Role of Correlation and Exchange for Quasi-particle Spectra of Magnetic and Diluted Magnetic Semiconductors

A. L. Kuzemsky†

Bogoliubov Laboratory of Theoretical Physics,
Joint Institute for Nuclear Research, 141980 Dubna, Russia

(June 11, 2018)

Abstract

Theoretical foundation and application of the generalized spin-fermion (sp−d) exchange lattice model to magnetic and diluted magnetic semiconductors are discussed. The capabilities of the model to describe spin quasi-particle spectra are investigated. The main emphasis is made on the dynamic behavior of two interacting subsystems, the localized spins and spin density of itinerant carriers. A nonperturbative many-body approach, the Irreducible Green Functions (IGF) method, is used to describe the quasi-particle 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 quasi-particle excitations with special attention given to diluted magnetic semiconductors. For this, to include the effects of disorder, modified mean fields are determined self-consistently. The role of the Coulomb correlation and exchange is clarified by comparing of both the cases.

75.50.Pp, 75.10.-b, 75.30.Ds
I. INTRODUCTION

There is considerable current interest in the properties of magnetic [1,2] and diluted magnetic semiconductors [3]- [8]. This field is very active and there are many aspects to the problem. A lot of materials were synthesized and tested [9]- [12]. The new materials design approach to fabrication of new functional diluted magnetic semiconductors (DMS) resulted in producing a variety of compounds. Diluted magnetic semiconductors are semiconducting alloys whose lattice contains magnetic atoms as randomly distributed substitutional impurities such as Mn-doped InAs or GaAs (general formula $A_{1-x}^\text{III}Mn_x^\text{II}B^\text{V}$). A fraction of A sublattice which is substituted at random by Mn changes the carrier density from the low doping (nearly insulating regime) to the large doping (metallic regime). 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 semiconducting properties as well as a rich field of interplay between them. 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 [13], [14]. Behavior and the true nature of the electronic and spin states, and their quasi-particle dynamics are of central importance to the understanding of physics of correlated systems such as magnetism and Mott-Hubbard metal-insulator transition in metals and oxides, magnetism and heavy fermions (HF) in rare-earths compounds, and anomalous transport properties in perovskite manganites. This class of systems is characterized by the complex, many-branch spectra of elementary excitations. Moreover, the correlations effects are essential [15], [16].

Recently, there has been considerable interest in identifying the microscopic origin of quasiparticle states in such systems and a few model approaches have been proposed. Many
magnetic and electronic properties of magnetic semiconductors and related materials may be interpreted reasonably in terms of combined spin-fermion models (SFM) which include the interacting spin and charge subsystems [13], [14], [15]. This approach permits one to describe significant and interesting physics, e.g., the bound states and magnetic polarons [17], [18], anomalous transport properties, etc.

The problem of adequate physical description within various types of generalized spin-fermion model 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 [29], [19] and magnetic semiconductors [15]-[18], [20]-[25]. For DMS the continuous analog of the Zener model was proposed recently by Dietl et al. [4]. The interplay of magnetic and semiconducting behavior was considered within a phenomenological mean field scheme.

The majority of theoretical papers on DMS studied its properties mainly within the mean field approximation and continuous media terms. In such a picture the disorder effects, which play an essential role [30]-[32], can be taken into account roughly only. However, many experimental investigations call for a better understanding of the relevant physics and nature of solutions (especially magnetic) in terms of the lattice spin-fermion model [19], [33]. In the previous papers, we set up the formalism of the method of Irreducible Green Functions (IGF) [16]. This IGF method allows one to describe the quasi-particle spectra with damping for a many-particle system 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 [26] and permits construction of the relevant dynamical 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 the quasi-particle 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 Generalized Mean Fields (GMF) [16] 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. Theoretical
foundation and application of the generalized spin-fermion (sp-d) exchange model to mag-
netic and diluted magnetic semiconductors are discussed in some detail. The capabilities of
the model to describe quasi-particle spectra are investigated. The purpose is to investigate
the quasi-particle spectra and GMF of the magnetic semiconductors consisting of two in-
teracting 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.

II. SPIN-FERMI ON MODEL

The concept of the sp − d ( or d − f ) model plays an important role in the quantum
theory of magnetism [13], [14], [19], [27], [28], [29]. In this section, we consider the generalized
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

\[ H = H_s + H_{s-d} + H_d \]  \hspace{1cm} (1)

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

\[ H_s = \sum_{ij} \sum_{\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + \frac{1}{2} \sum_{i\sigma} U n_{i\sigma} n_{i-\sigma} \]  \hspace{1cm} (2)

This is the Hubbard model. We adopt the notation

\[ a_{i\sigma} = N^{-1/2} \sum_{\vec{k}} a_{k\sigma} \exp(i\vec{k}\vec{R}_i) \quad a_{i\sigma}^\dagger = N^{-1/2} \sum_{\vec{k}} a_{k\sigma}^\dagger \exp(-i\vec{k}\vec{R}_i) \]

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 $\epsilon(\vec{k})$ is defined as follows:

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

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

$$\epsilon(\vec{k}) = 2 \sum_{\alpha} t(\vec{a}_\alpha) \cos(\vec{k}\vec{a}_\alpha)$$

(3)

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

The term $H_{s-d}$ describes the interaction of the total 3d(4f)-spin with the spin density of the itinerant carriers [28]

$$H_{s-d} = -2 \sum_i I\vec{\sigma}_i \vec{S}_i = -IN^{-1/2} \sum_{kq} [S^- \sigma_k a^\dagger_{k+q-\sigma} + z_\sigma S^z \sigma_k a^\dagger_{k+q\sigma}]$$

(4)

where sign factor $z_\sigma$ is given by

$$z_\sigma = (+ or -) \ f o r \ \sigma = (\uparrow \ o r \ \downarrow)$$

and

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

(5)

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

$$H_d = -\frac{1}{2} \sum_{ij} J_{ij} \vec{S}_i \vec{S}_j = -\frac{1}{2} \sum_q J_q \vec{S}_q \vec{S}_{-q}$$

Here we use the notation

$$S^\alpha_i = N^{-1/2} \sum_{\vec{k}} S^\alpha_i \exp(i\vec{k}\vec{R}_i) \ S^\alpha_k = N^{-1/2} \sum_{\vec{k}} S^\alpha_i \exp(-i\vec{k}\vec{R}_i)$$

$$[S^\pm_k, S^z_q] = \mp S^\pm_{k+q} \ [S^\pm_k, S^z_q] = \frac{2}{N^{1/2}} S^z_{k+q}$$

$$J_{ij} = N^{-1} \sum_k J_k \exp[i\vec{k}(\vec{R}_i - \vec{R}_j)],$$
This term describes the direct exchange interaction 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

\[ H_{RKKY} = -\sum_{i\neq j} K_{ij} \vec{S}_i \vec{S}_j \] (6)

We emphasize that \( K_{ij} \sim |I|^2 \sim V_{p-d}^4 \). To explain this, let us remind that the microscopic model [28], which contains the basic physics, is the Anderson-Kondo model

\[ H = \sum_{ij} \sum_{\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} - V \sum_{ij} \sum_{\sigma} (a_{i\sigma}^\dagger d_{j\sigma} + h.c.) - E_d \sum_i \sum_{\sigma} n_{i\sigma}^d + \frac{1}{2} \sum_{i\sigma} U n_{i\sigma}^d n_{i-\sigma}^d \] (7)

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

\[ H = \sum_{ij} \sum_{\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} - 2I \vec{\sigma}_i \vec{S}_i \] (8)

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

III. OUTLINE OF THE IGF METHOD

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

We reformulated the two-time GF method [16] to the form which is especially adjusted to correlated fermion systems on a lattice and systems with complex spectra [15]-[19]. A very important concept of the whole method is the Generalized Mean Fields (GMFs), as it was formulated in [16]. These GMFs 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.

