{-1}\left[(1/2N\Delta_I^2)\sum_q (f_{q\uparrow} + f_{q\downarrow})(\vec{k}\nabla_q)^2\varepsilon(\vec{q}) - (1/N\Delta_I^3)\sum_q (f_{q\uparrow} - f_{q\downarrow})(\vec{k}\nabla_q\varepsilon(\vec{q}))^2\right]}. \tag{52}$$

It follows from Eq. (52) that the stiffness constant D is proportional to the total magnetization of the system.

5.2.2. Zener or s–d exchange model

In the second case $I \neq 0,\ J \neq 0,\ U = 0$, we get

$$\langle\langle S_k^+ | S_{-k}^- \rangle\rangle^0 = \frac{2S_z}{\omega - Im - S_z(J_0 - J_k) - \frac{1}{2NS_z}\sum_q (J_q - J_{q-k})(2K_q^{zz} + K_q^{-+}) + 2I^2 S_z \chi_0^s(k,\omega)} \tag{53}$$

$$\langle\langle \sigma_k^+ | \sigma_{-k}^- \rangle\rangle^0 = \frac{\chi_0^s(k,\omega)}{1 - \dfrac{2I^2 S_z}{\omega - Im}\chi_0^s(k,\omega)}. \tag{54}$$

In order to calculate the acoustic pole of the GF (53), we make use of the small (k,ω) expansion again. We then get

$$\langle\langle S_k^+ | S_{-k}^- \rangle\rangle^0 \approx \frac{2S_z(1 + \frac{m}{2S_z})^{-1}}{\omega - (1 + \frac{m}{2S_z})^{-1} D_1 k^2 - (1 + \frac{m}{2S_z})^{-1}[\frac{1}{2N\Delta_I^2}\sum_q (f_{q\uparrow} + f_{q\downarrow})(\vec{k}\nabla_q)^2 \varepsilon(\vec{q}) - \frac{1}{N\Delta_I^3}\sum_q (f_{q\uparrow} - f_{q\downarrow})(\vec{k}\nabla_q \varepsilon(\vec{q}))^2]} \tag{55}$$

It follows from Eqs. (52) and (55) that the stiffness constant D is proportional to the total magnetization of the system.

5.2.3. Modified Zener model

The third case $I \neq 0,\ J = 0,\ U \neq 0$ corresponds to a model which is called the modified Zener lattice model [56]. It can be seen that in this case GFs (48) and (49) are equal to

$$\langle\langle S_k^+ | S_{-k}^- \rangle\rangle^0 = \frac{2S_z}{\omega - Im + 2I^2 S_z \chi^s(k,\omega)} \tag{56}$$

$$\langle\langle \sigma_k^+ | \sigma_{-k}^- \rangle\rangle^0 = \frac{\chi_0^s(k,\omega)}{1 - U_{\text{eff}}(\omega)\chi_0^s(k,\omega)}. \tag{57}$$

The results obtained here coincide with those of Bartel [56]. The excitation energies for the localized spin and spin densities of itinerant carriers are found from the zeros of the denominators of $\langle\langle S_k^+ | S_{-k}^- \rangle\rangle^0$ and $\langle\langle \sigma_k^+ | \sigma_{-k}^- \rangle\rangle^0$ which yield identical excitation spectra, consisting of three branches, the acoustic spin wave $E^{\text{ac}}(k)$, the optical spin wave $E^{\text{op}}(k)$, and the Stoner continuum $E^{\text{St}}(k)$

$$E^{\text{ac}}(k) = Dk^2,$$

$$E^{\text{op}}(k) = E_0^{\text{op}} - D\left(1 - \frac{UE^{\text{op}}}{I\Delta}\right)k^2; \quad E_0^{\text{op}} = I(m + 2S_z),\ E^{\text{St}}(k) = \varepsilon(k+q) - \varepsilon(q) + \Delta.$$

5.2.4. Generalized spin-fermion exchange model

The most general is the fourth case, $I \neq 0,\ J \neq 0,\ U \neq 0$. The total GF of the coupled system is given by Eq. (48). The magnetic excitation spectrum follows from the poles of the GF (32)

$$R = (1 - U\chi_0^s)\Omega_1 + \Omega_2 I N^{1/2}\chi_0^s = 0$$

and consists of three branches—the acoustic spin wave $E^{\text{ac}}(k)$, the optical spin wave $E^{\text{op}}(k)$, and the Stoner continuum $E^{\text{St}}(k)$.

