BOUND AND SCATTERING STATES OF ITINERANT CHARGE CARRIERS IN COMPLEX MAGNETIC MATERIALS

A. L. KUZEMSKY

Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research,
141980 Dubna, Moscow Region, Russia
kuzemsky@thsun1.jinr.ru

The concept of magnetic polaron is analyzed and developed to elucidate the nature of itinerant charge carrier states in magnetic semiconductors and similar complex magnetic materials. By contrasting the scattering and bound states of carriers within the s–d exchange model, the nature of bound states at finite temperatures is clarified. The free magnetic polaron at certain conditions is realized as a bound state of the carrier (electron or hole) with the spin wave. Quite generally, a self-consistent theory of a magnetic polaron is formulated within a nonperturbative many-body approach, the Irreducible Green Functions (IGF) method which is used to describe the quasiparticle many-body dynamics at finite temperatures. Within the above many-body approach we elaborate a self-consistent picture of dynamic behavior of two interacting subsystems, the localized spins and the itinerant charge carriers. In particular, we show that the relevant generalized mean fields emerges naturally within our formalism. At the same time, the correct separation of elastic scattering corrections permits one to consider the damping effects (inelastic scattering corrections) in the unified and coherent fashion. The damping of magnetic polaron state, which is quite different from the damping of the scattering states, finds a natural interpretation within the present self-consistent scheme.

Keywords: Spin-fermion model; itinerant charge carriers; bound and scattering states; magnetic polaron.

1. Introduction

The properties of itinerant charge carriers in complex magnetic materials are at the present time of much interest. The magnetic polaron problem is of particular interest because one can study how a magnetic ion subsystem influences electronic properties of complex magnetic materials. Recently, semiconducting ferro- and anti-ferromagnetic compounds have been studied very extensively.[1−5] 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. An itinerant carrier perturbs the magnetic lattice and is perturbed by the spin waves. It was shown that the effects of the sp–d or s–f exchange,[6−10] as well as the sp–$d(f)$ hybridization,[11] the electron-phonon interaction and disorder effects contributed to essential physics of these compounds and various anomalous properties are found. In these phenomena, the itinerant charge carriers play an important role and many of these anomalous properties may be attributed to the sp–$d(f)$ exchange interaction.[10,12] As a result, an electron travelling through a ferromagnetic crystal will in general couple to the magnetic subsystem. From the quantum mechanics point of view this means that the wave function of the electron would depend not only upon the electron coordinate but upon the state of the spin system as well. Recently, further attempts have been made to study and exploit carriers which are exchange-coupled to the localized spins.[13−17] The effect of carriers on the magnetic ordering temperature is now found to be very strong in diluted magnetic semiconductors (DMS).[4,13] Diluted magnetic semiconductors 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. The diluted magnetic semiconductors 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.

It was Kasuya[8,10,18−20] who first clarified that the s–f interaction works differently in magnetic semiconductors and in metals.[21] The effects of the sp–$d(f)$ exchange on the ferromagnetic state of a magnetic semiconductor were discussed in Refs. 22–26. It was shown that the effects of the sp–$d(f)$ exchange interaction are of a more variety in the magnetic semiconductors[10] than in the magnetic metals,[21] because in the former there are more parameters which can change over wide ranges.[10,18−20] The state of itinerant charge carriers may be greatly modified due to the scattering on the localized spins.[27−30] Interaction with the subsystem of localized spins leads to renormalization of bare states and the scattering and bound state regimes may occur.[31,32] Along with the scattering states, an additional dressing effect due to the sp–$d(f)$ exchange interaction can exist in some of these materials.[29,33,34] To some extent, the interaction of an itinerant carrier in a ferromagnet with spin waves is analogous to the polaron problem in polar crystals if we can consider the electron and spin waves to be separate subsystems.[22] Note, however, that the magnetic polaron differs from the ordinary polaron in a few important points.[25,26,34−36]

To describe this situation a careful analysis of the state of itinerant carriers in complex magnetic materials[37] is highly desirable. For this aim a few model approaches have been proposed. A basic model is a combined spin-fermion model (SFM) which includes interacting spin and charge subsystems.[25,27,38−40]

The problem of adequate physical description of itinerant carriers (including a self-trapped state) within various types of generalized spin-fermion models has intensively been studied during the last decades.[27,39−42] The dynamic interaction of an itinerant electron with the spin-wave system in a magnet has been studied by many authors,[8,10,22,25] including the effects of external fields. It was shown within the perturbation theory that the state of an itinerant charge carrier is renormalized due to the spin disorder scattering. The second order perturbation treatment leads to the lifetime of conduction electron and explains qualitatively the anomalous temperature dependence of the electrical resistivity.[43,44,31,32,25] The polaron formation in the concentrated systems leads to giant magneto-resistive effects in the Eu chalcogenides.[1,33]

The concept of magnetic polaron in the magnetic material was discussed and analyzed in Refs. 33, 38, 45, 25, 26. The future development of this concept was stimulated by many experimental results and observations on magnetic semiconductors.[3,46−48] A paramagnetic polaron in magnetic semiconductors was studied by Kasuya,[25] who argued on the basis of thermodynamics, that once electron is trapped into the spin cluster, the spin alignment within the spin cluster increases and thus the potential to trap an electron increases. The bound states around impurity ions of opposite charge and self-trapped carriers were discussed by de Gennes.[41] Emin[34] defined the self-trapped state and formulated that

> "the unit comprising the self-trapped carrier and the associated atomic deformation pattern is referred to as a polaron, with the adjective small or large denoting whether the spatial extent of the wave function of the self-trapped carrier is small or large compared with the dimensions of a unit cell".

In papers [Refs. 45, 49–52], a set of self-consistent equations for the self-trapped (magnetic polaron) state was derived and it was shown that the paramagnetic polaron appeared discontinuously with decreasing temperature. These studies were carried out for wide band materials and the thermodynamic arguments were mainly used in order to determine a stable configuration. Some specific points of spin-polaron and exiton magnetic polaron were discussed further in papers [Refs. 52–56].

Properties of the magnetic polaron in a paramagnetic semiconductor were studied by Yanase,[57] Kubler[58] and by Auslender and Katsnelson.[59] The later authors[60] developed a detailed theory of the states of itinerant charge carriers in ferromagnetic semiconductors in the spin-wave (low temperature) region within the framework of variational approach. The effect of the electron-phonon interaction on the self-trapped magnetic polaron state was investigated by Umehara.[61,62] A theory for self-trapped magnetic polaron in ferromagnetic semiconductor with a narrow band was formulated by Takeda and Kasuya.[63] The electron crystallization in antiferromagnetic semiconductors was studied by Umehara,[64,65] and a *dense magnetic polaron state* was conjectured to describe the physics of $Gd_{3-x}vS_4$.

A model of the bound magnetic polaron, i.e. electron trapped on impurity or by vacancy[48] was developed in papers [Refs. 66, 67]. The general thermodynamic model of the bound magnetic polaron and its stability was considered in Refs. 68–70. Then similar models were studied by several authors.[3,71,72]

The state of a conduction electron in a ferromagnetic crystal (magnetic polaron) was investigated by Richmond[73] who deduced an expression for one-electron Green function. Shastry and Mattis[74] presented a detailed analysis of the one-electron Green function at zero temperature. They constructed an exact Green function for a single electron in a ferromagnetic semiconductor and highlighted the crucial differences between bound- and scattering-state contributions to the electron spectral weight. A finite temperature self-consistent theory of magnetic polaron within the Green functions approach was developed in Ref. 75.

Recently, new interest in the problem of magnetic polaron was stimulated by the studies of magnetic and transport properties of the low-density carrier ferromagnets, diluted magnetic semiconductors (DMS).[76−78,4,5] The concept of the magnetic polaron, the self-trapped state of a carrier and spin wave, attracts increasing attention because of the anomalous magnetic, transport, and optical properties of DMS[77,79−83] and the perovskite manganites.[37,84,85] For example, a two-component phenomenological model, describing polaron formation in colossal magnetoresistive compounds, has been devised recently.[86] The paper [Ref. 78] includes a detailed analysis of the polaron-polaron interaction effects in DMS.

The purpose of the present work is to elucidate further the nature of itinerant carrier states in magnetic semiconductors and similar complex magnetic materials. An added motivation for performing new consideration and a careful analysis of the magnetic polaron problem arise from the circumstance that the various new materials were fabricated and tested, and a lot of new experimental facts were accumulated. This paper deals with the effects of the local exchange due to interaction of carrier spins with the ionic spins or the sp–d or s–f exchange interaction on the state of itinerant charge carriers. We develop in some detail a many-body approach to the calculation of the quasiparticle energy spectra of itinerant carriers so as to understand their quasiparticle many-body dynamics. The concept of the magnetic polaron is reconsidered and developed and the scattering and bound states are thoroughly analyzed. In the previous papers, we set up the formalism of the method of Irreducible Green Functions (IGF).[87] 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[88] 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 of charge carriers for the lattice spin-fermion model consisting of two interacting subsystems. The concepts of magnetic polaron and the scattering and bound states are

analyzed and developed in some detail. We consider thoroughly a self-consistent calculation of quasiparticle energy spectra of the itinerant carriers. We are particularly interested in how the scattering state appears differently from the bound state in magnetic semiconductor.

The key problem of most of this work is the formation of magnetic polaron under various conditions on the parameters of the spin-fermion model. It is the purpose of this paper to explore more fully the effects of the sp–$d(f)$ exchange interaction on the state of itinerant charge carriers in magnetic semiconductors and similar complex magnetic materials.

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.[9,10,18,12,40] 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 (for simplicity we shall call it the s–d model) is given by

$$H = H_s + H_{s-d} + H_d \,. \tag{1}$$

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

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

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

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

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[11]

$$H_{s-d} = -2 \sum_i I \vec{\sigma}_i \vec{S}_i = -IN^{-1/2} \sum_{kq} \sum_\sigma [S_{-q}^{-\sigma} a_{k\sigma}^\dagger a_{k+q-\sigma} + z_\sigma S_{-q}^z a_{k\sigma}^\dagger a_{k+q\sigma}] \quad (4)$$

where sign factor z_σ is given by

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

and

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

For example, in DMS[4] the local exchange coupling resulted from the p–d hybridization between the Mn d levels and the p valence band $I \sim V_{p-d}^2$. In magnetic semiconductors this interaction can lead to the formation of the bound electron-magnon (polaron-like) bound state due to the effective attraction of the electron and magnon in the case of antiferromagnetic coupling ($I < 0$).