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

\[ G^r = \langle\langle A(t), A^\dagger(t') \rangle\rangle = -i\theta(t - t') \langle A(t)A^\dagger(t') \rangle_\eta, \eta = \pm 1 \]  

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

\[ \omega G(\omega) = \langle [A, A^\dagger]_\eta \rangle + \langle\langle [A, H] - zA^\dagger [A, H] - zA \rangle\rangle \]

The essence of the method is as follows [16]:

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

\[ ^{\text{ir}}\langle\langle [A, H]_\eta A^\dagger \rangle\rangle = \langle\langle [A, H] - zA \rangle A^\dagger \rangle \]

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

\[ \langle [A, H]_\eta A^\dagger \rangle = 0 \]  

which is an analogue of the orthogonality condition in the Mori formalism. From the condition (12) one can find

\[ z = \frac{\langle [A, H]_\eta A^\dagger \rangle}{\langle [A, A^\dagger]_\eta \rangle} = \frac{M_1}{M_0} \]  

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 the 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

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

(14)

To calculate the IGF $<A, H(t), A^\dagger(t')>$ 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

$$G = G^0 + G^0 P G^0$$

(15)

The scattering operator $P$ is given by

$$P = (M_0)^{-1} (<A, H|A^\dagger, H>_<>^{(ir)})(M_0)^{-1}$$

(16)

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

$$P = M + MG^0 P$$

(17)

From the 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

$$G = G^0 + G^0 M G$$

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

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

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

$$(G^0)^{-1} - G^{-1} = PG^0G^{-1}$$

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

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. Notice that all quantities thus considered are exact. Approximations can be generated not by truncating the set of coupled equations of motions but by a specific approximation of the functional form of the mass operator $M$ within a self-consistent scheme expressing $M$ in terms of 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 the constraint (12) in our approach we emphasize the fundamental and central role of the Dyson equation for the 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 through the diagrammatic expansion for the causal GF.

It is important to note that for the retarded and advanced GFs, the notion of the proper part \( M = (P)^p \) is symbolic in nature [16]. In a certain sense, it is possible to say that it is defined here by analogy with the irreducible many-particle \( T \)-matrix. Furthermore, by analogy with the diagrammatic technique, we can also introduce the proper part defined as a solution to the integral equation (17). These analogues allow us to understand better the formal structure of the Dyson equation for the double-time thermal GF but only in a symbolic form. However, because of the identical form of the equations for GFs for all three types (advanced, retarded, and causal), we can convert in each stage of calculations to causal GF and, thereby, confirm the substantiated nature of definition (17)! We therefore should speak of an analogy of the Dyson equation. Hereafter, we drop this stipulating, since it does not cause any misunderstanding. In a sense, the IGF method is a variant of the Gram-Schmidt orthogonalization procedure.

It should be emphasized that the scheme presented above gives just a general idea of the IGF method. A more exact explanation why one should not introduce the approximation already in \( P \), instead of having to work out \( M \), is given below when working out the application of the method to specific problems.

The general philosophy of the IGF method is in the separation and identification of elastic scattering effects and inelastic ones. This latter point is quite often underestimated, and both effects are mixed. However, as far as the right definition of quasi-particle damping is concerned, the separation of elastic and inelastic scattering processes is believed to be cru-
cially important for many-body systems with complicated spectra and strong interaction. From a technical point of view, the elastic GMF renormalizations can exhibit quite a non-trivial structure. To obtain this structure correctly, one should construct the full GF from the complete algebra of relevant operators and develop a special projection procedure for higher-order GFs, in accordance with a given algebra. Then a natural question arises how to select the relevant set of operators \( \{A_1, A_2, \ldots, A_n\} \) describing the "relevant degrees of freedom". The above consideration suggests an intuitive and heuristic way to the suitable procedure as arising from an infinite chain of equations of motion (10). Let us consider the column

\[
\begin{pmatrix}
A_1 \\
A_2 \\
\vdots \\
A_n
\end{pmatrix}
\]

where

\[
A_1 = A, \quad A_2 = [A, H], \quad A_3 = [[A, H], H], \ldots A_n = [[[...[A, H]...H]...H]_n]
\]

Then the most general possible Green function can be expressed as a matrix

\[
\hat{G} = \langle\langle \begin{pmatrix}
A_1 \\
A_2 \\
\vdots \\
A_n
\end{pmatrix} | (A_1^\dagger \ A_2^\dagger \ \ldots \ A_n^\dagger) \rangle\rangle
\]

This generalized Green function describes the one-, two- and \( n \)-particle dynamics. The equation of motion for it includes, as a particular case, the Dyson equation for single-particle Green function, and the Bethe-Salpeter equation which is the equation of motion for the two-particle Green function and which is an analogue of the Dyson equation, etc. The corresponding reduced equations should be extracted from the equation of motion for the generalized GF with the aid of the special techniques such as the projection method and similar techniques. This must be a final goal towards a real understanding of the true many-body dynamics. At this point, it is worthwhile to underline that the above discussion is a
heuristic scheme only but not a straightforward recipe. The specific method of introducing the IGFs depends on the form of operators $A_n$, the type of the Hamiltonian, and conditions of the problem.

Here a sketchy form of the IGF method is presented. The aim is to introduce the general scheme and to lay the groundwork for generalizations. We demonstrated in [16] that the IGF method is a powerful tool for describing the quasi-particle excitation spectra, allowing a deeper understanding of elastic and inelastic quasi-particle 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 generalized mean fields of the complicated many-body models.

IV. QUASI-PARTICLE 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 the quasi-particle spectra of two interacting subsystem.