Let us consider, as a first approximation, the last term in its denominator which is the dynamic spin susceptibility of itinerant carriers in the static limit without any frequency dependence. The GF, Eq. (48), then becomes equal to

$$\langle\langle S_k^+|S_{-k}^-\rangle\rangle^0 \approx \frac{2S_z}{\omega - Im - S_z(J_0 - J_k) - \frac{1}{2NS_z}\sum_q (J_q - J_{q-k})(2K_q^{zz} + K_q^{-+}) + 2I^2 S_z \chi^s(k,0)}. \tag{58}$$

It is possible to verify that in the limit $k \to 0$

$$2I^2 S_z \chi^s(k,0) \approx Im - \frac{1}{2S_z N}\sum_q (f_{q\uparrow} + f_{q\downarrow})(\vec{k}\nabla_q)^2 \varepsilon(\vec{q}) + \frac{1}{2S_z N\Delta}\sum_q (f_{q\uparrow} - f_{q\downarrow})(\vec{k}\nabla_q \varepsilon(\vec{q}))^2. \tag{59}$$

Then for $\omega, k \to 0$ Eq. (58) becomes

$$\langle\langle S_k^+|S_{-k}^-\rangle\rangle^0 \approx \frac{2S_z}{\omega - D_1 k^2 - \frac{1}{2S_z 2N}\sum_q (f_{q\uparrow} + f_{q\downarrow})(\vec{k}\nabla_q)^2 \varepsilon(\vec{q}) + \frac{1}{2S_z N\Delta}\sum_q (f_{q\uparrow} - f_{q\downarrow})(\vec{k}\nabla_q \varepsilon(\vec{q}))^2}. \tag{60}$$

This expression can be expected to be qualitatively correct in spite of the primitive approximation. The spectrum of Stoner excitations is given by

$$E^{\mathrm{St}}(k) = \varepsilon(k+q) - \varepsilon(q) + \Delta. \tag{61}$$

In addition to the acoustic branch there is an optical branch of spin excitations. This can be seen from the following: For $k = 0$ we get for $R = 0$ the quadratic equation in ω with two solutions, $\omega = 0$ and $\omega = I(m + 2S_z) = E_0^{\mathrm{op}}$. In the hydrodynamic limit, $k \to 0$, $\omega \to 0$ the GF (47) can be written as

$$\langle\langle S_k^+|S_{-k}^-\rangle\rangle^0 \simeq \frac{2S_z}{\omega - E^{ac}(k)}, \tag{62}$$

where the acoustic spin wave energies are given by

$$E^{\mathrm{ac}}(k) = Dk^2 = \left(\frac{S_z}{2}\left[\psi_0 + \frac{1}{2NS_z^2}\sum_q \psi_q(2K_q^{zz} + K_q^{-+})\right] + \frac{1}{2N}\frac{1}{2S_z}\sum_q (f_{q\uparrow} + f_{q\downarrow})(\vec{n}\nabla_q)^2 \varepsilon(\vec{q}) + \frac{1}{N\Delta}\frac{1}{2S_z}\sum_q (f_{q\uparrow} - f_{q\downarrow})(\vec{n}\nabla_q \varepsilon(\vec{q}))^2\right) k^2. \tag{63}$$

For the optical spin wave branch the estimations can be carried out as in paper [2]

$$E^{\mathrm{op}}(k) = E_0^{\mathrm{op}} - D^{\mathrm{op}} k^2. \tag{64}$$

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

$$n_\sigma = \frac{1}{N}\sum_k [\exp(\beta(\varepsilon(k) + Un_{-\sigma} - IS_z - \varepsilon_F)) + 1]^{-1}. \tag{65}$$

Hence, the stiffness constant D can be expressed by the parameters of the sp–d model Hamiltonian.

6. Effects of disorder in DMS

We now proceed to a simple and qualitative discussion of the effects of disorder in DMS to give just a flavor of ideas how the disorder can be included in the IGF scheme. The full treatment of disorder effects requires the consideration of damping effects and will be considered separately.

The main aim of the investigation of DMS is to give a successful microscopic picture of the ferromagnetic ordering of localized spins induced by the interaction with the spin density of itinerant charge carriers. As it has been stated above, a suitable model, which may be used for investigation of this problem (at least at the initial stage), is a modified Kondo lattice model (8)

$$H = \sum_{ij} \sum_{\sigma} t_{ij} a^{\dagger}_{i\sigma} a_{j\sigma} - \sum_{i} 2I v_i \vec{\sigma}_i \vec{S}_i. \tag{66}$$

Here v_i projects out sites occupied by Mn atoms, i.e.,

$$v_i = \begin{cases} 1 & \text{if site } i \text{ is occupied by Mn} \\ 0 & \text{if site } i \text{ is occupied by Ga.} \end{cases}$$