For the subsystem of localized spins we have

$$H_d = -\frac{1}{2} \sum_{ij} J_{ij} \vec{S}_i \vec{S}_j = -\frac{1}{2} \sum_q J_q \vec{S}_q \vec{S}_{-q}. \quad (5)$$

Here we use the notation

$$S_i^\alpha = N^{-1/2} \sum_{\vec{k}} S_k^\alpha \exp(i\vec{k}\vec{R}_i), \quad S_k^\alpha = N^{-1/2} \sum_{\vec{i}} S_i^\alpha \exp(-i\vec{k}\vec{R}_i)$$

$$[S_k^\pm, S_q^z] = \frac{1}{N^{1/2}} \mp S_{k+q}^\pm, \quad [S_k^+, S_q^-] = \frac{2}{N^{1/2}} S_{k+q}^z$$

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

This term describes a 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 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 local moments[7,8,21,12]

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

We emphasize that $K_{ij} \sim |I^2| \sim V_{p-d}^4$. To explain this, let us remind that the microscopic model,[11] which contains basic physics, is the Anderson–Kondo model[12]

$$H = \sum_{ij} \sum_\sigma t_{ij} a_{i\sigma}^\dagger a_{j\sigma} - V \sum_{ij} \sum_\sigma (a_{i\sigma}^+ d_{j\sigma} + h.c.)$$

$$- E_d \sum_i \sum_\sigma n_{i\sigma}^d + \frac{1}{2} \sum_{i\sigma} U n_{i\sigma}^d n_{i-\sigma}^d. \quad (7)$$

For the symmetric case $U = 2E_d$ and for $U \gg V$ Eq. (7) can be mapped onto the Kondo lattice model[12] (KLM)

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

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

We follow the previous treatments and take as our model Hamiltonian expression (1). For the sake of brevity we omit in this paper the U-term (low-concentration limit). This U-term can be included into consideration straightforwardly (see Ref. 40). 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[87] 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* (GMFs), as it was formulated in Ref. 87. These GMFs have a complicated structure for a 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[88]

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

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

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

Here we use the notation $\langle\langle A(t), A^{\dagger}(t') \rangle\rangle$ for the time-dependent GF and $\langle\langle A | A^{\dagger} \rangle\rangle_{\omega}$ for its Fourier transform.[88] The notation $[A, B]_{\eta}$ refers to commutation and anti-commutation depending on the value of $\eta = \pm$.

The essence of the method is as follows[87]:

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

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

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

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

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 $(^{(ir)}\langle\langle [A, H]_- | A^\dagger \rangle\rangle)$ and operators $(^{(ir)}[A, H]_- \equiv ([A, H]_-)^{(ir)})$ we will use both the notation freely $(^{(ir)}\langle\langle A | B \rangle\rangle$ is the same as $\langle\langle (A)^{(ir)} | B \rangle\rangle)$. A choice one notation over another is determined by the brevity and clarity of notation only. From the 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 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

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

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

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

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

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

We use here the notation M for self-energy (mass operator in quantum field theory). 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

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

The difference between P and M can be regarded as two different solutions of two integral equations (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

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

Equation (19) can be regarded as an alternative form of the 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. 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 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 the 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 the 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.

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.[87] 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 better understand 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 our calculations to causal GF at each stage of calculations 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 crucially 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 nontrivial 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

$$A_1 = A \,, \quad A_2 = [A, H] \,, \quad A_3 = [[A, H], H], \ldots, A_n = [[\cdots [A, \underbrace{H] \cdots H]}_{n}\,.$$

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

$$\hat{G} = \left\langle\!\left\langle \begin{pmatrix} A_1 \\ A_2 \\ \vdots \\ A_n \end{pmatrix} | (A_1^\dagger A_2^\dagger \cdots A_n^\dagger) \right\rangle\!\right\rangle .$$

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 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 Ref. 87 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 a clear link between the equation-of-motion approach and the diagrammatic methods due to derivation of the Dyson equation. Moreover, due to the fact that it allows the approximate treatment of the self-energy effects on a final stage, it yields a systematic way of the construction of approximate solutions.

4. Charge and Spin Degrees of Freedom

Our attention will be focused on the quasiparticle many-body dynamics of the s–d model. To describe self-consistently the charge dynamics of the s–d model, one should take into account the full algebra of relevant operators of the suitable "charge modes" which are appropriate when the goal is to describe self-consistently the quasi-particle spectra of two interacting subsystems.

The simplest case is to consider a situation when a single electron is injected into an otherwise perfectly pure and insulating magnetic semiconductor. The behavior of charge carriers can be divided into two distinct limits based on interrelation between the band width W and the exchange interaction I:

$$|2IS| \gg W ; \quad |2IS| \ll W .$$

Exact solution for the s–d model is known only in the strong-coupling limit, where the band width is small compared to the exchange interaction. This case can be

considered as a starting point for the description of narrow band materials. The case of intermediate coupling, when $|2IS| \simeq W$, makes serious difficulties.

To understand how the itinerant charge carriers behave in a wide range of values of model parameters, consider the equations of motion for the charge and spin variables.

$$[a_{k\sigma}, H_s]_- = \epsilon_k a_{k\sigma} \tag{20}$$

$$[a_{k\sigma}, H_{s-d}]_- = -IN^{-1/2} \sum_q (S^{-\sigma}_{-q} a_{q+k-\sigma} + z_\sigma S^z_{-q} a_{q+k\sigma}) \tag{21}$$

$$[S^+_k, H_{s-d}]_- = -IN^{-1} \sum_{pq} [2S^z_{k-q} a^\dagger_{p\uparrow} a_{p+q\downarrow} - S^+_{k-q}(a^\dagger_{p\uparrow} a_{p+q\uparrow} - a^\dagger_{p\downarrow} a_{p+q\downarrow})] \tag{22}$$

$$[S^-_{-k}, H_{s-d}]_- = -IN^{-1} \sum_{pq} [2S^z_{k-q} a^\dagger_{p\downarrow} a_{p+q\uparrow} - S^-_{k-q}(a^\dagger_{p\uparrow} a_{p+q\uparrow} - a^\dagger_{p\downarrow} a_{p+q\downarrow})] \tag{23}$$

$$[S^z_k, H_{s-d}]_- = -IN^{-1} \sum_{pq} (S^+_{k-q} a^\dagger_{p\downarrow} a_{p+q\uparrow} - S^-_{k-q} a^\dagger_{p\uparrow} a_{p+q\downarrow}) \tag{24}$$

$$[S^+_k, H_d]_- = N^{-1/2} \sum_q J_q (S^z_q S^+_{k-q} - S^z_{k-q} S^+_q) \tag{25}$$

$$[S^-_{-k}, H_{s-d}]_- = -IN^{-1} \sum_{pq} [2S^z_{k-q} a^\dagger_{p\downarrow} a_{p+q\uparrow} - S^-_{k-q}(a^\dagger_{p\uparrow} a_{p+q\uparrow} - a^\dagger_{p\downarrow} a_{p+q\downarrow})] \tag{26}$$

From Eqs. (20)–(26) it follows that the localized spin and itinerant charge variables are coupled.

We have the following kinds of charge

$$a_{k\sigma}, \quad a^\dagger_{k\sigma}, \quad n_{k\sigma} = a^\dagger_{k\sigma} a_{k\sigma}$$

and spin operators

$$S^+_k, \quad S^-_{-k} = (S^+_k)^\dagger,$$

$$\sigma^+_k = \sum_q a^\dagger_{k\uparrow} a_{k+q\downarrow}; \quad \sigma^-_k = \sum_q a^\dagger_{k\downarrow} a_{k+q\uparrow}.$$

There are additional combined operators

$$b_{k\sigma} = \sum_q (S^{-\sigma}_{-q} a_{q+k-\sigma} + z_\sigma S^z_{-q} a_{q+k\sigma}).$$

In the lattice (Wannier) representation the operator $b_{k\sigma}$ reads

$$b_{i\sigma} = (S^{-\sigma}_i a_{i-\sigma} + z_\sigma S^z_i a_{i\sigma}). \tag{27}$$

It was clearly shown in Refs. 8, 9, 22, 27, 43 that the calculation of the energy of itinerant carriers involves the dynamics of the ion spin system. In the approximation of rigid ion spins,[27] i.e.:

$$S^x_j = S^y_j = 0, \quad S^z_j = S$$

the energy shift of electron was estimated as

$$\Delta\varepsilon(k\sigma) \sim -I\frac{\sigma}{2}S + \frac{S^2}{4}\sum_{q\neq 0}\frac{|I_q|^2}{\epsilon(k)-\epsilon(k-q)}\ .$$

The dynamic term was estimated as

$$\Delta\varepsilon(k\ \uparrow)$$
$$\sim \frac{S^2}{4}\sum_{Q\neq 0}\frac{|I_Q|^2}{\epsilon(k)-\epsilon(k-Q)} + \frac{S}{2N}\frac{1}{(2\pi)^3}\int d^3q\frac{|I_q|^2 N(\omega(q))}{\epsilon(k)-\epsilon(k-q)-I\langle S^z\rangle + Dq^2}\ .$$

For the case of rare-earth metals, the electron-magnon interaction in the s–d model within a second-order perturbation theory was studied by Liu and Davis[89] and by Kim[90,91] within the Bogoliubov–Tyablikov[88] GFs method.

To describe self-consistently the charge carrier dynamics of the s–d model within a sophisticated many-body approach, one should take into account the full algebra of relevant operators of the suitable "modes" (degrees of freedom) which are appropriate when the goal is to describe self-consistently quasiparticle spectra of two interacting subsystems. 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 due to the interaction of the "modes". Since our goal is to calculate the quasiparticle spectra of the itinerant charge carriers, including bound carrier-spin states, a suitable algebra of the relevant operators should be constructed. In principle, the complete algebra of the relevant "modes" should include the spin variables too. The most full relevant set of the operators is

$$\{a_{i\sigma},\ S_i^z,\ S_i^{-\sigma},\ S_i^z a_{i\sigma},\ S_i^{-\sigma}a_{i-\sigma}\}\ .$$

That means that the corresponding relevant GF for interacting charge and spin degrees of freedom should have the form

$$\begin{pmatrix} \langle\langle a_{i\sigma}|a_{j\sigma'}^\dagger\rangle\rangle & \langle\langle a_{i\sigma}|S_j^z\rangle\rangle & \langle\langle a_{i\sigma}|S_j^{\sigma'}\rangle\rangle & \langle\langle a_{i\sigma}|a_{j\sigma'}^\dagger,S_j^z\rangle\rangle & \langle\langle a_{i\sigma}|a_{j-\sigma'}^\dagger,S_j^\sigma\rangle\rangle \\ \langle\langle S_i^z|a_{j\sigma'}^\dagger\rangle\rangle & \langle\langle S_i^z|S_j^z\rangle\rangle & \langle\langle S_i^z|S_j^{\sigma'}\rangle\rangle & \langle\langle S_i^z|a_{j\sigma'}^\dagger,S_j^z\rangle\rangle & \langle\langle S_i^z|a_{j-\sigma'}^\dagger,S_j^{\sigma'}\rangle\rangle \\ \langle\langle S_i^{-\sigma}|a_{j\sigma'}^\dagger\rangle\rangle & \langle\langle S_i^{-\sigma}|S_j^z\rangle\rangle & \langle\langle S_i^{-\sigma}|S_j^{\sigma'}\rangle\rangle & \langle\langle S_i^{-\sigma}|a_{j\sigma'}^\dagger,S_j^z\rangle\rangle & \langle\langle S_i^{-\sigma}|a_{j-\sigma'}^\dagger,S_j^{\sigma'}\rangle\rangle \\ \langle\langle S_i^z a_{i\sigma}|a_{j\sigma'}^\dagger\rangle\rangle & \langle\langle S_i^z a_{i\sigma}|S_j^z\rangle\rangle & \langle\langle S_i^z a_{i\sigma}|S_j^{\sigma'}\rangle\rangle & \langle\langle S_i^z a_{i\sigma}|a_{j\sigma'}^\dagger,S_j^z\rangle\rangle & \langle\langle S_i^z a_{i\sigma}|a_{j-\sigma'}^\dagger,S_j^\sigma\rangle\rangle \\ \langle\langle S_i^{-\sigma}a_{i-\sigma}|a_{j\sigma'}^\dagger\rangle\rangle & \langle\langle S_i^{-\sigma}a_{i-\sigma}|S_j^z\rangle\rangle & \langle\langle S_i^{-\sigma}a_{i-\sigma}|S_j^{\sigma'}\rangle\rangle & \langle\langle S_i^{-\sigma}a_{i-\sigma}|a_{j\sigma'}^\dagger,S_j^z\rangle\rangle & \langle\langle S_i^{-\sigma}a_{i-\sigma}|a_{j-\sigma'}^\dagger,S_j^{\sigma'}\rangle\rangle \end{pmatrix}\ . \tag{28}$$

However, to make the problem more easily tractable, we will consider below the shortest algebra of the relevant operators $(a_{k\sigma}, a_{k\sigma}^\dagger, b_{k\sigma}, b_{k\sigma}^\dagger)$. However, this choice requires a separate treatment of the spin dynamics.