We have two kinds of spin variables

$$S_k^+, \quad S_{-k} = (S_k^+)^\dagger$$

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

Let us consider the equations of motion

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

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

$$[S_k^z, H_{s-d}] = -IN^{-1} \sum_{pq} (S_{k-q}^+ a_{p\uparrow}^+ a_{p+q\uparrow} - S_{k-q}^- a_{p\downarrow}^+ a_{p+q\downarrow})$$
\[ [S^+_k, H_d]_- = N^{-1/2} \sum_q J_q (S^z_q S^+_k - S^z_k S^+_q) \]  

(23)

\[ [S^-_k, H_d]_- = N^{-1/2} \sum_q J_q (S^z_q S^-_{k+q} - S^z_{k+q} S^-_q) \]  

(24)

\[ [a^\dagger_{q\uparrow} a_{q+k\downarrow}, H_s]_+ = (\epsilon(q + k) - \epsilon(q))a^\dagger_{q\uparrow} a_{q+k\downarrow} + \]  

\[ UN^{-1} \sum_{pq'} (a^\dagger_{q\uparrow} a^\dagger_{p'+p\uparrow} a_{p+q'} - a^\dagger_{q+p\uparrow} a^\dagger_{p'-p\downarrow} a_{q+k\downarrow}) \]  

(25)

\[ [a^\dagger_{q\uparrow} a_{q+k\downarrow}, H_{s-d}]_+ = IN^{-1/2} \sum_{pq'} [S^+_{p'} (a^\dagger_{q\uparrow} a_{p'+p\uparrow} \delta_{p,q,k} - a^\dagger_{p\uparrow} a_{q+k\downarrow} \delta_{q,p+q'}) - S^z_{p'} (a^\dagger_{q\uparrow} a_{p'+p\uparrow} \delta_{p+q+k} + a^\dagger_{p\uparrow} a_{q+k\downarrow} \delta_{q,p+q'})) \]  

(26)

From Eq.(20) - Eq.(26) it follows that the localized and itinerant spin variables are coupled. Suitable algebra of relevant operators should be described by the ‘spinor’ \( (\vec{S}_i \vec{\sigma}_i) \) ("relevant degrees of freedom"), according to the IGF strategy.

The model Hamiltonian \( H = H_s + H_{s-d} + H_d \) was used in [34], [35] 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 \( H_{s-d} \). Because of the inequivalent spin systems, localized and itinerant, a consequence of the model is the existence of acoustic and optic branches of the quasi-particle spectrum of spin excitations. In DMS the local antiferromagnetic interaction \( H_{s-d} \) produces the coupling between the carriers (which are holes in GaMnAs) and the Mn magnetic moments \( (s = 5/2) \) 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 [3]. An important question in this context is the self-consistent picture of the quasi-particle many-body dynamics which takes into account the complex structure of the spectra.
A. Spin Dynamics of the \( s-d \) Model. Scattering Regime.

In this section, we discuss the spectrum of spin excitations in the \( sp-d \) model. We consider the double-time thermal GF of localized spins [26] which is defined as

\[
G^{+-}(k; t-t') = \langle \langle S^+_k(t), S^-_k(t') \rangle \rangle = -i\theta(t-t') \langle [S^+_k(t), S^-_k(t')] \rangle - 1/2\pi \int_{-\infty}^{+\infty} d\omega \exp(-i\omega t)G^{+-}(k; \omega) \quad (27)
\]

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 quasi-particle spectra of two interacting subsystems. We introduce the generalized matrix GF of the form

\[
\begin{pmatrix}
\langle \langle S^+_k | \sigma^-_k \rangle \rangle & \langle \langle S^+_k | \sigma^-_k \rangle \rangle \\
\langle \langle \sigma^+_k | \sigma^-_k \rangle \rangle & \langle \langle \sigma^+_k | \sigma^-_k \rangle \rangle
\end{pmatrix} = \hat{G}(k; \omega) \quad (28)
\]

Here

\[
\sigma^+_k = \sum_q a^\dagger_{k+q}a_{k}; \quad \sigma^-_k = \sum_q a^\dagger_{k}a_{k+q}
\]

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

\[
\begin{pmatrix}
\langle \langle S^+_k | S^-_k \rangle \rangle & \langle \langle S^+_k | a^\dagger_{k+q}a_{q} \rangle \rangle \\
\langle \langle a^\dagger_{q}a_{k+q} | S^-_k \rangle \rangle & \langle \langle a^\dagger_{q}a_{k+q} | a^\dagger_{k+q}a_{q} \rangle \rangle
\end{pmatrix} = \hat{G}'(k; \omega), \quad (29)
\]

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

Let us consider the equation of motion for the GF \( \hat{G}(k; \omega) \). By differentiation of the GF \( \langle \langle S^+_k(t) | B(t') \rangle \rangle \) with respect to the first time, \( t \), we find

\[
\omega \langle \langle S^+_k | B \rangle \rangle = \left\{ \begin{array}{ll}
2N^{-1/2} \langle S^+_0 \rangle \\
0
\end{array} \right\} + \frac{I}{N} \sum_{pq} \langle \langle S^+_k a^\dagger_{p+q}a_{p+q} - a^\dagger_{p}a_{p+q} | S^+_k \rangle \rangle \langle \langle a^\dagger_{p}a_{p+q} | B \rangle \rangle + \frac{N^{-1/2}}{J} \sum_q \langle \langle \sigma^+_k - S^+_k S^-_k \rangle \rangle \langle \langle \sigma^-_k - S^+_k S^-_k \rangle \rangle B \rangle \rangle \quad (30)
\]

\[
\frac{1}{N} \sum_{pq} \langle \langle S^+_k a^\dagger_{p+q}a_{p+q} - a^\dagger_{p}a_{p+q} | S^+_k \rangle \rangle \langle \langle a^\dagger_{p}a_{p+q} | B \rangle \rangle + \frac{N^{-1/2}}{J} \sum_q \langle \langle \sigma^+_k - S^+_k S^-_k \rangle \rangle \langle \langle \sigma^-_k - S^+_k S^-_k \rangle \rangle B \rangle \rangle \quad (31)
\]

14
where

\[ B = \left\{ S_{-k}^-, \sigma_{-k} \right\} \]

Let us introduce by definition irreducible (ir) operators as

\[
(S_q^z)^{ir} = S_q^z - < S_0^z > \delta_{q,0}; \quad (a_{p+q\sigma}^{\dagger}a_{p\sigma})^{ir} = a_{p+q\sigma}^{\dagger}a_{p\sigma} - < a_{p\sigma}a_{p\sigma} > \delta_{q,0} \tag{32}
\]

\[
((S_q^z)^{ir} S_{k-q}^+ - (S_{k-q}^z)^{ir} S_q^+)^{ir} = ((S_q^z)^{ir} S_{k-q}^+ - (S_{k-q}^z)^{ir} S_q^+) - (\phi_q - \phi_{k-q})S_k^+ \tag{33}
\]

From the condition (12)

\[
< [(S_q^z)^{ir} S_{k-q}^+ - (S_{k-q}^z)^{ir} S_q^+] - (\phi_q - \phi_{k-q})S_k^+] - > = 0
\]

one can find

\[
\phi_q = \frac{2K_q^{zz} + K_q^{-+}}{2 < S_0^z >} \tag{34}
\]

\[
K_q^{zz} = < (S_q^z)^{ir} (S_q^z)^{ir} >; \quad K_q^{-+} = < S_q^- S_q^+ > \tag{35}
\]