This model is relevant for the doped II–VI or III–V compound. The essential feature of the model is that it describes a mechanism of how the spins of carriers (electrons or holes) become polarized due to the local antiferromagnetic exchange interactions with localized spins. In $A^{\mathrm{III}}_{1-x}\mathrm{Mn}_x B^{\mathrm{V}}$ the main magnetic interaction is an antiferromagnetic exchange between the Mn spins and the charge-carrier spins. The superexchange term $H_{\mathrm{d}} = -\frac{1}{2}\sum_{ij} J_{ij}\vec{S}_i\vec{S}_j$ is antiferromagnetic too, but is as a rule rather small in the concentration range of interest ($x \approx 0.05$). In the case of Mn-doped III–V compounds the antiferromagnetic superexchange interaction will generally reduce the ferromagnetic ordering temperature. As a result, the carrier-induced ferromagnetism in DMS arises due to the effective ferromagnetic interaction between the Mn spins. In other words, the ferromagnetism in this system is most probably related to the uncompensated Mn spins and is mediated by holes. The density of Mn ions c_{Mn} is greater than the hole density p, $c_{\mathrm{Mn}} \gg p$. The optimal interrelation of both the magnitudes is a delicate and subtle question and was recently analyzed in paper [49]. It was shown that the concentration of free holes and ferromagnetically active Mn spins was governed by the position of the Fermi level which controls the formation energy of compensating interstitial Mn donors. The experimental evidence has been provided that the upper limit of the Curie temperature is caused by Fermi-level-induced hole saturation. In order to provide a suitable treatment of the spin quasiparticle dynamics it is necessary to take into account the effects of disorder since the Mn ions are assumed to be distributed randomly with concentration c. This is positional disorder. There is variation of site-energy of nonmagnetic origin due to the substitution of A atom with Mn ion. The detailed nature of the disorder is not fully clear. In paper [49], it was shown that the dominant fraction of the Mn atoms was on either substitutional sites or specific sites shadowed by the host atoms. This reveals that the majority of the Mn atoms are on specific (nonrandom) sites commensurate with the lattice, but this does not necessarily imply that all of the Mn atoms are in substitutional positions. For $x > 0.05$ an increasing fraction of Mn spins does not participate in ferromagnetism. It can be related with an increase in the concentration of Mn interstitials accompanied by a reduction of T_{c}.There are indications of an increase in Mn atoms in the form of random clusters not commensurate with the GaAs lattice. However, these results require independent confirmation. The conclusion that there is a maximum in T_{c} due to that the Fermi level pinning is a conjection only. There are evidences that the largest values of T_{c} have been found to be considerably larger than 110 K [33,34,45].

It follows from Eq. (66) that the spin dynamics of a modified KLM will be described by the GFs in the lattice site representation for a given configuration

$$\langle\langle S_i^+|S_j^-\rangle\rangle \quad \langle\langle \sigma_i^+|\sigma_j^-\rangle\rangle$$

and instead of Eq. (28) the lattice GF should be considered

$$\begin{pmatrix} \langle\langle S_i^+|S_j^-\rangle\rangle & \langle\langle S_i^+|\sigma_j^-\rangle\rangle \\ \langle\langle \sigma_i^+|S_j^-\rangle\rangle & \langle\langle \sigma_i^+|\sigma_j^-\rangle\rangle \end{pmatrix} = \hat{G}_{ij}(\omega). \tag{67}$$

In order to provide a simultaneous and self-consistent treatment of the quasiparticle dynamics including the effects of disorder, a sophisticated description of disorder should be done. Most treatments remove disorder by making a virtual-crystal-like approximation in which the Mn ion distribution is replaced by a continuum. A more sophisticated approach for treating the positional disorder of the magnetic impurities inside the host semiconductor is the CPA [58]. The CPA replaces the initial Hamiltonian of a disordered system by an effective one which is assumed to produce no further scattering [58]. It describes reasonably well the state of itinerant charge scattering in disordered substitutional alloys $A_{1-x}B_x$.

In order to simplify the discussion, we will deal with a much simpler and less sophisticated description. The approximation discussed below should be considered as a first, crude approximation to a theory of disorder effects in DMS. Since the detailed nature of disorder in DMS is not yet established completely, we will confine ourselves to the simplest possible approximation. Let us remind that the IGF method is based on the suitable definition of the GMF [9]. To demonstrate the flexibility of the IGF method, we show below how the mean field should be redefined to include the disorder in an effective way. The previous definition of the irreducible spin operator, Eq. (31), should be replaced by

$$(S_q^z)^{\mathrm{ir}} = S_q^z - c\overline{\langle S_z\rangle}\delta_{q,0}; \quad (a_{p+q\sigma}^\dagger a_{p\sigma})^{\mathrm{ir}} = a_{p+q\sigma}^\dagger a_{p\sigma} - \langle a_{p\sigma}^\dagger a_{p\sigma}\rangle\delta_{q,0}. \tag{68}$$