Here we reproduce very briefly the description of the spin dynamics of the s–d model for the sake of self-contained formulation. The spin quasiparticle dynamics of the s–d model was considered in detail in papers.[39,40,92] We consider the double-time thermal GF of localized spins[88] which is defined as

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

$$= 1/2\pi \int_{-\infty}^{+\infty} d\omega \exp(-i\omega t)\mathcal{G}^{+-}(k; \omega). \tag{29}$$

The next step is to write down the equation of motion for the GF. To describe self-consistently the spin dynamics of the s–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 used the following generalized matrix GF of the form[39,40,92]:

$$\begin{pmatrix} \langle\langle S_k^+|S_{-k}^-\rangle\rangle & \langle\langle S_k^+|\sigma_{-k}^-\rangle\rangle \\ \langle\langle \sigma_k^+|S_{-k}^-\rangle\rangle & \langle\langle \sigma_k^+|\sigma_{-k}^-\rangle\rangle \end{pmatrix} = \hat{\mathcal{G}}(k; \omega). \tag{30}$$

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

$$\omega\langle\langle S_k^+|B\rangle\rangle_\omega = \left\{ \begin{matrix} 2N^{-1/2}\langle S_0^z\rangle \\ 0 \end{matrix} \right\}$$

$$+ \frac{I}{N} \sum_{pq} \langle\langle S_{k-q}^+(a_{p\uparrow}^\dagger a_{p+q\uparrow} - a_{p\downarrow}^\dagger a_{p+q\downarrow}) - 2S_{k-q}^z a_{p\uparrow}^\dagger a_{p+q\downarrow}|B\rangle\rangle_\omega$$

$$+ N^{-1/2} \sum_q J_q\langle\langle(S_q^z S_{k-q}^+ - S_{k-q}^z S_q^+)|B\rangle\rangle_\omega \tag{31}$$

where

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

Let us introduce by definition irreducible (ir) operators as

$$(S_q^z)^{ir} = S_q^z - \langle S_0^z\rangle\delta_{q,0};$$

$$(a_{p+q\sigma}^\dagger a_{p\sigma})^{ir} = a_{p+q\sigma}^\dagger a_{p\sigma} - \langle a_{p\sigma}^\dagger a_{p\sigma}\rangle\delta_{q,0} \tag{32}$$

$$((S_q^z)^{ir} S_{k-q}^+ - (S_{k-q}^z)^{ir} S_q^+)^{ir}$$

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

From the condition (12)

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

one can find

$$\phi_q = \frac{2K_q^{zz} + K_q^{-+}}{2\langle S_0^z\rangle} \tag{34}$$

$$K_q^{zz} = \langle(S_q^z)^{ir}(S_q^z)^{ir}\rangle; \quad K_q^{-+} = \langle S_{-q}^- S_q^+\rangle. \tag{35}$$

Using the definition of the mass operator Eq. (17) the equation of motion, Eq. (31), can be exactly transformed to the Dyson equation, Eq. (18)

$$\hat{\mathcal{G}} = \hat{\mathcal{G}}_0 + \hat{\mathcal{G}}_0 \hat{M} \hat{\mathcal{G}} . \tag{36}$$

Hence, the determination of the full GF $\hat{G}$ has been reduced to that of $\hat{\mathcal{G}}_0$ and $\hat{M}$. The GF matrix $\mathcal{G}_0$ in the generalized mean field approximation reads

$$\hat{\mathcal{G}}_0 = R^{-1} \begin{pmatrix} I^{-1} N^{1/2} \Omega_2 & \Omega_2 N \chi_0^s \\ \Omega_2 N \chi_0^s & -\Omega_1 N \chi_0^s \end{pmatrix} \tag{37}$$

where

$$R = \Omega_1 + \Omega_2 I N^{1/2} \chi_0^s . \tag{38}$$

The diagonal matrix elements $\mathcal{G}_0^{11}$ read

$$\langle\langle S_k^+ | S_{-k}^- \rangle\rangle^0 = \frac{2 S_z}{\Omega_1 + 2 I^2 S_z \chi_0^s(k,\omega)} \tag{39}$$

where

$$\Omega_1 = \omega - \frac{\langle S_0^z \rangle}{N^{1/2}} (J_0 - J_k) - N^{-1/2}$$

$$\times \sum_q (J_q - J_{q-k}) \frac{2 K_q^{zz} + K_q^{-+}}{2 \langle S_0^z \rangle} - I(n_\uparrow - n_\downarrow) \tag{40}$$

$$\Omega_2 = \frac{2 \langle S_0^z \rangle I}{N} \tag{41}$$

$$\chi_0^s(k,\omega) = N^{-1} \sum_p \frac{(f_{p+k\downarrow} - f_{p\uparrow})}{\omega_{p,k}^s} . \tag{42}$$

Here the notation was used

$$\omega_{p,k}^s = (\omega + \epsilon_p - \epsilon_{p+k} - \Delta_I)$$

$$\Delta_I = 2 I S_z \tag{43}$$

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

$$\varepsilon(q\sigma) = \epsilon_q - z_\sigma I S_z$$

$$\bar{n} = \sum (n_\uparrow + n_\downarrow); \quad 0 \le \bar{n} \le 2$$

$$S_z = N^{-1/2} \langle S_0^z \rangle .$$

We assume then that the local exchange parameter $I = 0$. In this limiting case we have

$$\langle\langle S_k^+ | S_{-k}^- \rangle\rangle^0 = \frac{2 S_z}{\omega - S_z(J_0 - J_k) - \frac{1}{2 N S_z} \sum_q (J_q - J_{q-k})(2 K_q^{zz} + K_q^{-+})} . \tag{44}$$

The spectrum of quasiparticle excitations of localized spins without damping follows from the poles of the generalized mean-field GF (44)

$$\omega(k) = S_z(J_0 - J_k) + \frac{1}{2NS_z}\sum_q (J_q - J_{q-k})(2K_q^{zz} + K_q^{-+}) . \tag{45}$$

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:

$$J_k = \sum_i \exp\left(-i\vec{k}\vec{R}_i\right) J(|\vec{R}_i|) . \tag{46}$$

The expansion in small $\vec{k}$ gives[92]

$$\langle\langle S_k^+ | S_{-k}^-\rangle\rangle^0 = \frac{2S_z}{\omega - \omega(k)} \tag{47}$$

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

$$= \left(\frac{S_z}{2}\eta_0 + \frac{N}{2S_z^2}\sum_q \eta_q(2K_q^{zz} + K_q^{-+})\right)k^2$$

$$\eta_q = \sum_i (\vec{k}\vec{R}_i)^2 J(|\vec{R}_i|)\exp\left(-i\vec{q}\vec{R}_i\right) .$$

It is easy to analyze the quasiparticle spectra of the $(s\text{--}d)$ model in the case of nonzero coupling I. The full generalized mean field GFs can be rewritten as

$$\langle\langle S_k^+ | S_{-k}^-\rangle\rangle^0$$

$$= \frac{2S_z}{\omega - Im - S_z(J_0 - J_k) - \frac{1}{2NS_z}\sum_q (J_q - J_{q-k})(2K_q^{zz} + K_q^{-+}) + 2I^2 S_z \chi_0^s(k,\omega)} \tag{48}$$

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

Here the notation was used

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

The precise significance of this description of spin quasiparticle dynamics appears in the next sections.

5. Charge Dynamics of the *s–d* Model. Scattering Regime

In order to discuss the charge quasiparticle dynamics of the *s–d* model, we can use the whole development in Sec. 3. The concept of a magnetic polaron requires that we should have also precise knowledge about the scattering charge states. By contrasting the bound and scattering state regime, the properties of itinerant charge carriers and their quasiparticle many-body dynamics can be substantially clarified. We consider again the double-time thermal GF of charge operators[88] which is defined as

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

$$= 1/2\pi \int_{-\infty}^{+\infty} d\omega \exp(-i\omega t)g_{k\sigma}(\omega). \tag{50}$$

To describe the quasiparticle charge dynamics or dynamics of carriers of the *s–d* model self-consistently, we should consider the equation of motion for the GF *g*:

$$\omega\langle\langle a_{k\sigma}|a_{k\sigma}^{\dagger}\rangle\rangle_{\omega} = 1 + \epsilon_k\langle\langle a_{k\sigma}|a_{k\sigma}^{\dagger}\rangle\rangle_{\omega}$$

$$- IN^{-1/2}\sum_{q}\langle\langle(S_{-q}^{-\sigma}a_{q+k-\sigma} + z_{\sigma}S_{-q}^{z}a_{q+k\sigma})|a_{k\sigma}^{\dagger}\rangle\rangle_{\omega}$$

$$= IN^{-1/2}\langle\langle b_{k\sigma}|a_{k\sigma}^{\dagger}\rangle\rangle_{\omega}. \tag{51}$$

Let us introduce by definition irreducible (*ir*) spin operators as

$$(S_q^z)^{ir} = S_q^z - \langle S_0^z\rangle\delta_{q,0}$$
$$(S_q^\sigma)^{ir} = S_q^\sigma - \langle S_0^\sigma\rangle\delta_{q,0} = S_q^\sigma. \tag{52}$$

By this definition we suppose that there is a long-range magnetic order in the system under consideration with the order parameter $\langle S_0^z\rangle$. The irreducible operator for the transversal spin components coincides with the initial operator.