Using the definition of the irreducible parts the equation of motion Eq.(30) can be exactly transformed to the following form:

\[
\Omega_1 < S_k^+ | B > >_\omega + \Omega_2 < \sigma_k^+ | B > >_\omega = \left\{ \begin{array}{l}
\left( \frac{N^{1/2}}{T} \right) \Omega_2 \\
0
\end{array} \right\} + < A_1 | B > >_\omega \tag{36}
\]

where

\[
\Omega_1 = \omega - < S_0^z > \frac{1}{N^{1/2}} (J_0 - J_k) - N^{-1/2} \sum_q (J_q - J_{q-k}) \frac{2K_q^{zz} + K_q^{-+}}{2 < S_0^z >} - I(n_\uparrow - n_\downarrow) \tag{37}
\]

\[
\Omega_2 = \frac{2 < S_0^z > I}{N} \tag{38}
\]

\[
n_\sigma = \frac{1}{N} \sum_q < a_{q\sigma}^{\dagger}a_{q\sigma} > = \frac{1}{N} \sum_q f_{q\sigma} = \sum_q (\exp(\beta \epsilon(q\sigma)) + 1)
\]

\[
\epsilon(q\sigma) = \epsilon(q) - z_\sigma IN^{-1/2} < S_0^z > + Un_{-\sigma}
\]

\[
\bar{n} = \sum(n_\uparrow + n_\downarrow); \quad 0 \leq \bar{n} \leq 2
\]

The many-particle operator $A_1$ reads
\[ A_1 = \frac{I}{N} \sum_{pq} [S_{k-q}^+ (a^\dagger_{p+q} a^\dagger_{p+q} - a^\dagger_{p} a^\dagger_{p+q}) \text{ir} - 2(S_{k-q}^z) \text{ir} a^\dagger_{p+q} a^\dagger_{p+q}] \]
\[ + N^{-1/2} \sum_{q} J_q ((S_q^z) \text{ir} S_{k-q}^+ - (S_{k-q}^z) \text{ir} S_q^+) \text{ir} \] 

(39)

and it satisfies the conditions

\[ < [A_1, S^{-}_q]_\text{-} >= < [A_1, \sigma^{-}_q]_\text{-} >= 0 \]

To write down the equation of motion for the Fourier transform of the GF \( <\sigma^+_k(t), B(t')>\), we need the following auxiliary equation of motion:

\[
(\omega + \epsilon(p) - \epsilon(p + k) - 2IN^{-1/2} < S_0^z > - U(n^\uparrow - n^\downarrow)) <a^\dagger_{p+q} B> \omega + \] 

(40)

\[
UN^{-1}(f_{p+q} - f_{p+q}) <\sigma^+_k B> \omega + IN^{-1/2}(f_{p+q} - f_{p+q}) <S^+_k B> \omega = \]

\[
\left\{ \begin{array}{l}
0 \\
IN^{-1/2} \sum_{qr} <S^+_{-r}(a^\dagger_{q+r} a^\dagger_{p+q+r} \delta_{p+k,q} + a^\dagger_{p+q+r} \delta_{p,q+r}) \text{ir} [B] > \omega - \end{array} \right. \]

\[
IN^{-1/2} \sum_{qr} <(S^z_{-r}) \text{ir} (a^\dagger_{q+r} a^\dagger_{p+q+r} \delta_{p,q+r} + a^\dagger_{p+q+r} \delta_{p,q+r}) [B] > \omega + \]

\[
UN^{-1} \sum_{qr} <(a^\dagger_{p+q+r} a^\dagger_{p+q+r} a^\dagger_{q+r} a^\dagger_{p+q+r} \delta_{p,q+r}) \text{ir} [B] > \omega \]

Let us use the following notation:

\[
A_2 = -IN^{-1/2} \sum_{qr} [S^+_{-r}(a^\dagger_{q+r} a^\dagger_{p+q+r} \delta_{p+k,q} + a^\dagger_{p+q+r} \delta_{p,q+r}) \text{ir} - \]

\[
(S^z_{-r}) \text{ir} (a^\dagger_{q+r} a^\dagger_{p+q+r} \delta_{p,q+r} + a^\dagger_{p+q+r} \delta_{p,q+r})] + \]

(41)

\[
UN^{-1} \sum_{qr} (a^\dagger_{p+q+r} a^\dagger_{p+q+r} a^\dagger_{q+r} a^\dagger_{p+q+r} \delta_{p,q+r} \text{ir} - a^\dagger_{p+q+r} a^\dagger_{q+r} a^\dagger_{p+q+r} \text{ir}) \omega_{p,k} = (\omega + \epsilon(p) - \epsilon(p + k) - \Delta) \]

(42)

\[
\Delta = 2IN^{-1/2} < S_0^z > - U(n^\uparrow - n^\downarrow) = 2I \tilde{S} - Um = \Delta_I + \Delta_U \]

(43)

\[
\chi_0^s(k, \omega) = N^{-1} \sum_p \frac{(f_{p+k} - f_{p+q})}{\omega_{p,k}} \]

(44)

Now we consider the GF \( <\sigma^+_k(t), B(t')>\). Similarly to Eq. (36), we have

\[
-N^{1/2} I \chi_0^s(k, \omega) < S_{k}^+ [B] > \omega + (1 - U \chi_0^s(k, \omega)) <\sigma^+_k B > \omega = \]

\[
\left\{ \begin{array}{l}
0 \\
-N \chi_0^s(k, \omega) \end{array} \right\} + \sum_p \frac{1}{\omega_{p,k}} <A_2 [B] > \omega \]

(45)

Here the following definition of the irreducible part for the Coulomb correlation term was used
(a_{p+r\uparrow}^\dagger a_{p+r\downarrow}^\dagger a_{p+r+k\downarrow} - a_{p+r\uparrow}^\dagger a_{p+r\downarrow}^\dagger a_{p+r+k\uparrow})^{ir} \\
= (a_{p+r\uparrow}^\dagger a_{p+r\downarrow}^\dagger a_{p+r+k\downarrow} - a_{p+r\uparrow}^\dagger a_{p+r\downarrow}^\dagger a_{p+r+k\uparrow}) \\
- < a_{p+r\uparrow}^\dagger a_{p+r\downarrow}^\dagger > \delta_{q+r,q} a_{p+r+k\downarrow}^\dagger \\
- < a_{p+r\uparrow}^\dagger a_{p+r\downarrow}^\dagger > \delta_{q+r,q} a_{p+r+k\uparrow}^\dagger \\
(46)

The operator $A_2$ satisfies the conditions

$$< [A_2, S_{-k}^\downarrow] >= < [A_2, \sigma_{-k}^\downarrow] > = 0$$

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

$$\hat{\Omega}\hat{G}(k; \omega) = \hat{I} + \sum_p \hat{\Phi}(p)\hat{D}(p; \omega)$$

$$(\hat{G}(k; \omega))^\dagger(\hat{\Omega}) = (\hat{I})^\dagger + \sum_p (\hat{D}(p; \omega))^\dagger(\hat{\Phi}(p))^\dagger$$

where

$$\hat{\Omega} = \begin{pmatrix} \Omega_1 & \Omega_2 \\ -IN^{1/2} \chi_0^s & (1 - U \chi_0^s) \end{pmatrix} \quad \hat{I} = \begin{pmatrix} I^{-1}N^{1/2} \Omega_2 & 0 \\ 0 & -N \chi_0^s \end{pmatrix}$$

$$\hat{D}(p; \omega) = \begin{pmatrix} << A_1 | S_{-k}^\downarrow >> & << A_1 | \sigma_{-k}^\downarrow >> \\ << A_2 | S_{-k}^\downarrow >> & << A_2 | \sigma_{-k}^\downarrow >> \end{pmatrix} \quad \hat{\Phi}(p) = \begin{pmatrix} N^{-1} & 0 \\ 0 & \omega_{p,k}^{-1} \end{pmatrix}$$