Here $\overline{\langle S_z\rangle} = N^{-1/2}\bar{S}_z$ corresponds to the configuration average. The average $\langle S_z\rangle$ denotes the mean value of S^z for a given configuration of all the spins. We omitted here the variation of site energy of nonmagnetic origin. The consequences of this choice manifest themselves. It means precisely that in a random system the mean field is weaker as compared to a regular system. The approximation is conceptually as simple as an ordinary mean-field approximation and corresponds to the VCA. The situation is then completely analogous to the previous one considered in the preceding sections. For the configurationally averaged GFs we get

$$\overline{\langle\langle S_i^+|S_j^-\rangle\rangle^0} = \langle\langle S_k^+|S_{-k}^-\rangle\rangle^0 \approx \frac{2c\bar{S}_z}{\omega - Im + 2I^2c\bar{S}_z\chi_0^s(k,\omega)}, \tag{69}$$

$$\overline{\langle\langle \sigma_i^+|\sigma_j^-\rangle\rangle^0} = \langle\langle \sigma_k^+|\sigma_{-k}^-\rangle\rangle^0 \approx \frac{\chi_0^s(k,\omega)}{\omega + \frac{2I^2c\bar{S}_z}{\omega - Im}\chi_0^s(k,\omega)}. \tag{70}$$

These simple results are fully tractable and are the reason for their derivation.

It is worth noting that in the case of the modified Zener model, which contains the correlation (Hubbard) term, the effects of disorder should be considered on the basis of a similar model [59]

$$H = \sum_{ij}\sum_{\sigma} t_{ij}a_{i\sigma}^\dagger a_{j\sigma} + U\sum_i v_i n_{i\uparrow}n_{i\downarrow} - \sum_i 2Iv_i\vec{\sigma}_i\vec{S}_i. \tag{71}$$

The Coulomb repulsion is assumed to exist only on lattice sites occupied at random by Mn atoms. The approach mostly used [59] to calculate a stiffness constant within a random version of the Hubbard model

was based on the random phase approximation, where the electron–electron interaction in the Hartree-Fock approximation and the disorder in the CPA were taken into account. It is therefore very probable that within this approach the formation of magnetic clusters can be reproduced; the formation of the clusters is thus strongly enviromental dependent. However, the calculation of the spatial GF, Eq. (67), for the model, Eq. (71), is rather a long and nontrivial task and we must avoid considering this problem here. We hope, nevertheless, that the description of the disorder effects, as given above, gives a good first approximation as far as the IGF method is concerned. A more detail consideration of the state of itinerant carriers in DMS, including a more sophisticated treatment of disorder effects will be carried out separately.

7. Conclusions

In summary, we have presented an analytical approach to treating the spin quasiparticle dynamics of the generalized spin-fermion model, which provides a basis for description of the physical properties of magnetic and diluted magnetic semiconductors. We have investigated the influence of the correlation and exchange effects on interacting systems of itinerant carriers and localized spins. The workable and self-consistent IGF approach to the decoupling problem for the equation-of-motion method for double-time temperature Green functions has been presented. The main achievement of this formulation is the derivation of the Dyson equation for double-time retarded Green functions instead of causal ones. That formulation permits one to unify convenient analytical properties of retarded and advanced GF and the formal solution of the Dyson equation which, in spite of the required approximations for the self-energy, provides the correct functional structure of single-particle GF. The main advantage of the mathematical formalism is brought out by showing how elastic scattering corrections (generalized mean fields) and inelastic scattering effects (damping and finite lifetimes) could be self-consistently incorporated in a general and compact manner. In this paper, we have confined ourselves to the elastic scattering corrections and have not considered the damping effects. This approach gives a workable scheme for definition of relevant generalized mean fields written in terms of appropriate correlators. A comparative study of real many-body dynamics of the generalized spin-fermion model is important to characterize the true quasiparticle excitations and the role of magnetic correlations. It was shown that the magnetic dynamics of the generalized spin-fermion model can be understood in terms of combined dynamics of itinerant carriers, and of localized spins and magnetic correlations of various nature. The two other principal distinctive features of our calculation were, first, the use of correct analytic definition of the relevant GMF and, second, the explicit calculation of the spin-wave quasiparticle spectra and its analysis for the two interacting subsystems. This analysis includes all of the interaction terms that can contribute to essential physics. Thus, the present consideration is the most complete analysis of the quasiparticle spectra of the spin-fermion model of magnetism within the generalized mean-field approximation. These applications illustrate some of subtle details of the IGF approach and exhibit their physical significance in a representative form.