Equivalently, one can write down by definition irreducible GFs:

$$(^{ir}\langle\langle S_{-q}^{-\sigma}a_{q+k-\sigma}|a_{k\sigma}^{\dagger}\rangle\rangle_{\omega}) = \langle\langle S_{-q}^{-\sigma}a_{q+k-\sigma}|a_{k\sigma}^{\dagger}\rangle\rangle_{\omega}$$
$$(^{ir}\langle\langle S_{-q}^{z}a_{q+k\sigma}|a_{k\sigma}^{\dagger}\rangle\rangle_{\omega}) = \langle\langle S_{-q}^{z}a_{q+k\sigma}|a_{k\sigma}^{\dagger}\rangle\rangle_{\omega}$$
$$- \langle S_0^z\rangle\delta_{q,0}\langle\langle a_{k\sigma}|a_{k\sigma}^{\dagger}\rangle\rangle_{\omega}. \tag{53}$$

Then the equation of motion for the GF $g_{k\sigma}(\omega)$ can be exactly transformed to the following form:

$$(\omega - \varepsilon(k\sigma))\langle\langle a_{k\sigma}|a_{k\sigma}^{\dagger}\rangle\rangle_{\omega} + IN^{-1/2}\langle\langle C_{k\sigma}|a_{k\sigma}^{\dagger}\rangle\rangle = 1. \tag{54}$$

Here the notation was used

$$C_{k\sigma} = b_{k\sigma}^{ir} = \sum_{q}(S_{-q}^{-\sigma}a_{q+k-\sigma} + z_{\sigma}(S_{-q}^{z})^{ir}a_{q+k\sigma}). \tag{55}$$

Following the IGF strategy we should perform the differentiation of the higher-order GFs on the second time t' and introduce the irreducible GFs (operators) for the

"right" side. Using this approach the equation of motion, Eq. (34), can be exactly transformed into the Dyson equation Eq. (18)

$$g_{k\sigma}(\omega) = g_{k\sigma}^0(\omega) + g_{k\sigma}^0(\omega)M_{k\sigma}(\omega)g_{k\sigma}(\omega) \tag{56}$$

where

$$g_{k\sigma}^0(\omega) = \langle\langle a_{k\sigma}|a_{k\sigma}^\dagger\rangle\rangle^0 = (\omega - \varepsilon(k\sigma))^{-1}. \tag{57}$$

The mean-field GF Eq. (57) contains all the mean-field renormalizations or elastic scattering corrections. The inelastic scattering corrections, according to Eq. (56), are separated to the mass operator $M_{k\sigma}(\omega)$. Here the mass operator has the following exact representation (scattering regime):

$$
\begin{aligned}
M_{k\sigma}(\omega) &= M_{k\sigma}^{e-m}(\omega) \\
&= \frac{I^2}{N}\sum_{qs}(({}^{(ir)}\langle\langle S_{-q}^{-\sigma}a_{k+q-\sigma}|S_s^\sigma a_{k+s-\sigma}^+\rangle\rangle^{(ir),p}) \\
&\quad + ({}^{(ir)}\langle\langle S_{-q}^z a_{k+q\sigma}|S_s^z a_{k+s\sigma}^+\rangle\rangle^{(ir),p})).
\end{aligned}
\tag{58}
$$

To calculate the mass operator $M_{k\sigma}(\omega)$, we express the GF in terms of the correlation functions. In order to calculate the mass operator self-consistently, we shall use approximation of two interacting modes for M^{e-m}. Then the corresponding expression can be written as

$$
\begin{aligned}
M_{k\sigma}^{e-m}(\omega) &= \frac{I^2}{N}\sum_q \int \frac{d\omega_1 d\omega_2}{\omega - \omega_1 - \omega_2}F_1(\omega_1,\omega_2) \\
&\quad \times \left(\frac{-1}{\pi}Im\, g_{k+q,-\sigma}(\omega_2)\left(\frac{-1}{\pi}Im\langle\langle S_{-q}^\sigma|S_q^{-\sigma}\rangle\rangle_{\omega_1}\right)\right. \\
&\quad \left. + \frac{-1}{\pi}Im\, g_{k+q,\sigma}(\omega_2)\left(\frac{-1}{\pi}Im\langle\langle (S_q^z)^{ir}|(S_{-q}^z)^{ir}\rangle\rangle_{\omega_1}\right)\right)
\end{aligned}
\tag{59}
$$

where

$$F_1(\omega_1,\omega_2) = (1 + N(\omega_1) - f(\omega_2))$$
$$N(\omega(k)) = [\exp(\beta\omega(k)) - 1]^{-1}.$$

Equations (56) and (59) form a closed self-consistent system of equations for one-fermion GF of the carriers for the s–d model in the scattering regime. It clearly shows that the charge quasiparticle dynamics couples intrinsically with the spin quasiparticle dynamics in a self-consistent way.

To find explicit expressions for the mass operator, Eq. (43), we choose for the first iteration step in its r.h.s. the following trial expressions:

$$-\frac{1}{\pi}Im\, g_{k\sigma}(\omega) = \delta(\omega - \varepsilon(k\sigma)) \tag{60}$$

$$\frac{-1}{\pi} Im\langle\langle S_q^\sigma | S_{-q}^{-\sigma}\rangle\rangle \approx z_\sigma (2S_z)\delta(\omega - z_\sigma\omega(q)). \tag{61}$$

Here $\omega(q)$ is given by the expression Eq. (45). Then we obtain

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

$$M_{k\downarrow}^{e-m}(\omega) = \frac{2I^2\langle S_0^z\rangle}{N^{3/2}} \sum_q \frac{1 - f_{k-q,\uparrow} + N(\omega(q))}{\omega - \varepsilon(k-q,\uparrow) - \omega(q)}. \tag{62}$$

This result was written for the low temperature region when one can drop the contributions from the dynamics of longitudinal spin GF. The last is essential at high temperatures and in some special cases. The obtained formulas generalize the zero-temperature calculations of Davis and Liu[89] and the approach of papers.[27,90,91] The numerical calculations of the typical behaviour of the real and imaginary parts of the self-energy in generalized Born approximation were carried out in Refs. 28, 30.

6. Charge Quasiparticle Dynamics of the s–d Model. Bound State Regime

In this section, we further discuss the spectrum of charge carrier excitations in the s–d model and describe bound state regime. As previously, consider the double-time thermal GF of charge operators $\langle\langle a_{k\sigma}(t), a_{k\sigma}^\dagger(t')\rangle\rangle$. The next step is to write down the equation of motion for the GF g:

$$(\omega - \varepsilon(k\sigma))\langle\langle a_{k\sigma} | a_{k\sigma}^\dagger\rangle\rangle_\omega + IN^{-1/2}\langle\langle C_{k\sigma} | a_{k\sigma}^\dagger\rangle\rangle_\omega = 1. \tag{63}$$

We also have

$$(\omega - \varepsilon(k\sigma))\langle\langle a_{k\sigma} | C_{k\sigma}^\dagger\rangle\rangle_\omega + IN^{-1/2}\langle\langle C_{k\sigma} | C_{k\sigma}^\dagger\rangle\rangle_\omega = 0. \tag{64}$$

It follows from Eqs. (63) and (64) that to take into account both the regimes, scattering and bound state, properly, we should treat the operators $a_{k\sigma}, a_{k\sigma}^\dagger$ and $C_{k\sigma}, C_{k\sigma}^\dagger$ on the equal footing. That means that one should consider the new relevant operator, a kind of "spinor" $\begin{pmatrix} a_{k\sigma} \\ C_{k\sigma} \end{pmatrix}$ ("relevant degrees of freedom") to construct a suitable Green function. Thus, according to the IGF strategy, to describe the bound state regime properly, contrary to the scattering regime, one should consider the generalized matrix GF of the form

$$\begin{pmatrix} \langle\langle a_{k\sigma} | a_{k\sigma}^\dagger\rangle\rangle_\omega & \langle\langle a_{k\sigma} | C_{k\sigma}^\dagger\rangle\rangle_\omega \\ \langle\langle C_{k\sigma} | a_{k\sigma}^\dagger\rangle\rangle_\omega & \langle\langle C_{k\sigma} | C_{k\sigma}^\dagger\rangle\rangle_\omega \end{pmatrix} = \hat{G}(k;\omega). \tag{65}$$

Equivalently, we can do the calculations in the Wannier representation with the matrix of the form

$$\begin{pmatrix} \langle\langle a_{i\sigma} | a_{j\sigma}^\dagger\rangle\rangle & \langle\langle a_{i\sigma} | C_{j\sigma}^\dagger\rangle\rangle \\ \langle\langle C_{i\sigma} | a_{j\sigma}^\dagger\rangle\rangle & \langle\langle C_{i\sigma} | C_{j\sigma}^\dagger\rangle\rangle \end{pmatrix} = \hat{G}(ij;\omega). \tag{66}$$

The form of Eq. (66) is more convenient for considering the effects of disorder. Let us consider now the equation of motion for the GF $\hat{G}(k;\omega)$. To write down the equation of motion for the Fourier transform of the GF $\hat{G}(k;\omega)$, we need auxiliary equations of motion for the following GFs of the form

$$(\omega - \varepsilon(k + q - \sigma))\langle\langle S_{-q}^{-\sigma} a_{k+q-\sigma} | a_{k\sigma}^{\dagger}\rangle\rangle_{\omega}$$

$$= -IN^{-1/2}\langle\langle S_{-q}^{-\sigma} C_{k+q-\sigma} | a_{k\sigma}^{\dagger}\rangle\rangle_{\omega}$$

$$- z_{\sigma} N^{-1/2} \sum_{p} J_{p}\langle\langle (S_{-(p+q)}^{-\sigma} S_{p}^{z} - S_{p}^{-\sigma} S_{-(p+q)}^{z}) a_{q+k-\sigma} | a_{k\sigma}^{\dagger}\rangle\rangle_{\omega}$$

$$= -IN^{-1/2} \sum_{p} \langle\langle S_{-q}^{-\sigma}(S_{-p}^{\sigma} a_{p+k+q\sigma} + z_{-\sigma}(S_{-p}^{z})^{ir} a_{p+k+q-\sigma}) | a_{k\sigma}^{\dagger}\rangle\rangle_{\omega}$$

$$- z_{\sigma} N^{-1/2} \sum_{p} J_{p}\langle\langle (S_{-(p+q)}^{-\sigma} S_{p}^{z} - S_{p}^{-\sigma} S_{-(p+q)}^{z}) a_{q+k-\sigma} | a_{k\sigma}^{\dagger}\rangle\rangle_{\omega} . \quad (67)$$

To separate the elastic and inelastic scattering corrections, it is convenient to introduce by definition the following set of irreducible operators:

$$(S_{-p}^{\sigma} S_{-q}^{-\sigma})^{ir} = S_{-p}^{\sigma} S_{-q}^{-\sigma} - \langle S_{q}^{\sigma} S_{-q}^{-\sigma}\rangle \delta_{-q,p}$$

$$(S_{-(p+q)}^{-\sigma} S_{p}^{z} - S_{p}^{-\sigma} S_{-(p+q)}^{z})^{ir} = (S_{-(p+q)}^{-\sigma} S_{p}^{z} - S_{p}^{-\sigma} S_{-(p+q)}^{z})$$

$$- (\langle S_{0}^{z}\rangle(\delta_{p,0} - \delta_{p,-q})$$

$$+ (\phi_{-p} - \phi_{-(p+q)}))S_{-q}^{-\sigma}) . \quad (68)$$

This is the standard way of introducing the "irreducible" parts of operators or GFs.[87] However, we are interested here in describing the bound electron-magnon states correctly. Thus, the definition of the relevant generalized mean field is more tricky for this case. It is important to note that *before* introducing the irreducible parts, Eq. (68), one has to extract from the GF $\langle\langle S_{-q}^{-\sigma} C_{k+q-\sigma} | a_{k\sigma}^{\dagger}\rangle\rangle$ the terms proportional to the initial GF $\langle\langle S_{-q}^{-\sigma} a_{k+q-\sigma} | a_{k\sigma}^{\dagger}\rangle\rangle$. That means that we should project the higher-order GF onto the initial one.[87] This projection should be performed using the spin commutation relations:

$$[S_{-q}^{-\sigma}, S_{-p}^{z}] = z_{\sigma} N^{-1/2} S_{-(q+p)}^{-\sigma} ;$$

$$[S_{-q}^{-\sigma}, S_{-p}^{\sigma}] = z_{-\sigma} 2N^{-1/2} S_{-(q+p)}^{z} .$$

In other words, this procedure introduces effectively the spin-operator ordering rule into the calculations. Roughly speaking, we should construct the relevant mean field not for spin or electron alone, but for the complex object, the "spin-electron", or for the operator $(S_{-q}^{-\sigma} a_{k+q-\sigma})$. This is the crucial point of the whole treatment, which leads to the correct definition of the generalized mean field in which the free magnetic polaron will propagate. We have then

$$\langle\langle S^{-\sigma}_{-q} S^{z}_{-p} a_{k+q+p-\sigma}|a^{\dagger}_{k\sigma}\rangle\rangle_{\omega} = z_{\sigma} N^{-1/2}\langle\langle S^{-\sigma}_{-(q+p)} a_{k+q+p-\sigma}|a^{\dagger}_{k\sigma}\rangle\rangle_{\omega}$$

$$+ \langle\langle S^{z}_{-p} S^{-\sigma}_{-q} a_{k+q+p-\sigma}|a^{\dagger}_{k\sigma}\rangle\rangle_{\omega} \tag{69}$$