To calculate the higher order GFs in (47), 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

$$<< A | S_{-k}^\downarrow >>_\omega \Omega_1 = \frac{I}{N} \sum_{p'q'} << A | S_{-(k-q')}^\downarrow (a_{p'\uparrow}^\dagger a_{p'\downarrow}^\dagger - a_{p'\downarrow}^\dagger a_{p'\uparrow}^\dagger) \ ir - 2S_{-(k-q')}^z a_{p'\uparrow}^\dagger a_{p'\downarrow}^\dagger >>_\omega \\
+ N^{-1/2} \sum_{q'} J_{q'p} << A | [(S_{q'}^z)^{ir} S_{-(k+q')}^\downarrow - (S_{-(k+q')}^\downarrow)^{ir} S_{q'}^z]^{ir} >>_\omega$$

(50)

Here, the quantity $A$ in the l.h.s. should be substituted by

$$A = \begin{cases} 
((S_{q}^z)^{ir} S_{k-q}^+ - (S_{k-q}^z)^{ir} S_{q}^+)^{ir} \\
S_{k-q}^+(a_{p\uparrow}^\dagger a_{p+q\uparrow}^\dagger - a_{p\downarrow}^\dagger a_{p+q\downarrow})^{ir} \\
2S_{k-q}^z a_{p\uparrow}^\dagger a_{p+q\downarrow} \end{cases}$$
In the matrix notation the full equation of motion for the GF $\hat{D}(k;\omega)$ can now be written in the following form:

$$\hat{\Omega}\hat{D}(p;\omega) = \sum_{p'} \hat{\Phi}(p')\hat{D}_1(p';\omega)$$  \hspace{1cm} (51)

where

$$\hat{D}_1 = \begin{pmatrix} <<A_1|A_1^\dagger>> & <<A_1|A_2^\dagger>> \\ <<A_2|A_1^\dagger>> & <<A_2|A_2^\dagger>> \end{pmatrix}$$  \hspace{1cm} (52)

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

$$\hat{\Omega}\hat{G}(k;\omega) = \hat{I} + \sum_{pp'} \hat{\Phi}(p)\hat{P}(p,p')\hat{\Phi}(p')(\hat{\Omega}^\dagger)^{-1}$$  \hspace{1cm} (53)

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

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

$$\hat{G} = \hat{G}_0 + \hat{G}_0\hat{P}\hat{G}_0$$  \hspace{1cm} (54)

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

$$\hat{G}_0 = \hat{\Omega}^{-1}\hat{I}$$  \hspace{1cm} (55)

The scattering operator $P$ has the form

$$\hat{P} = \hat{I}^{-1}\sum_{pp'} \hat{\Phi}(p)\hat{P}(p,p')\hat{\Phi}(p')\hat{I}^{-1}$$  \hspace{1cm} (56)

Here we have used the obvious notation

$$\hat{P}(p,p';\omega) = \begin{pmatrix} <<A_1|A_1^\dagger>> & <<A_1|A_2^\dagger>> \\ <<A_2|A_1^\dagger>> & <<A_2|A_2^\dagger>> \end{pmatrix}$$  \hspace{1cm} (57)

As is shown above, Eq.(54) can be transformed exactly into the Dyson equation (18)

$$\hat{G} = \hat{G}_0 + \hat{G}_0\hat{M}\hat{G}_0$$  \hspace{1cm} (58)

with the self-energy operator $M$ given as

$$\hat{M} = (\hat{P})^p$$  \hspace{1cm} (59)

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

From the definition (55), the GF matrix in the generalized mean-field approximation reads

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

(60)

where

\[
R = (1 - U\chi_0)\Omega_1 + \Omega_2 IN^{1/2}\chi_0^s
\]

Let us write down explicitly the diagonal matrix elements \(G_{01}^{11}\) and \(G_{02}^{22}\)

\[
<< S_k^+ | S_{-k}^- >>^0 = \frac{2\bar{S}}{\Omega_1 + 2I^2S\chi^s(k,\omega)}
\]

(61)

\[
<< \sigma_k^+ | \sigma_{-k}^- >>^0 = \frac{\Omega_1\chi^s(k,\omega)}{\Omega_1 + 2I^2S\chi^s(k,\omega)}
\]

(62)

where

\[
\chi^s(k,\omega) = \chi_0^s(k,\omega)(1 - U\chi_0^s(k,\omega))^{-1}
\]

(63)

\[
\bar{S} = N^{-1/2} < S_0^z >
\]

To clarify the functional structure of the generalized mean-field GFs (61) and (62), let us consider a few limiting cases.

A. 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

\[
<< S_k^+ | S_{-k}^- >>^0 = \frac{2\bar{S}}{\omega - \bar{S}(J_0 - J_k) - \frac{1}{2NS}\sum_q(J_q - J_{q-k})(2K_q^{zz} + K_q^{zz})}
\]

(64)
\[ \langle \sigma_k^+ | \sigma_{-k}^- \rangle^0 = \chi^s(k; \omega) \] (65)

The spectrum of quasi-particle excitations of localized spins without damping follows from the poles of the generalized mean-field GF (64)

\[ \omega(k) = \tilde{S}(J_0 - J_k) + \frac{1}{2NS} \sum_q (J_q - J_{q-k}) (2K^zz_q + K^{-+}_q) \] (66)

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:

\[ J_k = \sum_i \exp \left(-i\bar{k}\bar{R}_i\right) J(|\bar{R}_i|) \] (67)

The expansion in small \( \bar{k} \) gives

\[ J_k = \sum_i J(|\bar{R}_i|) - \frac{1}{2} \sum_i (\bar{k}\bar{R}_i)^2 J(|\bar{R}_i|) = J_0 - \frac{k^2}{2} \sum_i (\bar{n}\bar{R}_i)^2 J(|\bar{R}_i|) \] (68)

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

\[ J_{k-q} = J_q - (\bar{k}\nabla_q)J_q + \frac{1}{2}(\bar{k}\nabla_q)^2 J_q + \cdots \] (69)

\[ (\bar{k}\nabla_q)J_q = -i \sum_i (\bar{k}\bar{R}_i) J(|\bar{R}_i|) \exp(-i\bar{q}\bar{R}_i) \]

\[ (\bar{k}\nabla_q)^2 J_q = -\frac{1}{2} \sum_i (\bar{k}\bar{R}_i)^2 J(|\bar{R}_i|) \exp(-i\bar{q}\bar{R}_i) \]