As it is seen, this treatment has advantages in comparison with the standard methods of decoupling of higher order GFs within the equation-of-motion approach, namely, the following: At the mean-field level, the GF one obtains, is richer than that following from the standard procedures. The generalized mean fields represent all elastic scattering renormalizations in a compact form. The approximations (the decoupling) are introduced at a later stage with respect to other methods, i.e., only into the rigorously obtained self-energy.

The physical picture of elastic and inelastic scattering processes in the interacting many-particle systems is clearly seen at every stage of calculations, which is not the case with the standard methods of decoupling.

Many results of the previous works are reproduced mathematically more simply.

The main advantage of the whole method is the possibility of a *self-consistent* description of quasiparticle spectra and their damping in a unified and coherent fashion. However, in the present paper, for the sake of

clarity, we concentrated on the clear presentation of the quasiparticle many-body dynamics within a generalized mean-field approximation. This explains why we confine ourselves to consideration of disorder effects in the simplest VCA. The consideration of disorder effects beyond VCA includes many intrinsic specific problems and deserves a separate investigation. The irreducible GFs methods will be generalized to treat these problems in separate publications.

Thus, this new picture of an interacting spin-fermion system on a lattice is far richer and gives more possibilities for analysis of phenomena which can actually take place. In this sense, the approach we suggest produces a more advanced physical picture of the quasiparticle many-body dynamics. Our main results reveal the fundamental importance of the adequate definition of generalized mean fields at finite temperatures which results in a deeper insight into the nature of quasiparticle states of the correlated lattice fermions and spins. The key to understanding of the situation in DMS lies in the right description of the interplay of interactions and disorder effects for coupled spin and charge subsystems. Consequently, it is crucial that the correct functional structure of generalized mean fields is calculated in a closed and compact form. The detailed consideration of the state of itinerant charge carriers in DMS along this line will be considered separately.

Appendix A. Dyson equation for the s–d model

In this Appendix, we present details of the derivation of the Dyson equation (30) for the sp–d model. Let us consider the equation of motion for the GF $\hat{G}(k;\omega)$ Eq. (28). By differentiation of the GF $\langle\langle S_k^+(t)|B(t')\rangle\rangle$ with respect to the first time, t, we find

$$\begin{aligned}\omega\langle\langle S_k^+|B\rangle\rangle_\omega = &\left\{\begin{array}{c} 2N^{-1/2}\langle S_0^z\rangle \\ 0 \end{array}\right\} \\ &+\frac{I}{N}\sum_{pq}\langle\langle S_{k-q}^+(a_{p\uparrow}^\dagger a_{p+q\uparrow} - a_{p\downarrow}^\dagger a_{p+q\downarrow}) \\ &- 2S_{k-q}^z a_{p\uparrow}^\dagger a_{p+q\downarrow}|B\rangle\rangle_\omega + N^{-1/2}\sum_q J_q\langle\langle(S_q^z S_{k-q}^+ - S_{k-q}^z S_q^+)|B\rangle\rangle_\omega \end{aligned} \tag{A.1}$$

where

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

Let us introduce by definition irreducible (ir) operators as

$$(S_q^z)^{\mathrm{ir}} = S_q^z - \langle S_0^z\rangle\delta_{q,0}; \quad (a_{p+q\sigma}^\dagger a_{p\sigma})^{\mathrm{ir}} = a_{p+q\sigma}^\dagger a_{p\sigma} - \langle a_{p\sigma}^\dagger a_{p\sigma}\rangle\delta_{q,0} \tag{A.2}$$

$$((S_q^z)^{\mathrm{ir}} S_{k-q}^+ - (S_{k-q}^z)^{\mathrm{ir}} S_q^+)^{\mathrm{ir}} = ((S_q^z)^{\mathrm{ir}} S_{k-q}^+ - (S_{k-q}^z)^{\mathrm{ir}} S_q^+) - (\phi_q - \phi_{k-q})S_k^+ \tag{A.3}$$

From the condition (12)

$$\langle[((S_q^z)^{\mathrm{ir}} S_{k-q}^+ - (S_{k-q}^z)^{\mathrm{ir}} S_q^+ - (\phi_q - \phi_{k-q})S_k^+), S_{-k}^-]_-\rangle = 0$$

one can find

$$\phi_q = \frac{2K_q^{zz} + K_q^{-+}}{2\langle S_0^z\rangle}, \tag{A.4}$$

$$K_q^{zz} = \langle (S_q^z)^{\rm ir}(S_q^z)^{\rm ir}\rangle; \quad K_q^{-+} = \langle S_{-q}^- S_q^+\rangle. \tag{A.5}$$