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

$$+ \langle S^{z}_{0}\rangle\delta_{p,0}\langle\langle S^{-\sigma}_{-q} a_{k+q-\sigma}|a^{\dagger}_{k\sigma}\rangle\rangle_{\omega} \tag{70}$$

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

$$+ \langle S^{-\sigma}_{-q} S^{\sigma}_{q}\rangle\delta_{p,-q}\langle\langle a_{k\sigma}|a^{\dagger}_{k\sigma}\rangle\rangle \tag{71}$$

$$\langle\langle (S^{-\sigma}_{-(p+q)} S^{z}_{p} - S^{-\sigma}_{p} S^{z}_{-(p+q)})a_{k+q-\sigma}|a^{\dagger}_{k\sigma}\rangle\rangle_{\omega}$$

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

$$+ \langle S^{z}_{0}\rangle(\delta_{p,0} - \delta_{p,-q})\langle\langle S^{-\sigma}_{-q} a_{k+q-\sigma}|a^{\dagger}_{k\sigma}\rangle\rangle_{\omega}. \tag{72}$$

Finally, by differentiation of the GF $\langle\langle S^{-\sigma}_{-q} a_{k+q-\sigma}(t), a^{\dagger}_{k\sigma}(0)\rangle\rangle$ with respect to the first time, t, and using the definition of the irreducible parts, Eqs. (69)–(72), the equation of motion, Eq. (67), can be exactly transformed to the following form:

$$(\omega + z_{\sigma}\omega(q) - \varepsilon(k+q-\sigma))\langle\langle S^{-\sigma}_{-q} a_{k+q-\sigma}|a^{\dagger}_{k\sigma}\rangle\rangle_{\omega}$$

$$+ IN^{-1/2}\langle S^{-\sigma}_{-q} S^{\sigma}_{q}\rangle\langle\langle a_{k\sigma}|a^{\dagger}_{k\sigma}\rangle\rangle_{\omega}$$

$$= IN^{-1/2}\sum_{p}\langle\langle S^{-\sigma}_{-p} a_{k+p-\sigma}|a^{\dagger}_{k\sigma}\rangle\rangle_{\omega} + \langle\langle A_{q}|a^{\dagger}_{k\sigma}\rangle\rangle_{\omega} \tag{73}$$

where

$$A_{q} = -IN^{-1/2}\sum_{p}\{(S^{-\sigma}_{-q} S^{-\sigma}_{-p} a_{k+q+p\sigma})^{ir} + z_{-\sigma}(S^{z}_{-p})^{ir} S^{-\sigma}_{-q} a_{k+q+p-\sigma}\}$$

$$- z_{\sigma} N^{-1/2}\sum_{p} J_{p}(S^{-\sigma}_{-(p+q)}(S^{z}_{p})^{ir} - S^{-\sigma}_{p}(S^{z}_{q+p})^{ir})^{ir} a_{k+q-\sigma}$$

$$= -IN^{-1/2} C_{k+q-\sigma} S^{-\sigma}_{-q}$$

$$- z_{\sigma} N^{-1/2}\sum_{p} J_{p}(S^{-\sigma}_{-(p+q)}(S^{z}_{p})^{ir} - S^{-\sigma}_{p}(S^{z}_{q+p})^{ir})^{ir} a_{k+q-\sigma}. \tag{74}$$

It is easy to see that

$$\langle\langle S_{-q}^{-\sigma} a_{k+q-\sigma} | a_{k\sigma}^\dagger \rangle\rangle_\omega + IN^{-1/2} \frac{\langle S_{-q}^{-\sigma} S_q^\sigma \rangle}{(\omega + z_\sigma \omega(q) - \varepsilon(k+q-\sigma))} \langle\langle a_{k\sigma} | a_{k\sigma}^\dagger \rangle\rangle_\omega$$

$$= IN^{-1/2} \frac{1}{(\omega + z_\sigma \omega(q) - \varepsilon(k+q-\sigma))} \sum_p \langle\langle S_{-p}^{-\sigma} a_{k+p-\sigma} | a_{k\sigma}^\dagger \rangle\rangle_\omega$$

$$+ \frac{1}{(\omega + z_\sigma \omega(q) - \varepsilon(k+q-\sigma))} \langle\langle A_q | a_{k\sigma}^\dagger \rangle\rangle_\omega \,. \tag{75}$$

After summation with respect to q we find

$$\left\{ IN^{-1/2} \sum_q \frac{\langle S_{-q}^{-\sigma} S_q^\sigma \rangle}{(\omega + z_\sigma \omega(q) - \varepsilon(k+q-\sigma))} \right\} \langle\langle a_{k\sigma} | a_{k\sigma}^\dagger \rangle\rangle_\omega$$

$$+ \left\{ 1 - IN^{-1} \sum_q \frac{1}{(\omega + z_\sigma \omega(q) - \varepsilon(k+q-\sigma))} \right\} \sum_p \langle\langle S_{-p}^{-\sigma} a_{k+p-\sigma} | a_{k\sigma}^\dagger \rangle\rangle_\omega$$

$$= \sum_q \frac{1}{(\omega + z_\sigma \omega(q) - \varepsilon(k+q-\sigma))} \langle\langle A_q | a_{k\sigma}^\dagger \rangle\rangle_\omega \,. \tag{76}$$

Then Eq. (75) can be exactly rewritten in the following form:

$$\sum_q \langle\langle S_{-p}^{-\sigma} a_{k+p-\sigma} | a_{k\sigma}^\dagger \rangle\rangle_\omega$$

$$= - \left\{ IN^{-1/2} \sum_q \frac{\langle S_{-q}^{-\sigma} S_q^\sigma \rangle}{(1 - I\Lambda_{k\sigma}(\omega))(\omega + z_\sigma \omega(q) - \varepsilon(k+q-\sigma))} \right\} \langle\langle a_{k\sigma} | a_{k\sigma}^\dagger \rangle\rangle_\omega$$

$$+ \sum_q \frac{1}{(1 - I\Lambda_{k\sigma}(\omega))(\omega + z_\sigma \omega(q) - \varepsilon(k+q-\sigma))} \langle\langle A_q | a_{k\sigma}^\dagger \rangle\rangle_\omega \tag{77}$$

where

$$\Lambda_{k\sigma}(\omega) = \frac{1}{N} \sum_q \frac{1}{(\omega + z_\sigma \omega(q) - \varepsilon(k+q-\sigma))} \,. \tag{78}$$

To write down the equation of motion for the matrix GF $\hat{G}(k;\omega)$ Eq. (65) it is necessary to return to the operators $C_{k\sigma}$. We find

$$IN^{-1/2} \sum_q \left\{ \frac{\langle S_{-q}^{-\sigma} S_q^\sigma \rangle}{(1 - I\Lambda_{k\sigma}(\omega))(\omega + z_\sigma \omega(q) - \varepsilon(k+q-\sigma))} \right.$$

$$\left. + \frac{\langle (S_{-q}^z)^{ir} (S_q^z)^{ir} \rangle}{\omega - \varepsilon(k+q\sigma)} \right\} \langle\langle a_{k\sigma} | a_{k\sigma}^\dagger \rangle\rangle_\omega + \langle\langle C_{k\sigma} | a_{k\sigma}^\dagger \rangle\rangle_\omega$$

$$= \sum_q \left\{ \frac{\langle\langle A_q | a_{k\sigma}^\dagger \rangle\rangle_\omega}{(1 - I\Lambda_{k\sigma}(\omega))(\omega + z_\sigma \omega(q) - \varepsilon(k+q-\sigma))} + \frac{\langle\langle B_q | a_{k\sigma}^\dagger \rangle\rangle_\omega}{\omega - \varepsilon(k+q\sigma)} \right\} \tag{79}$$

$$IN^{-1/2} \sum_q \left\{ \frac{\langle S^{-\sigma}_{-q} S^{\sigma}_q \rangle}{(1 - I\Lambda_{k\sigma}(\omega))(\omega + z_\sigma \omega(q) - \varepsilon(k + q - \sigma))} \right.$$

$$\left. + \frac{\langle (S^z_{-q})^{ir} (S^z_q)^{ir} \rangle}{\omega - \varepsilon(k + q\sigma)} \right\} \langle\langle a_{k\sigma} | C^{\dagger}_{k\sigma} \rangle\rangle_\omega$$

$$+ \langle\langle C_{k\sigma} | C^{\dagger}_{k\sigma} \rangle\rangle_\omega = \sum_q \left\{ \frac{\langle S^{-\sigma}_{-q} S^{\sigma}_q \rangle}{(1 - I\Lambda_{k\sigma}(\omega))(\omega + z_\sigma \omega(q) - \varepsilon(k + q - \sigma))} \right.$$

$$\left. + \frac{\langle (S^z_{-q})^{ir} (S^z_q)^{ir} \rangle}{\omega - \varepsilon(k + q\sigma)} \right\}$$

$$+ \sum_q \left\{ \frac{\langle\langle A_q | C^{\dagger}_{k\sigma} \rangle\rangle_\omega}{(1 - I\Lambda_{k\sigma}(\omega))(\omega + z_\sigma \omega(q) - \varepsilon(k + q - \sigma))} + \frac{\langle\langle B_q | C^{\dagger}_{k\sigma} \rangle\rangle_\omega}{\omega - \varepsilon(k + q\sigma)} \right\} \quad (80)$$

where

$$B_q = -IN^{-1/2} \sum_p [(S^z_{-q} S^z_{-p} a_{k+q+p\sigma})^{ir} + z_\sigma (S^z_{-q})^{ir} S^{-\sigma}_{-p} a_{k+q+p-\sigma}]$$

$$= -z_\sigma IN^{-1/2} (S^z_{-q})^{ir} C_{k+q\sigma} \,. \quad (81)$$

The irreducible operators Eq. (68), Eqs. (69)–(72) have been introduced in such a way that the the operators A_q and B_q satisfy the conditions

$$\langle [A_q, a^{\dagger}_{k\sigma}]_+ \rangle = \langle [A_q, C^{\dagger}_{k\sigma}]_+ \rangle = 0$$
$$\langle [B_q, a^{\dagger}_{k\sigma}]_+ \rangle = \langle [B_q, C^{\dagger}_{k\sigma}]_+ \rangle = 0 \,. \quad (82)$$