Combining Eq.(69), Eq.(68), and Eq.(66) we get

\[ \langle \sigma_k^+ | \sigma_{-k}^- \rangle^0 = \frac{2\tilde{S}}{\omega - \omega(k)} \] (70)

\[ \omega(k \to 0) = \left( \tilde{S}(J_0 - J_k) + \frac{1}{2NS} \sum_q (J_q - J_{q-k}) (2K^zz_q + K^{-+}_q) \right) \approx D_1 k^2 \]

\[ = \left( \frac{\tilde{S}}{2} \psi_0 + \frac{N}{2S^2} \sum_q \psi_q (2K^zz_q + K^{-+}_q) \right) k^2 \]

\[ \psi_q = \sum_i (\bar{k}\bar{R}_i)^2 J(|\bar{R}_i|) \exp(-i\bar{q}\bar{R}_i) \]
Let us now consider the spin susceptibility of itinerant carriers Eq. (65) in the hydrodynamic limit $k \to 0$, $\omega \to 0$. It is convenient to consider the static limit of Eq. (65)

$$
<< \sigma^+_k | \sigma^-_k >>^0 |_{\omega=0} = \frac{\chi^s_{0}(k, 0)}{1 - U \chi^s_{0}(k, 0)}
$$  \hspace{1cm} (71)

$$
\chi^s_{0}(k, 0) = \frac{1}{N} \sum_q \frac{f_{q+k} - f_{q\uparrow}}{\epsilon(q) - \epsilon(q + k) - \Delta_U}
$$  \hspace{1cm} (72)

$$
\Delta_U = U(n_\uparrow - n_\downarrow) = Um
$$

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

$$
\epsilon(q + k) - \epsilon(q) = (\vec{k} \nabla_q)\epsilon(q) + \frac{1}{2}(\vec{k} \nabla_q)^2\epsilon(q) + \cdots
$$  \hspace{1cm} (73)

$$
\chi^s_{0}(k, 0) = \frac{1}{N \Delta_U} \sum_q (f_{q\uparrow} - f_{q\downarrow}) - \frac{1}{N \Delta_U^2} \sum_q (f_{q\uparrow} + f_{q\downarrow}) \frac{1}{2}(\vec{k} \nabla_q)^2\epsilon(q) + \frac{1}{N \Delta_U^2} \sum_q (f_{q\uparrow} - f_{q\downarrow}) (\vec{k} \nabla_q \epsilon(q))^2 + \cdots
$$

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

$$
1 - U \chi^s_{0}(k, \omega) = 0
$$  \hspace{1cm} (74)

In another form this reads in detail

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

If we set $\omega = E(k)$ and put then $k = 0$, 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.(73) exists which has the property

$$
\lim_{k \to 0} E(k) = 0
$$

and this solution corresponds to an acoustic spin-wave branch of excitations

$$
E(k) = D_2 k^2 = -\frac{U}{2N \Delta_U} \sum_q (f_{q\uparrow} + f_{q\downarrow})(\vec{k} \nabla_q)^2\epsilon(q) + \frac{U}{N \Delta_U^2} \sum_q (f_{q\uparrow} - f_{q\downarrow})(\vec{k} \nabla_q \epsilon(q))^2
$$

$$
\omega = \epsilon(k + q) - \epsilon(q) + \Delta_U
$$

It is seen that the stiffness constant $D_2$ can be interpreted as expanded in $\frac{1}{\Delta_U}$. For the tight-binding electrons in s.c. lattice the spin wave dispersion relation $D_2 k^2$ becomes
\[ D_2k^2 = (3(n^+ - n^-))^{-1} \sum_q \left( \frac{(f_{q}^+ - f_{q}^-)}{\Delta_U} \right) |\nabla_q \epsilon(q)|^2 - \frac{(f_{q}^+ + f_{q}^-)}{2} \nabla_q^2 \epsilon(q) = \] (75)

\[ (3(n^+ - n^-))^{-1}(\frac{2t^2a^2}{\Delta_U} \sum_q (f_{q}^+ - f_{q}^-) (k_x \sin(q_x a) + k_y \sin(q_y a) + k_z \sin(q_z a))^2 - \]
\[ ta^2 \sum_q (f_{q}^+ + f_{q}^-) (k_x^2 \cos q_x a + k_y^2 \cos q_y a + k_z^2 \cos q_z a)) \]

**B. Coupled Subsystems**

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

\[ << S^+_k | S^-_{-k} >>^0 = \frac{2\bar{S}}{\omega - Im - \bar{S}(J_0 - J_k) - \frac{1}{2N\bar{S}} \sum_q (J_q - J_{-q-k}) (2K_q^{zz} + K_{q}^{-+}) + 2t^2S\chi^s(k,\omega) \] (76)

\[ << \sigma^+_k | \sigma^-_{-k} >>^0 = \frac{\chi^s_0(k,\omega)}{1 - U_{eff}(\omega)\chi^s_0(k,\omega)} \] (77)

Here the notation is used

\[ U_{eff} = U - \frac{2t^2\bar{S}}{\omega - Im}; \quad m = (n^+ - n^-) \]

The expression Eq.(77) coincides with that for the itinerant spin susceptibility as calculated in [13]. 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) \( I \neq 0, J \neq 0, U \neq 0 \)
1.

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 (76) and (77) are then equal to

\[
\langle \langle S^+_k | S^-_k \rangle \rangle^0 = \frac{2\bar{S}}{\omega - Im + 2I^2S\chi^0_0(k, \omega)}
\]

\[
\langle \langle \sigma^+_k | \sigma^-_k \rangle \rangle^0 = \frac{\chi^0_0(k, \omega)}{\omega + 2I^2S\chi^0_0(k, \omega)}
\]

In order to calculate the acoustic pole of the GF (78), we make use of the small \((k, \omega)\) expansion. Hence we get

\[
\langle \langle S^+_k | S^-_k \rangle \rangle^0 \approx \frac{2\bar{S}(1 + \frac{m}{2\bar{S}})^{-1}}{\omega - (1 + \frac{m}{2\bar{S}})^{-1}[\frac{1}{2N\Delta f} \sum_q (f^q_\uparrow + f^q_\downarrow)(\vec{k} \nabla^q)^2\epsilon(\vec{q}) - \frac{1}{N\Delta f} \sum_q (f^q_\uparrow - f^q_\downarrow)(\vec{k} \nabla^q\epsilon(\vec{q}))^2]}
\]

It follows from Eq.(80) that the stiffness constant \( D \) is proportional to the total magnetization of the system.

2.

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

\[
\langle \langle S^+_k | S^-_k \rangle \rangle^0 = \frac{2\bar{S}}{\omega - Im - S(J_0 - J_k) - \frac{1}{2NSB} \sum_q (J_q - J_{q-k})(2K^{zz}_q + K^{-+}_q) + 2I^2S\chi^0_0(k, \omega)}
\]

\[
\langle \langle \sigma^+_k | \sigma^-_k \rangle \rangle^0 = \frac{\chi^0_0(k, \omega)}{1 - \frac{2I^2S}{\omega - Im}\chi^0_0(k, \omega)}
\]

In order to calculate the acoustic pole of the GF (81), we make use of the small \((k, \omega)\) expansion again. We then get

\[
\langle \langle S^+_k | S^-_k \rangle \rangle^0 \approx \frac{2\bar{S}(1 + \frac{m}{2\bar{S}})^{-1}}{\omega - (1 + \frac{m}{2\bar{S}})^{-1}[\frac{1}{2N\Delta f} \sum_q (f^q_\uparrow + f^q_\downarrow)(\vec{k} \nabla^q)^2\epsilon(\vec{q}) - \frac{1}{N\Delta f} \sum_q (f^q_\uparrow - f^q_\downarrow)(\vec{k} \nabla^q\epsilon(\vec{q}))^2]}
\]

It follows from Eqs.(80) and (83) that the stiffness constant \( D \) is proportional to the total magnetization of the system.
3.