Using the definition of the irreducible parts the equation of motion, Eq. (A.1) can be exactly transformed to the following form:

$$\Omega_1 \langle\langle S_k^+|B\rangle\rangle_\omega + \Omega_2 \langle\langle \sigma_k^+|B\rangle\rangle_\omega = \left\{ \begin{matrix} \left(\frac{N^{1/2}}{I}\right)\Omega_2 \\ 0 \end{matrix} \right\} + \langle\langle A_1|B\rangle\rangle_\omega \tag{A.6}$$

where

$$\Omega_1 = \omega - \frac{\langle S_0^z\rangle}{N^{1/2}}(J_0 - J_k) - N^{-1/2}\sum_q (J_q - J_{q-k})\frac{2K_q^{zz} + K_q^{-+}}{2\langle S_0^z\rangle} - I(n_\uparrow - n_\downarrow), \tag{A.7}$$

$$\Omega_2 = \frac{2\langle S_0^z\rangle I}{N}, \tag{A.8}$$

$$n_\sigma = \frac{1}{N}\sum_q \langle a_{q\sigma}^\dagger a_{q\sigma}\rangle = \frac{1}{N}\sum_q f_{q\sigma} = \sum_q (\exp(\beta\varepsilon(q\sigma)) + 1)^{-1},$$

$$\varepsilon(q\sigma) = \varepsilon(q) - z_\sigma I N^{-1/2}\langle S_0^z\rangle, + U n_{-\sigma} \quad \bar{n} = \sum (n_\uparrow + n_\downarrow); \quad 0 \leqslant \bar{n} \leqslant 2.$$

The many-particle operator A_1 reads

$$\begin{aligned} A_1 = {} & \frac{I}{N}\sum_{pq}[S_{k-q}^+(a_{p\uparrow}^\dagger a_{p+q\uparrow} - a_{p\downarrow}^\dagger a_{p+q\downarrow})^{\rm ir} - 2(S_{k-q}^z)^{\rm ir} a_{p\uparrow}^\dagger a_{p+q\downarrow}] \\ & + N^{-1/2}\sum_q J_q((S_q^z)^{\rm ir} S_{k-q}^+ - (S_{k-q}^z)^{\rm ir} S_q^+)^{\rm ir} \end{aligned} \tag{A.9}$$

and it satisfies the conditions

$$\langle [A_1, S_{-q}^-]_-\rangle = \langle [A_1, \sigma_{-q}^-]_-\rangle = 0.$$

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 an auxiliary equation of motion for the GF of the form $\langle\langle a_{p\uparrow}^\dagger a_{p+k\downarrow}(t), B(t')\rangle\rangle$. For this we have to write the equation of motion for it after differentiation with respect to the first time variable t and extract the corresponding irreducible parts. Then, we obtain, after the Fourier transformation, the following equation:

$$\begin{aligned} & (\omega + \varepsilon(p) - \varepsilon(p+k) - 2IN^{-1/2}\langle S_0^z\rangle - U(n_\uparrow - n_\downarrow)) \times \langle\langle a_{p\uparrow}^\dagger a_{p+k\downarrow}|B\rangle\rangle_\omega \\ & \quad + UN^{-1}(f_{p\uparrow} - f_{p+k\downarrow})\langle\langle \sigma_k^+|B\rangle\rangle_\omega + IN^{-1/2}(f_{p\uparrow} - f_{p+k\downarrow})\langle\langle S_k^+|B\rangle\rangle_\omega \\ & = \left\{ \begin{matrix} 0 \\ (f_{p\uparrow} - f_{p+k\downarrow}) \end{matrix} \right\} - IN^{-1/2}\sum_{qr}\langle\langle S_{-r}^+(a_{p\uparrow}^\dagger a_{q+r\uparrow}\delta_{p+k,q} - a_{q\downarrow}^\dagger a_{p+k\downarrow}\delta_{p,q+r})^{\rm ir}|B\rangle\rangle_\omega \\ & \quad - IN^{-1/2}\sum_{qr}\langle\langle (S_{-r}^z)^{\rm ir}(a_{q\uparrow}^\dagger a_{p+k\downarrow}\delta_{p,q+r} + a_{p\uparrow}^\dagger a_{q+r\downarrow}\delta_{p+k,q})|B\rangle\rangle_\omega \\ & \quad + UN^{-1}\sum_{qr}\langle\langle (a_{p\uparrow}^\dagger a_{q+r\uparrow}^\dagger a_{q\uparrow} a_{p+r+k\downarrow} - a_{p+r\uparrow}^\dagger a_{q-r\downarrow}^\dagger a_{q\downarrow} a_{p+k\downarrow})^{\rm ir}|B\rangle\rangle_\omega. \end{aligned} \tag{A.10}$$