The equations of motion, Eqs. (79) and (80) can be rewritten in the following form:

$$IN^{-1/2} \chi^b_{k\sigma}(\omega) \langle\langle a_{k\sigma} | a^{\dagger}_{k\sigma} \rangle\rangle_\omega + \langle\langle C_{k\sigma} | a^{\dagger}_{k\sigma} \rangle\rangle_\omega$$

$$= \sum_q \left\{ \frac{\langle\langle A_q | a^{\dagger}_{k\sigma} \rangle\rangle_\omega}{(1 - I\Lambda_{k\sigma}(\omega))(\omega + z_\sigma \omega(q) - \varepsilon(k + q - \sigma))} \right.$$

$$\left. + \frac{(1 + I\Lambda_{k\sigma}(\omega)) \langle\langle B_q | a^{\dagger}_{k\sigma} \rangle\rangle_\omega}{(1 - I\Lambda_{k\sigma}(\omega))(\omega - \varepsilon(k + q\sigma))} \right\} \quad (83)$$

$$IN^{-1/2} \chi^b_{k\sigma}(\omega) \langle\langle a_{k\sigma} | C^{\dagger}_{k\sigma} \rangle\rangle_\omega + \langle\langle C_{k\sigma} | C^{\dagger}_{k\sigma} \rangle\rangle_\omega$$

$$= \sum_q \left\{ \frac{\langle\langle A_q | C^{\dagger}_{k\sigma} \rangle\rangle_\omega}{(1 - I\Lambda_{k\sigma}(\omega))(\omega + z_\sigma \omega(q) - \varepsilon(k + q - \sigma))} \right.$$

$$\left. + \frac{(1 + I\Lambda_{k\sigma}(\omega)) \langle\langle B_q | C^{\dagger}_{k\sigma} \rangle\rangle_\omega}{(1 - I\Lambda_{k\sigma}(\omega))(\omega - \varepsilon(k + q\sigma))} \right\} \quad (84)$$

$$\times \sum_q \left\{ \frac{\langle\langle A_q | C_{k\sigma}^\dagger \rangle\rangle_\omega}{(1 - I\Lambda_{k\sigma}(\omega))(\omega + z_\sigma \omega(q) - \varepsilon(k + q - \sigma))} \right.$$

$$\left. + \frac{(1 + I\Lambda_{k\sigma}(\omega))\langle\langle B_q | C_{k\sigma}^\dagger \rangle\rangle_\omega}{(1 - I\Lambda_{k\sigma}(\omega))(\omega - \varepsilon(k + q\sigma))} \right\}$$

where

$$\chi_{k\sigma}^b(\omega) = \sum_q \left\{ \frac{\langle S_{-q}^{-\sigma} S_q^\sigma \rangle}{(1 - I\Lambda_{k\sigma}(\omega))(\omega + z_\sigma \omega(q) - \varepsilon(k + q - \sigma))} \right.$$

$$\left. + \frac{(1 + I\Lambda_{k\sigma}(\omega))\langle (S_{-q}^z)^{ir} (S_q^z)^{ir} \rangle}{(1 - I\Lambda_{k\sigma}(\omega))(\omega - \varepsilon(k + q\sigma))} \right\}. \tag{85}$$

Here $\chi_{k\sigma}^b(\omega)$ plays the role of the generalized "susceptibility" of the spin-electron bound states instead of the electron susceptibility $\chi_0^s(k, \omega)$ in the scattering-state regime Eq. (40) (see also Refs. 39, 40). Analogously, one can write the equation for the GF $\langle\langle C_{k\sigma} | C_{k\sigma}^\dagger \rangle\rangle$.

Now we are ready to write down the equation of motion for the matrix GF $\hat{G}(k; \omega)$, Eq. (65), after differentiation with respect to the first time, t. Using the equations of motion (80), (83), (84) and (63), we find

$$\hat{\Omega}\hat{G}(k; \omega) = \hat{I} + \sum_p \hat{\Phi}(p)\hat{D}(p; \omega) \tag{86}$$

where

$$\hat{\Omega} = \begin{pmatrix} \omega - \varepsilon(k\sigma) & IN^{1/2} \\ IN^{1/2}\chi_{k\sigma}^b(\omega) & 1 \end{pmatrix}, \quad \hat{I} = \begin{pmatrix} 1 & 0 \\ 0 & \chi_{k\sigma}^b(\omega) \end{pmatrix} \tag{87}$$

$$\hat{D}(p; \omega) = \begin{pmatrix} \langle\langle A_p | a_{k\sigma}^\dagger \rangle\rangle_\omega & \langle\langle A_p | C_{k\sigma}^\dagger \rangle\rangle_\omega \\ \langle\langle B_p | a_{k\sigma}^\dagger \rangle\rangle_\omega & \langle\langle B_p | C_{k\sigma}^\dagger \rangle\rangle_\omega \end{pmatrix}, \quad \hat{\Phi}(p) = \begin{pmatrix} 0 & 0 \\ \dfrac{1}{\omega_{k,p}^b} & \dfrac{1}{\Omega_{k,p}} \end{pmatrix} \tag{88}$$

with the notation

$$\omega_{k,q}^b = (1 - I\Lambda_{k\sigma}(\omega))(\omega + z_\sigma \omega(q) - \varepsilon(k + q - \sigma)) \tag{89}$$

$$\Omega_{k,q} = \frac{(1 - I\Lambda_{k\sigma}(\omega))}{(1 + I\Lambda_{k\sigma}(\omega))}(\omega - \varepsilon(k + q\sigma)). \tag{90}$$

To calculate the higher order GFs $\hat{D}(p; \omega)$ in Eq. (86), we differentiate its r.h.s. with respect to the second-time variable (t'). After introducing the irreducible parts as discussed above, but this time for the "right" operators, and combining both (the first- and second-time differentiated) equations of motion, we get the "exact" (no approximation has been made till now) "scattering" equation

$$\hat{G}(k; \omega) = \hat{G}^0(k; \omega) + \hat{G}^0(k; \omega)\hat{P}\hat{G}^0(k; \omega). \tag{91}$$

Here the generalized mean-field GF was defined as

$$\hat{G}^0(k;\omega) = \Omega_{k,p}^{-1}\hat{I}.$$

(92)

Note that it is possible to arrive at Eq. (91) using the symmetry properties too. We have

$$\hat{G}^\dagger\hat{\Omega}^\dagger = \hat{I}^\dagger + \sum_q \hat{D}^\dagger\hat{\Phi}^\dagger(q)$$

$$\hat{G} = \hat{I}^\dagger(\hat{\Omega}^\dagger)^{-1} + \sum_q \hat{D}^\dagger\hat{\Phi}^\dagger(q)(\hat{\Omega}^\dagger)^{-1}$$

$$\Omega\hat{D}^\dagger = \sum_p \hat{\Phi}(p)\hat{P}(pq) \quad \hat{G}^\dagger = \hat{G} = (\hat{\Omega}^{-1}\hat{I})$$

$$\hat{G} = (\hat{\Omega}^{-1}\hat{I})^\dagger + (\hat{\Omega}^{-1}\hat{I})\sum_{pq}\hat{I}^{-1}\hat{\Phi}(p)\hat{P}(pq)\hat{\Phi}^\dagger(q)(\hat{I}^{-1})^\dagger(\hat{\Omega}^{-1}\hat{I})^\dagger$$

$$\hat{P} = \hat{I}^{-1}\left\{\sum_{pq}\hat{\Phi}(p)\hat{P}(pq)\hat{\Phi}^\dagger(q)\right\}\hat{I}^{-1}$$

(93)

$$\hat{P}(pq) = \begin{pmatrix} \langle\langle A_p|A_q^\dagger\rangle\rangle & \langle\langle A_p|B_q^\dagger\rangle\rangle \\ \langle\langle B_p|A_q^\dagger\rangle\rangle & \langle\langle B_p|B_q^\dagger\rangle\rangle \end{pmatrix}.$$

(94)

We shall now consider the magnetic polaron state in the generalized mean field approximation and estimate the binding energy of the magnetic polaron.

7. Magnetic Polaron in Generalized Mean Field

From the definition, Eq. (92), the generalized mean-field GF matrix reads

$$\hat{G}^0(k;\omega) = \begin{pmatrix} \langle\langle a_{k\sigma}|a_{k\sigma}^\dagger\rangle\rangle^0 & \langle\langle a_{k\sigma}|C_{k\sigma}^\dagger\rangle\rangle^0 \\ \langle\langle C_{k\sigma}|a_{k\sigma}^\dagger\rangle\rangle^0 & \langle\langle C_{k\sigma}|C_{k\sigma}^\dagger\rangle\rangle^0 \end{pmatrix}$$

$$= \frac{1}{\det\hat{\Omega}}\begin{pmatrix} 1 & -IN^{-1/2}\chi_{k\sigma}^b(\omega) \\ -IN^{-1/2}\chi_{k\sigma}^b(\omega) & (\omega-\varepsilon(k\sigma))\chi_{k\sigma}^b(\omega) \end{pmatrix}$$

(95)

where

$$\det\hat{\Omega} = \omega - \varepsilon(k\sigma) - I^2N^{-1}\chi_{k\sigma}^b(\omega).$$

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

$$\langle\langle a_{k\sigma}|a_{k\sigma}^\dagger\rangle\rangle^0 = (\det\hat{\Omega})^{-1} = (\omega-\varepsilon(k\sigma) - I^2N^{-1}\chi_{k\sigma}^b(\omega))^{-1}.$$

(96)

The corresponding GF for the scattering regime are given by Eq. (57). As it follows from Eqs. (57) and (96) the mean-field GF $\langle\langle a_{k\sigma}|a_{k\sigma}^\dagger\rangle\rangle^0$ in the bound-state regime has a very nontrivial structure which is quite different from the scattering-state regime form. This was achieved by a suitable reconstruction of the generalized

mean field and by a sophisticated redefinition of the relevant irreducible Green functions! We have also

$$\langle\langle C_{k\sigma}|C_{k\sigma}^\dagger\rangle\rangle^0 = (\det\hat\Omega)^{-1}(\omega - \varepsilon(k\sigma))(\omega - \varepsilon(k\sigma) - \det\hat\Omega))\frac{N}{I^2}. \tag{97}$$

It follows from Eq. (96) that the quasiparticle spectrum of the electron-magnon bound states in the generalized mean field renormalization are determined by the equation

$$E_{k\sigma} = \varepsilon(k\sigma) + I^2 N^{-1}\chi_{k\sigma}^b(E_{k\sigma}). \tag{98}$$

The bound polaron-like electron-magnon energy spectrum consists of two branches for any electron spin projection. At the so-called "atomic limit" (when $\epsilon_k = 0$) and in the limit $k \to 0$, $\omega \to 0$ we obtain the exact analytical representation for the single-particle GF of the form

$$\langle\langle a_{k\sigma}|a_{k\sigma}^\dagger\rangle\rangle^0 = \frac{S + z_\sigma S_z}{2S + 1}(\omega + IS)^{-1} + \frac{S - z_\sigma S_z}{2S + 1}(\omega - I(S + 1))^{-1}. \tag{99}$$

Here the notation S and $S_z = \frac{\langle S_0^z\rangle}{\sqrt{N}}$ means the spin-value and magnetization, respectively. This result was derived previously in paper.[60]

However, our approach is the closest to the seminal paper of Shastry and Mattis,[74] where the Green function treatment of the magnetic polaron problem was formulated for zero temperature. Our generalized mean-field solution is reduced exactly to the Shastry–Mattis result if we put in our expression for the spectrum, Eq. (97), the temperature $T = 0$

$$\langle\langle a_{k\sigma}|a_{k\sigma}^\dagger\rangle\rangle^0|_{T=0} = \left\{\omega - \varepsilon(k\sigma) - \delta_{\sigma\downarrow}2I^2S\frac{\Lambda_{k\sigma}(\omega)}{(1 - I\Lambda_{k\sigma}(\omega))}\right\}^{-1}. \tag{100}$$

We can see that the magnetic polaron states are formed for antiferromagnetic s–d coupling ($I < 0$) only when there is a lowering of the band of the uncoupled itinerant charge carriers due to the effective attraction of the carrier and magnon.

The derivation of Eq. (100) was carried out for arbitrary interrelations between the s–d model parameters. Let us consider now the two limiting cases where analytical calculations are possible.