The third case \( I \neq 0, J = 0, U \neq 0 \) corresponds to a model which is called the modified Zener lattice model \([34]\). It can be seen that in this case GFs (76) and (77) are equal to

\[
<< S^+_k | S^-_k >>^0 = \frac{2\bar{S}}{\omega - Im + 2I^2 S \chi_s(k, \omega)} \quad (84)
\]

\[
<< \sigma^+_k | \sigma^-_k >>^0 = \frac{\chi^s_0(k, \omega)}{1 - U_{eff}(\omega) \chi_0(k, \omega)} \quad (85)
\]

The results obtained here coincide with those of Bartel \([34]\). The excitation energies for the localized spin and spin densities of itinerant carriers are found from the zeros of the denominators of \( << S^+_k | S^-_k >>^0 \) and \( << \sigma^+_k | \sigma^-_k >>^0 \) which yield identical excitation spectra, consisting of three branches, the acoustic spin wave \( E^{ac}(k) \), the optical spin wave \( E^{op}(k) \), and the Stoner continuum \( E^{St}(k) \)

\[
E^{ac}(k) = Dk^2
\]

\[
E^{op}(k) = E_0^{op} - D(1 - \frac{UE^{op}}{I\Delta})k^2; \quad E_0^{op} = I(m + 2\bar{S})
\]

\[
E^{St}(k) = \epsilon(k + q) - \epsilon(q) + \Delta
\]

4.

The most general is the forth case, \( I \neq 0, J \neq 0, U \neq 0 \). The total GF of the coupled system is given by Eq.(76). The magnetic excitation spectrum follows from the poles of the GF (60)

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

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

Let us, as a first approximation, consider 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.(76) then becomes equal to
\[ \langle\langle S_k^+ | S_{-k}^- \rangle\rangle^0 \approx \frac{2 \tilde{S}}{\omega - Im - S(J_0 - J_k) - \frac{1}{2NS} \sum q (J_q - J_{q-k})(2K_q^{zz} + K_q^{-+}) + 2I^2 S X^*(k, 0)} \]

(86)

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

\[ 2I^2 \tilde{S} X^*(k, 0) \approx Im - \frac{1}{2SN} \sum q (f_q^\uparrow + f_q^\downarrow)(k \nabla q)^2 \epsilon(q) + \frac{1}{2SN \Delta} \sum q (f_q^\uparrow - f_q^\downarrow)(k \nabla q \epsilon(q))^2 \]

(87)

Then for \( \omega, k \to 0 \) Eq.(87) becomes

\[ \langle\langle S_k^+ | S_{-k}^- \rangle\rangle^0 \approx \frac{2 \tilde{S}}{\omega - D_1 k^2 - \frac{1}{2SN} \sum q (f_q^\uparrow + f_q^\downarrow)(k \nabla q)^2 \epsilon(q) + \frac{1}{2SN \Delta} \sum q (f_q^\uparrow - f_q^\downarrow)(k \nabla q \epsilon(q))^2} \]

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

\[ E_{St}(k) = \epsilon(k + q) - \epsilon(q) + \Delta \]

(89)

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 \( \omega \) with two solutions, \( \omega = 0 \) and \( \omega = I(m + 2 \tilde{S}) = E_{op}^0 \). In the hydrodynamic limit, \( k \to 0, \omega \to 0 \) the GF (75) can be written as

\[ \langle\langle S_k^+ | S_{-k}^- \rangle\rangle^0 \approx \frac{2 \tilde{S}}{\omega - E_{ac}^0(k)} \]

(90)

where the acoustic spin wave energies are given by

\[ E_{ac}^0(k) = Dk^2 = \left( \tilde{S}^2 [\psi_0 + \frac{1}{2NS^2} \sum q \psi_q (2K_q^{zz} + K_q^{-+})] + \frac{1}{2N} \frac{1}{2S} \sum q (f_q^\uparrow + f_q^\downarrow)(\bar{n} \nabla q)^2 \epsilon(q) + \frac{1}{N \Delta 2S} \sum q (f_q^\uparrow - f_q^\downarrow)(\bar{n} \nabla q \epsilon(q))^2 \right) k^2 \]

(91)

For the optical spin wave branch the estimations can be carried out as in paper [13]

\[ E_{op}^0(k) = E_{op}^0 - D_{op}^0 k^2 \]

(92)

In the GMF approximation the density of itinerant electrons (and the band splitting \( \Delta \)) can be evaluated by solving the equation
\[
n_\sigma = \frac{1}{N} \sum_k \left[ \exp(\beta(\epsilon(k) + U n_{-\sigma} - IS - \epsilon_F)) + 1 \right]^{-1}
\]  

(93)

Hence, the stiffness constant \( D \) can be expressed by the parameters of the \( sp - d \) model Hamiltonian.

VI. EFFECTS OF DISORDER IN DMS

We now proceed to give a simple and qualitative discussion of the effects of disorder in DMS. 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. The big amount of information was accumulated on the problem of ordering of localized spins of \( Mn^{2+} \) ions in \( Cd_{1-x} Mn_x Te \) and similar compounds [1], [37]. Recently, main attention was directed to studying III-V semiconducting alloys doped with Mn. As it was 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)

\[
H = \sum_{ij} \sum_\sigma t_{ij} a_i^{\dagger} a_j - \sum_i 2I \nu_i \vec{\sigma}_i \vec{S}_i
\]

(94)

Here \( \nu_i \) projects out sites occupied by Mn atoms, i.e.:

\[
\nu_i = \begin{cases} 
1 & \text{if site } i \text{ is occupied by Mn} \\
0 & \text{if site } i \text{ is occupied by Ga}
\end{cases}
\]

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 \( A_{1-x}^{III} Mn_x B^V \) the main magnetic interaction is an antiferromagnetic exchange between the Mn spins and the charge-carrier spins. The superexchange term \( H_d = -\frac{1}{2} \sum_{ij} J_{ij} \vec{S}_i \vec{S}_j \) is antiferromagnetic also 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 may arise 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 $p$, $c_{Mn} \gg p$. The optimal interrelation of both the magnitudes is a delicate and subtle question and was analyzed recently in paper [36]. It was shown that the concentration of free holes and ferromagnetically active Mn spins were 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 [36], it was shown that the dominant fraction of the Mn atoms are 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 that does not necessarily imply that all of the Mn atoms are in substitutional positions. For $x > 0.05$ an increasing fraction of Mn spins do 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. It follows from Eq.(94) that the spin dynamics of a modified KLM will be described by the GFs in the lattice site representation for a given configuration

$$<< S^+_i | S^-_j >> << \sigma^+_i | \sigma^-_j >>$$

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

$$\begin{pmatrix}
<< S^+_i | S^-_j >> & << S^+_i | \sigma^-_j >> \\
<< \sigma^+_i | S^-_j >> & << \sigma^+_i | \sigma^-_j >>
\end{pmatrix} = \hat{G}_{ij}(\omega)$$

(95)
In order to provide a simultaneous and self-consistent treatment of the quasi-particle 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 [30]-[32]. The CPA replaces the initial Hamiltonian of disordered system by an effective one which is assumed to produce no further scattering [38]. 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 here, 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 generalized mean fields [16]. 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.(32), should be replaced by

$$
(S^z_q)^{ir} = S^z_q - c< \bar{S}_z > \delta_{q,0}; \quad (a^\dagger_{p+q\sigma}a_{p\sigma})^{ir} = a^\dagger_{p+q\sigma}a_{p\sigma} - \bar{a}_{p\sigma}^\dagger\bar{a}_{p\sigma} \delta_{q,0}
$$

(96)

Here $< S_z > = \bar{S}_z$ corresponds to the configuration average. The average $< S_z >$ 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 virtual crystal approximation. The situation is then completely analogous to the previous one considered in the preceding sections. We get for the configurationally averaged GFs

$$
<< S^+_j | S^-_j >>^0 = << S^+_k | S^-_{-k} >>^0 \approx \frac{2c\bar{S}_z}{\omega - Im + 2I^2c\bar{S}_z\chi_0^*(k,\omega)}
$$

(97)
Here $\bar{S}_z = N^{-1/2} < S_z >$. These simple results are fully tractable and are the reason for their derivation.