Let us use the following notation:

$$A_2 = -IN^{-1/2}\sum_{qr}[S^{+}_{-r}(a^{\dagger}_{p\uparrow}a_{q+r\uparrow}\delta_{p+k,q} - a^{\dagger}_{q\downarrow}a_{p+k\downarrow}\delta_{p,q+r})^{\mathrm{ir}} - (S^{z}_{-r})^{\mathrm{ir}} \times(a^{\dagger}_{q\uparrow}a_{p+k\downarrow}\delta_{p,q+r} + a^{\dagger}_{p\uparrow}a_{q+r\downarrow}\delta_{p+k,q})] + UN^{-1}\sum_{qr}(a^{\dagger}_{p\uparrow}a^{\dagger}_{q+r\uparrow}a_{q\uparrow}a_{p+r+k\downarrow} - a^{\dagger}_{p+r\uparrow}a^{\dagger}_{q-r\downarrow}a_{q\downarrow}a_{p+k\downarrow})^{\mathrm{ir}}, \tag{A.11}$$

$$\omega_{p,k} = (\omega + \varepsilon(p) - \varepsilon(p+k) - \Delta), \tag{A.12}$$

$$\Delta = 2IN^{-1/2}\langle S^{z}_{0}\rangle - U(n_{\uparrow} - n_{\downarrow}) = 2IS_z - Um = \Delta_I + \Delta_U, \tag{A.13}$$

$$\chi^{s}_{0}(k,\omega) = N^{-1}\sum_{p}\frac{(f_{p+k\downarrow} - f_{p\uparrow})}{\omega_{p,k}}. \tag{A.14}$$

Now we consider the GF $\langle\langle\sigma^{+}_{k}(t), B(t')\rangle\rangle$. Similarly to Eq. (A.6), we have

$$-N^{1/2}I\chi^{s}_{0}(k,\omega)\langle\langle S^{+}_{k}|B\rangle\rangle_{\omega} + (1 - U\chi^{s}_{0}(k,\omega))\langle\langle\sigma^{+}_{k}|B\rangle\rangle_{\omega} = \left\{\begin{array}{c} 0 \\ -N\chi^{s}_{0}(k,\omega)\end{array}\right\} + \sum_{p}\frac{1}{\omega_{p,k}}\langle\langle A_2|B\rangle\rangle_{\omega}. \tag{A.15}$$

Here the following definition of the irreducible part for the Coulomb correlation term was used:

$$(a^{\dagger}_{p\uparrow}a^{\dagger}_{q+r\uparrow}a_{q\uparrow}a_{p+r+k\downarrow} - a^{\dagger}_{p+r\uparrow}a^{\dagger}_{q-r\downarrow}a_{q\downarrow}a_{p+k\downarrow})^{\mathrm{ir}} = (a^{\dagger}_{p\uparrow}a^{\dagger}_{q+r\uparrow}a_{q\uparrow}a_{p+r+k\downarrow} - a^{\dagger}_{p+r\uparrow}a^{\dagger}_{q-r\downarrow}a_{q\downarrow}a_{p+k\downarrow}) - \langle a^{\dagger}_{q+r\uparrow}a_{q\uparrow}\rangle\delta_{q+r,q}a^{\dagger}_{p\uparrow}a_{p+r+k\downarrow} - \langle a^{\dagger}_{q-r\downarrow}a_{q\downarrow}\rangle\delta_{q-r,q}a^{\dagger}_{p+r\uparrow}a_{p+k\downarrow}. \tag{A.16}$$

The operator A_2 satisfies the conditions

$$\langle[A_2, S^{-}_{-k}]_{-}\rangle = \langle[A_2, \sigma^{-}_{-k}]_{-}\rangle = 0$$

In the matrix notation the full equation of motion for the GF $\hat{G}(k;\omega)$ can now be summarized in the following form:

$$\hat{\Omega}\hat{G}(k;\omega) = \hat{I} + \sum_{p}\hat{\Phi}(p)\hat{D}(p;\omega),\ (\hat{G}(k;\omega))^{\dagger}(\hat{\Omega})^{\dagger} = (\hat{I})^{\dagger} + \sum_{p}(\hat{D}(p;\omega))^{\dagger}(\hat{\Phi}(p))^{\dagger}, \tag{A.17}$$

where

$$\hat{\Omega} = \begin{pmatrix}\Omega_1 & \Omega_2 \\ -IN^{1/2}\chi^{s}_{0} & (1 - U\chi^{s}_{0})\end{pmatrix},\quad \hat{I} = \begin{pmatrix}I^{-1}N^{1/2}\Omega_2 & 0 \\ 0 & -N\chi^{s}_{0}\end{pmatrix}, \tag{A.18}$$

$$\hat{D}(p;\omega) = \begin{pmatrix}\langle\langle A_1|S^{-}_{k}\rangle\rangle & \langle\langle A_1|\sigma^{-}_{-k}\rangle\rangle \\ \langle\langle A_2|S^{-}_{-k}\rangle\rangle & \langle\langle A_2|\sigma^{-}_{-k}\rangle\rangle\end{pmatrix},\quad \hat{\Phi}(p) = \begin{pmatrix}N^{-1} & 0 \\ 0 & \omega^{-1}_{p,k}\end{pmatrix}. \tag{A.19}$$