(i) a wide-band semiconductor ($|I|S \ll W$)

$$E_{k\downarrow} \simeq \epsilon_k + I\frac{S(S + S_z + 1) + S_z(S - S_z + 1)}{2S}$$

$$+ \frac{(-I)}{N}\sum_q \frac{(\epsilon_{k-q} - \epsilon_k + 2I(S - S_z))}{(\epsilon_{k-q} - \epsilon_k + 2IS_z)}\frac{\langle S_q^+ S_{-q}^-\rangle}{2S}; \tag{101}$$

(ii) a narrow-band semiconductor ($|I|S \gg W$)

$$E_{k\downarrow} \simeq I(S+1) + \frac{2(S+1)(S+S_z)}{(2S+1)(S+S_z+1)}\epsilon_k$$

$$+ \frac{1}{N}\sum_q \frac{(\epsilon_{k-q} - \epsilon_k)}{(2S+1)}\frac{\langle S_q^+ S_{-q}^-\rangle}{(S+S_z+1)}. \tag{102}$$

In the above formulae the correlation function of the longitudinal spin components K_q^{zz} was omitted for the sake of simplicity. Here W is the bandwidth in the limit $I = 0$.

Let us now consider in more detail the low-temperature spin-wave limit in Eqs. (101) and (102). In that limit it is reasonable to suppose that $S_z \simeq S$. In the spin-wave approximation we also have

$$\langle S_q^+ S_{-q}^-\rangle \simeq 2S(1 + N(\omega(q))).$$

Thus, we obtain (c.f. Refs. 27, 60).

(i) a wide-band semiconductor ($|I|S \ll W$)

$$E_{k\downarrow} \simeq \epsilon_k + IS + \frac{2I^2S}{N}\sum_q \frac{1}{(\epsilon_k - \epsilon_{k-q} + 2IS)}$$

$$+ \frac{(-I)}{N}\sum_q \frac{(\epsilon_{k-q} - \epsilon_k)}{(\epsilon_{k-q} - \epsilon_k - 2IS)}N(\omega(q)); \tag{103}$$

(ii) a narrow-band semiconductor ($|I|S \gg W$)

$$E_{k\downarrow} \simeq I(S+1) + \frac{2S}{(2S+1)}\epsilon_k + \frac{1}{N}\sum_q \frac{2S}{(2S+1)}\frac{(\epsilon_{k-q} - \epsilon_k)}{(2S+1)}N(\omega(q)). \tag{104}$$

We shall now estimate the binding energy of the magnetic polaron bound state. The binding energy of the magnetic polaron is convenient to define as

$$\varepsilon_B = \varepsilon_{k\downarrow} - E_{k\downarrow}. \tag{105}$$

This definition is quite natural and takes into account the fact that in the simple Hartree–Fock approximation the spin-down band is given by the expression

$$\varepsilon_{k\downarrow} = \epsilon_k + IS.$$

Then the binding energy ε_B behaves according to the formula:

(i) a wide-band semiconductor ($|I|S \ll W$)

$$\varepsilon_B = \varepsilon_{B1}^0 - \frac{(-I)}{N}\sum_q \frac{(\epsilon_{k-q} - \epsilon_k)}{(\epsilon_{k-q} - \epsilon_k - 2IS)}N(\omega(q)); \tag{106}$$

(ii) a narrow-band semiconductor ($|I|S \gg W$)

$$\varepsilon_B = \varepsilon_{B2}^0 - \frac{1}{N}\sum_q \frac{2S}{(2S+1)}\frac{(\epsilon_{k-q} - \epsilon_k)}{(2S+1)}N(\omega(q)) \tag{107}$$

where

$$\varepsilon_{B1}^0 = \frac{(2I^2S)}{N} \sum_q \frac{1}{(\epsilon_{k-q} - \epsilon_k - 2IS)} \simeq \frac{|I|S}{W}|I|$$

$$\varepsilon_{B2}^0 = -I + \frac{\epsilon_k}{(2S+1)} \simeq |I| \,. \tag{108}$$

The present consideration gives the generalization of the thermodynamic study of the magnetic polaron. Clearly, local magnetic order lowers the state energy of the dressed itinerant carrier, with respect to some conduction or valence band. It is obvious that below T_N of the antiferromagnet the mobility of spin polarons will be less than of bare carriers,[93] since they have to drag their polarization cloud along. Experimental evidence for magnetic polarons in concentrated magnetic semiconductors came from optical studies of EuTe, an antiferromagnet.[94] Direct measurements of the polaron-binding energy were carried out in Ref. 95.

8. Quasiparticle Many-Body Dynamics and Damping of Quasiparticle States

8.1. *Green function picture of quasiparticles*

An effective way of viewing quasiparticles, quite general and consistent, is via the Green function scheme of many-body theory[87] which we sketch below for completeness.

At sufficiently low temperatures, a few quasiparticles are excited and, therefore, this dilute quasiparticle gas is nearly a noninteracting gas in the sense that the quasiparticles rarely collide. The success of the quasiparticle concept in an interacting many-body system is particularly striking because of a great number of various applications. However, the range of validity of the quasiparticle approximation, especially for strongly interacting lattice systems, was not discussed properly in many cases. In systems like simple metals, quasiparticles constitute long-lived, weakly interacting excitations, since their intrinsic decay rate varies as the square of the dispersion law, thereby justifying their use as the building blocks for the low-lying excitation spectrum.

As we have mentioned earlier, to describe a quasiparticle correctly, the Irreducible Green functions method is a very suitable and useful tool.

It is known[87] that the GF is completely determined by the spectral weight function $A(\omega)$. To explain this, let us remind that the GFs are linear combinations of the time correlation functions

$$F_{AB}(t-t') = \langle A(t)B(t') \rangle = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega \exp[i\omega(t-t')]A_{AB}(\omega) \tag{109}$$

$$F_{BA}(t'-t) = \langle B(t')A(t) \rangle = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega \exp[i\omega(t'-t)]A_{BA}(\omega) \,. \tag{110}$$

Here, the Fourier transforms $A_{AB}(\omega)$ and $A_{BA}(\omega)$ are of the form

$$A_{BA}(\omega) = Q^{-1}2\pi \sum_{m,n} \exp(-\beta E_n)(\psi_n^\dagger B \psi_m)(\psi_m^\dagger A \psi_n)\delta(E_n - E_m - \omega) \quad (111)$$

$$A_{AB} = \exp(-\beta\omega)A_{BA}(-\omega). \quad (112)$$

Expressions (111) and (112) are spectral representations of the corresponding time correlation functions. The quantities A_{AB} and A_{BA} are spectral densities or spectral weight functions.

It is convenient to define

$$F_{BA}(0) = \langle B(t)A(t)\rangle = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega A(\omega) \quad (113)$$

$$F_{AB}(0) = \langle A(t)B(t)\rangle = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega \exp(\beta\omega)A(\omega). \quad (114)$$

Then, the spectral representations of the Green functions can be expressed in the form

$$G^r(\omega) = \langle\langle A|B\rangle\rangle_\omega^r$$
$$= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{d\omega'}{\omega - \omega' + i\epsilon}[\exp(\beta\omega') - \eta]A(\omega') \quad (115)$$

$$G^a(\omega) = \langle\langle A|B\rangle\rangle_\omega^a$$
$$= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{d\omega'}{\omega - \omega' - i\epsilon}[\exp(\beta\omega') - \eta]A(\omega'). \quad (116)$$

The most important practical consequence of spectral representations for the retarded and advanced GFs is the so-called *spectral theorem*. The spectral theorem can be written as

$$\langle B(t')A(t)\rangle = -\frac{1}{\pi}\int_{-\infty}^{+\infty} d\omega \exp[i\omega(t-t')][\exp(\beta\omega) - \eta]^{-1} Im G_{AB}(\omega + i\epsilon) \quad (117)$$

$$\langle A(t)B(t')\rangle = -\frac{1}{\pi}\int_{-\infty}^{+\infty} d\omega \exp(\beta\omega)$$
$$\times \exp[i\omega(t-t')][\exp(\beta\omega) - \eta]^{-1} Im G_{AB}(\omega + i\epsilon). \quad (118)$$

Expressions (117) and (118) are of fundamental importance. They directly relate the statistical averages with the Fourier transforms of the corresponding GFs. The problem of evaluating the latter is thus reduced to finding their Fourier transforms providing the practical usefulness of the Green functions technique.[88,87]

The spectral weight function reflects the microscopic structure of the system under consideration. Its Fourier transform origination is then the density of states that can be reached by adding or removing a particle of a given momentum and energy. Consider a system of interacting fermions as an example. For a noninteracting

system, the spectral weight function of the single-particle GF $G_k(\omega) = \langle\langle a_{k\sigma}; a_{k\sigma}^\dagger\rangle\rangle$ has a simple peaked structure

$$A_k(\omega) \sim \delta(\omega - \epsilon_k)\,.$$

For an interacting system, the spectral function $A_k(\omega)$ has no such a simple peaked structure, but it obeys the following conditions:

$$A_k(\omega) \geq 0\,; \quad \int A_k(\omega)d\omega = \langle[a_{k\sigma}, a_{k\sigma}^\dagger]_+\rangle = 1\,.$$

Thus, we can see from these expressions that for a noninteracting system, the sum rule is exhausted by a single peak. A sharply peaked spectral function for an interacting system means a long-lived single-particle-like excitation. Thus, the spectral weight function was established here as a physically significant attribute of GF. The question of what is the best way of extracting it from a microscopic theory is the main aim of the present theory.

The GF for a noninteracting system is $G_k(\omega) = (\omega - \epsilon_k)^{-1}$. For a weakly interacting Fermi system, we have $G_k(\omega) = (\omega - \epsilon_k - M_k(\omega))^{-1}$ where $M_k(\omega)$ is the mass operator. Thus, for a weakly interacting system, the δ-function for $A_k(\omega)$ is spread into a peak of finite width due to the mass operator. We have

$$M_k(\omega \pm i\epsilon) = ReM_k(\omega) \mp ImM_k(\omega) = \Delta_k(\omega) \mp \Gamma_k(\omega)\,.$$

The single-particle GF can be written in the form

$$G_k(\omega) = \{\omega - [\epsilon_k + \Delta_k(\omega)] \pm \Gamma_k(\omega)\}^{-1}\,. \tag{119}$$

In the weakly interacting case, we can thus find the energies of quasiparticles by looking for the poles of single-particle GF (119)

$$\omega = \epsilon_k + \Delta_k(\omega) \pm \Gamma_k(\omega)\,.$$

The dispersion relation of a quasiparticle

$$\epsilon(k) = \epsilon_k + \Delta_k[\epsilon(k)] \pm \Gamma_k[\epsilon(k)]$$

and the lifetime $1/\Gamma_k$ then reflects the inter-particle interaction. It is easy to see the connection between the width of the spectral weight function and decay rate. We can write

$$A_k(\omega) = (\exp(\beta\omega) + 1)^{-1}(-i)[G_k(\omega + i\epsilon) - G_k(\omega - i\epsilon)]$$

$$= (\exp(\beta\omega) + 1)^{-1}\frac{2\Gamma_k(\omega)}{[\omega - (\epsilon_k + \Delta_k(\omega))]^2 + \Gamma_k^2(\omega)}\,. \tag{120}$$

In other words, for this case, the corresponding propagator can be written in the form

$$G_k(t) \approx \exp(-i\epsilon(k)t)\exp(-\Gamma_k t)\,.$$

This form shows under which conditions, the time-development of an interacting system can be interpreted as the propagation of a quasiparticle with a reasonably well-defined energy and a sufficiently long lifetime. To demonstrate this, we consider the following conditions:

$$\Delta_k[\epsilon(k)] \ll \epsilon(k); \quad \Gamma_k[\epsilon(k)] \ll \epsilon(k).$$