It is worth to note 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 [39]

$$H = \sum_{ij} \sum_{\sigma} t_{ij} a_i^{\dagger} a_j^{\sigma} + U \sum_i \nu_i n_i^{\uparrow} n_i^{\downarrow} - \sum_i 2\nu_i \vec{\sigma}_i \vec{S}_i$$

(99)

The Coulomb repulsion is assumed to exist only on lattice sites occupied at random by Mn atoms. The approach mostly used [39] to calculate stiffness constant within a random version of the Hubbard model was based on the random phase approximation, where the electron-electron approximation was taken into account in the Hartree-Fock approximation and the disorder in the CPA. 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 environment-dependent. However, the calculation of the spatial GF Eq.(95), for the model, Eq.(99), 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 irreducible Green functions 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.

**VII. CONCLUSIONS**

In summary, we have presented an analytical approach for treating the spin quasi-particle 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 for interacting systems of itinerant carriers and localized spins using the ideas of quantum field theory for interacting electron and
spin systems on a lattice. 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 was the derivation of the Dyson equation for double-time retarded Green functions instead of causal ones. That formulation permits 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 quasi-particle 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. 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.

The main advantage of the whole method is the possibility of a self-consistent description of quasi-particle spectra and their damping in a unified and coherent fashion.

Many results of the previous works are reproduced mathematically more simply. 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 more advanced physical picture of the quasi-particle 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 quasi-particle states of the correlated lattice fermions and spins. The key to an 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 was 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.
REFERENCES

† Electronic address: kuzemsky@thsun1.jinr.ru; URL: http://thsun1.jinr.ru/~kuzemsky

[1] T. Dietl, in: Handbook on Semiconductors edited by T. S. Moss, (North-Holland, Amsterdam, 1994), Vol. 3, p.1251.

[2] A. Mauger and C. Godart, Phys. Rep. 141, 51 (1986).

[3] F. Matsukura, H. Ohno and T. Dietl, in: Handbook of Magnetic Materials edited by K. H. J. Buschow (North-Holland, Amsterdam, 2002), Vol. 14, p.1.

[4] T. Dietl, H. Ohno, F. Matsukura, J. Gibert and D. Ferrand, Science 287, 1019 (2000).

[5] P. Kacman, Semicond. Sci. Technol. 16, R25 (2001).

[6] T. Dietl, Physica E 10, 120 (2001).

[7] T. Dietl, H. Ohno and F. Matsukura, Phys. Rev. B 63, 195295 (2001).

[8] T. Dietl, Semicond. Sci. Technol. 17, 377 (2002).

[9] H. Ohno, J. Magn. Magn. Mater. 200, 110 (1999).

[10] K. Sato, H. Katayama-Yoshida, Mat. Res. Soc. Symp. Proc. 666, F4.6.1 (2001).

[11] K. Sato, H. Katayama-Yoshida, Semicond. Sci. Technol. 17, 367 (2001).

[12] Y. D. Park, A. T. Hanbicki, S. C. Erwin, C. S. Hellberg, J. M. Sullivan, J. E. Mattson, T. F. Ambrose, A. Wilson, G. Spanos and B. T. Jonker, Science 295, 651 (2002).

[13] S. Doniach and E. P. Wohlfarth, Proc. Roy. Soc., A 296, 442 (1967).

[14] A. J. Fedro, and T. Arai, Phys. Rev. 170, 583 (1968).

[15] D. Marvakov, J. Vlahov, and A. L. Kuzemsky, J. Physics C: Solid State Phys. 18, 2871 (1985).

[16] A. L. Kuzemsky, Rivista Nuovo Cimento 25, 1 (2002).
[17] B. S. Shastry, and D. C. Mattis, Phys. Rev. B 24, 5340 (1981).

[18] D. Marvakov, A. L. Kuzemsky, and J. Vlahov, Physica B 138, 129 (1986).

[19] A. L. Kuzemsky, Intern. J. Modern Phys. B 13, 2573 (1999).

[20] M. Takahashi, K. Mitsui, and M. Umehara, Phys. Rev. B 48, 17053 (1993).

[21] M. Takahashi, K. Mitsui, and M. Umehara, Phys. Rev. B 52, 16313 (1995).

[22] M. Takahashi, and K. Mitsui, Phys. Rev. B 54, 11298 (1996).

[23] M. Takahashi, Phys. Rev. B 55, 6950 (1997).

[24] M. Takahashi, Phys. Rev. B 56, 7389 (1997).

[25] A. Babcenco, and M. G. Cottam, J. Physics C: Solid State Phys. 14, 5347 (1981).

[26] S. V. Tyablikov, Methods in the Quantum Theory of Magnetism (Plenum Press, New York, 1967).

[27] O. Krisement, J. Magn. Magnet. Mat. 3, 7 (1976).

[28] B. E. Larson, K. C. Hass, H. Ehrenreich, and A. E. Carlson, Phys. Rev. B 37, 4137 (1988).

[29] B. Coqblin The Electronic Structure of Rare-Earth Metals and Alloys: the Magnetic Heavy Rare-Earths (Academic Press, N. Y., London, 1977).

[30] M. Takahashi, Phys. Rev. B 60, 15858 (1999).

[31] M. Takahashi, J. Phys. Condens. Matter 13, 3433 (2001).

[32] M. Takahashi, and K. Kubo, Phys. Rev. B 66, 153202 (2002).

[33] R. Eder, O. Stoica, and G. A. Sawatsky, Phys. Rev. B 55, R6109 (1997).
[34] L. C. Bartel, Phys. Rev. B 7, 3153 (1973).

[35] I. S. Tyagi, R. Kishore, and S. K. Joshi, Phys. Rev. B 10, 4050 (1974).

[36] K. M. Yu, W. Walukiewicz, W. L. Lim, X. Liu, U. Bindley, M. Dobrowolska, and J. K. Furdyna, Phys. Rev. B 68, 041308(R) (2003).

[37] M. Takahashi, J. Phys. Soc. Jpn. 70, 2224 (2001).

[38] P. Soven, Phys. Rev. 156, 809 (1967).

[39] E. Kolley, W. Kolley, and A. L. Kuzemsky, Solid State Physics, 21, 3100 (1979).