To calculate the higher-order GFs in (A.17), we differentiate its r.h.s. with respect to the second-time variable (t'). Let us give explicitly one of the four equations. After introducing the irreducible parts as

discussed above we get

$$\langle\langle A_i|S^-_{-k}\rangle\rangle_\omega \Omega_1 = \frac{I}{N}\sum_{p'q'}\langle\langle A_i|S^-_{-(k-q')}(a^\dagger_{p'\uparrow}a_{p'+q'\uparrow} - a^\dagger_{p'\downarrow}a_{p'+q'\downarrow})^{\rm ir} - 2S^z_{-(k-q')}a^\dagger_{p'\downarrow}a_{p'+q'\uparrow}\rangle\rangle_\omega$$
$$+ N^{-1/2}\sum_{q'} J_{q'}\langle\langle A_i|[(S^z_{q'})^{\rm ir}S^-_{-(k+q')} - (S^z_{-(k+q')})^{\rm ir}S^-_{q'}]^{\rm ir}\rangle\rangle_\omega. \tag{A.20}$$

Here the symbolic notation for the three equation of motions was used with $i = 1, 2, 3$. The quantity A_i in the l.h.s. of (A.20) should be substituted by

$$A_i = \begin{cases} A_1 = ((S^z_q)^{\rm ir}S^+_{k-q} - (S^z_{k-q})^{\rm ir}S^+_q)^{\rm ir}, \\ A_2 = S^+_{k-q}(a^\dagger_{p\uparrow}a_{p+q\uparrow} - a^\dagger_{p\downarrow}a_{p+q\downarrow})^{\rm ir}, \\ A_3 = 2S^z_{k-q}a^\dagger_{p\uparrow}a_{p+q\downarrow}. \end{cases}$$

In the matrix notation the full equation of motion for the GF $\hat{D}(k;\omega)$ can now be written in the following form:

$$\hat{\Omega}\hat{D}(p;\omega) = \sum_{p'}\hat{\Phi}(p')\hat{D}_1(p';\omega), \tag{A.21}$$

where

$$\hat{D}_1 = \begin{pmatrix} \langle\langle A_1|A_1^\dagger\rangle\rangle & \langle\langle A_1|A_2^\dagger\rangle\rangle \\ \langle\langle A_2|A_1^\dagger\rangle\rangle & \langle\langle A_2|A_2^\dagger\rangle\rangle \end{pmatrix}. \tag{A.22}$$

Combining both (the first- and second-time differentiated) equations of motion, we get the "exact" (no approximation has been made till now) "scattering" equation

$$\hat{\Omega}\hat{G}(k;\omega) = \hat{I} + \sum_{pp'}\hat{\Phi}(p)\hat{P}(p,p')\hat{\Phi}(p')(\hat{\Omega}^\dagger)^{-1}. \tag{A.23}$$

This equation can be identically transformed to the standard form Eq. (16)

$$\hat{G} = \hat{G}_0 + \hat{G}_0\left(\sum_{pp'}\hat{I}^{-1}\Phi(p)\hat{P}(p,p')\Phi(p')\hat{I}^{-1}\right)\hat{G}_0,$$

$$\hat{G} = \hat{G}_0 + \hat{G}_0\hat{P}\hat{G}_0. \tag{A.24}$$

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

$$\hat{G}_0 = \hat{\Omega}^{-1}\hat{I}. \tag{A.25}$$

The scattering operator P has the form

$$\hat{P} = \hat{I}^{-1}\sum_{pp'}\hat{\Phi}(p)\hat{P}(p,p')\hat{\Phi}(p')\hat{I}^{-1}. \tag{A.26}$$

Here we have used the obvious notation

$$\hat{P}(p,p';\omega) = \begin{pmatrix} \langle\langle A_1|A_1^\dagger\rangle\rangle & \langle\langle A_1|A_2^\dagger\rangle\rangle \\ \langle\langle A_2|A_1^\dagger\rangle\rangle & \langle\langle A_2|A_2^\dagger\rangle\rangle \end{pmatrix}. \tag{A.27}$$

As is shown above, Eq. (A.24) can be transformed exactly into the Dyson equation (18)

$$\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{M} \hat{G}_0 \tag{A.28}$$

with the self-energy operator M given as

$$\hat{M} = (\hat{P})^p. \tag{A.29}$$

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