Then we can write

$$G_k(\omega) = \frac{1}{[\omega - \epsilon(k)][1 - \frac{d\Delta_k(\omega)}{d\omega}|_{\omega=\epsilon(k)}] + i\Gamma_k[\epsilon(k)]} \tag{121}$$

where the renormalized energy of excitations is defined by

$$\epsilon(k) = \epsilon_k + \Delta_k[\epsilon(k)].$$

In this case, we have, instead of (121),

$$A_k(\omega) = [\exp(\beta\epsilon(k)) + 1]^{-1} \left[1 - \frac{d\Delta_k(\omega)}{d\omega}\bigg|_{\epsilon(k)}\right]^{-1} \frac{2\Gamma(k)}{(\omega - \epsilon(k))^2 + \Gamma^2(k)}. \tag{122}$$

As a result, we find

$$G_k(t) = \langle\langle a_{k\sigma}(t); a_{k\sigma}^\dagger\rangle\rangle$$

$$= -i\theta(t)\exp(-i\epsilon(k)t)\exp(-\Gamma(k)t) \left[1 - \frac{d\Delta_k(\omega)}{d\omega}\bigg|_{\epsilon(k)}\right]^{-1}. \tag{123}$$

A widely known strategy to justify this line of reasoning is the perturbation theory. In a strongly interacted system on a lattice with complex spectra, the concept of a quasiparticle needs a suitable adaptation and a careful examination. It is therefore useful to have a workable and efficient IGF method which, as we have seen, permits one to determine and correctly separate the elastic and inelastic scattering renormalizations by a correct definition of the generalized mean field and to calculate real quasiparticle spectra, including the damping and lifetime effects.

8.2. *Damping of magnetic polaron state*

We shall now calculate the damping of the magnetic polaron state due to the inelastic scattering effects. To obtain the Dyson equation from Eq. (91), we have to use the relation (17). Thus, we obtain the exact Dyson equation, Eq. (18),

$$\hat{G}(k;\omega) = \hat{G}^0(k;\omega) + \hat{G}^0(k;\omega)\hat{M}_{k\sigma}\hat{G}(k;\omega). \tag{124}$$

The mass operator has the following exact representation:

$$\hat{M}_{k\sigma} = \begin{pmatrix} 0 & 0 \\ 0 & \frac{\Pi_{k\sigma}(\omega)}{\chi_{k\sigma}^b(\omega)} \end{pmatrix}. \tag{125}$$

Here the notation was used

$$\Pi_{k\sigma}(\omega) = \sum_{pq} \left\{ \frac{\langle\langle A_p | A_q^\dagger \rangle\rangle^p}{\omega_{kp}^b \omega_{kq}^b} + \frac{\langle\langle A_p | B_q^\dagger \rangle\rangle^p}{\omega_{kp}^b \Omega_{kq}} + \frac{\langle\langle B_p | A_q^\dagger \rangle\rangle^p}{\Omega_{kp} \omega_{kq}^b} + \frac{\langle\langle B_p | B_q^\dagger \rangle\rangle^p}{\Omega_{kp} \Omega_{kq}} \right\} . \quad (126)$$

For the single-particle GF of itinerant carriers we have

$$\langle\langle a_{k\sigma} | a_{k\sigma}^\dagger \rangle\rangle = \{ (\langle\langle a_{k\sigma} | a_{k\sigma}^\dagger \rangle\rangle^0)^{-1} - \Sigma_{k\sigma}(\omega) \}^{-1} . \quad (127)$$

Here the self-energy operator $\Sigma_{k\sigma}(\omega)$ was defined as

$$\Sigma_{k\sigma}(\omega) = \frac{I^2}{N} \frac{\Pi_{k\sigma}(\omega)}{1 - (\chi_{k\sigma}^b(\omega))^{-1} \Pi_{k\sigma}(\omega)} . \quad (128)$$

We shall now use the exact representation, Eq. (128), to derive a suitable self-consistent approximate expression for the self-energy. Let us consider the GFs appearing in Eq. (126). According to the spectral theorem, Eqs. (117) and (118), it is convenient to write down the GF $\langle\langle A_p | A_q^\dagger \rangle\rangle^p$ in the following form:

$$\langle\langle A_p | A_q^\dagger \rangle\rangle^p$$
$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{d\omega'}{\omega - \omega' + i\epsilon} [\exp(\beta\omega') + 1] \int dt \exp(i\omega' t) \langle A_q^\dagger A_p(t) \rangle^p . \quad (129)$$

Then we obtain for the correlation function $\langle A_q^\dagger A_p(t) \rangle^p$

$$\langle A_q^\dagger A_p(t) \rangle^p = \frac{I^2}{N} \langle S_q^\sigma C_{k+q-\sigma}^\dagger C_{k+p-\sigma}(t) S_{-p}^{-\sigma}(t) \rangle$$
$$+ \langle a_{q+k-\sigma}^\dagger \Phi_{-q-\sigma}^\dagger \Phi_{-p-\sigma}(t) a_{p+k-\sigma}(t) \rangle . \quad (130)$$

A further insight is gained if we select a suitable relevant "trial" approximation for the correlation function in the r.h.s. of (130). In this paper, we show that our formulations based on the IGF method permit one to obtain an explicit approximate expression for the mass operator in a self-consistent way. It is clear that a relevant trial approximation for the correlation function in (130) can be chosen in various ways. For example, a reasonable and workable one can be the following "mode-mode coupling approximation" which is especially suitable for a description of two coupled subsystems. Then the correlation function $\langle A_q^\dagger A_p(t) \rangle^p$ could now be written in the approximate form using the following decoupling procedure (approximate trial solutions):

$$\langle S_q^\sigma C_{k+q-\sigma}^\dagger C_{k+p-\sigma}(t) S_{-p}^{-\sigma}(t) \rangle \simeq \delta_{q,p} \langle S_q^\sigma S_{-q}^{-\sigma}(t) \rangle \langle C_{k+q-\sigma}^\dagger C_{k+q-\sigma}(t) \rangle$$

$$\langle a_{q+k-\sigma}^\dagger \Phi_{-q-\sigma}^\dagger \Phi_{-p-\sigma}(t) a_{p+k-\sigma}(t) \rangle \simeq \delta_{q,p} \langle \Phi_{-q-\sigma}^\dagger \Phi_{-q-\sigma}(t) \rangle \langle a_{q+k-\sigma}^\dagger a_{q+k-\sigma}(t) \rangle .$$
$$(131)$$

Here the notation was introduced

$$\langle \Phi^{\dagger}_{-q-\sigma} \Phi_{-q-\sigma}(t) \rangle$$

$$= \frac{1}{N} \sum_{pp'} J_p J_{p'} \langle ((S^z_{-p})^{ir} S^{\sigma}_{q+p} - (S^z_{-(q+p)})^{ir} S^{\sigma}_{-p})^{ir}$$

$$\times (S^{-\sigma}_{-(p'+q)}(t)(S^z_{p'}(t))^{ir} - S^{-\sigma}_{p'}(t)(S^z_{-(q+p)}(t))^{ir})^{ir} \rangle. \qquad (132)$$

The approximation, Eq. (131), in the diagrammatic language corresponds to neglect of the vertex correction, i.e. the correlation between the propagation of the polaron and the magnetic excitation, and the electron and magnon, respectively. This can be performed since we already have in our exact expression (130) the terms proportional to I^2 and J^2. Taking into account the spectral theorem, Eqs. (117) and (118), we obtain from Eqs. (129)–(132)

$$\langle\langle A_p | A_q^{\dagger} \rangle\rangle^p \simeq \frac{I^2}{N} \delta_{q,p} \int \int \frac{d\omega_1 d\omega_2}{\omega - \omega_1 - \omega_2} F_1(\omega_1, \omega_2) \qquad (133)$$

$$\left(\frac{-1}{\pi} Im\langle\langle S^{-\sigma}_{-q} | S^{\sigma}_q \rangle\rangle_{\omega_1} \right) \left(\frac{-1}{\pi} Im\langle\langle C_{k+q-\sigma} | C^{\dagger}_{k+q-\sigma} \rangle\rangle_{\omega_2} \right)$$

$$+ \delta_{q,p} \frac{1}{N} \sum_{q'} (J_{q'} - J_{q-q'})^2 \int \int \int \frac{d\omega_1 d\omega_2 d\omega_3}{\omega - \omega_1 - \omega_2 - \omega_3} F_2(\omega_1, \omega_2, \omega_3)$$

$$\times \left(\frac{-1}{\pi} Im\langle\langle (S^z_{-q'})^{ir} | (S^z_{q'})^{ir} \rangle\rangle_{\omega_1} \right) \left(\frac{-1}{\pi} Im\langle\langle S^{-\sigma}_{-(q-q')} | S^{\sigma}_{q-q'} \rangle\rangle_{\omega_2} \right)$$

$$\times \left(\frac{-1}{\pi} Im\langle\langle a_{k+q-\sigma} | a^{\dagger}_{k+q-\sigma} \rangle\rangle_{\omega_3} \right)$$

$$\langle\langle B_p | B_q^{\dagger} \rangle\rangle^p \simeq \frac{I^2}{N} \delta_{q,p} \int \int \frac{d\omega_1 d\omega_2}{\omega - \omega_1 - \omega_2} F_1(\omega_1, \omega_2)$$

$$\times \left(\frac{-1}{\pi} Im\langle\langle (S^z_{-q})^{ir} | (S^z_q)^{ir} \rangle\rangle_{\omega_1} \right) \left(\frac{-1}{\pi} Im\langle\langle C_{k+q\sigma} | C^{\dagger}_{k+q\sigma} \rangle\rangle_{\omega_2} \right) \quad (134)$$

where

$$F_1(\omega_1, \omega_2) = (1 + N(\omega_1) - f(\omega_2)) \qquad (135)$$

$$F_2(\omega_1, \omega_2, \omega_3) = (1 + N(\omega_1))(1 + N(\omega_2) - f(\omega_3)) - N(\omega_2)f(\omega_3)$$

$$= (1 + N(\omega_1))(1 + N(\omega_2)) - (1 + N(\omega_1) + N(\omega_2))f(\omega_2). \qquad (136)$$

The functions $F_1(\omega_1, \omega_2)$, Eq. (136), and $F_2(\omega_1, \omega_2, \omega_3)$, Eq. (135), represent clearly the inelastic scattering of bosons and fermions. For estimation of the damping effects it is reasonably to accept that

$$\langle\langle A_p | B_q^{\dagger} \rangle\rangle^p \simeq \langle\langle B_p | A_q^{\dagger} \rangle\rangle^p \simeq 0. \qquad (137)$$

We have then

$$\Pi_{k\sigma} \simeq \sum_{qp} \left(\frac{\langle\langle A_p | A_q^\dagger \rangle\rangle^p}{\omega_{kp}^b \omega_{kq}^b} + \frac{\langle\langle B_p | B_q^\dagger \rangle\rangle^p}{\Omega_{kp} \Omega_{kq}} \right)$$

$$\simeq \sum_q \left(\frac{\langle\langle A_q | A_q^\dagger \rangle\rangle^p}{(\omega_{kq}^b)^2} + \frac{\langle\langle B_q | B_q^\dagger \rangle\rangle^p}{(\Omega_{kq})^2} \right). \tag{138}$$

We can see that there are two distinct contributions to the self-energy. Putting together formulae (133)–(138), we arrive at the following formulae for both the contributions

$$\Pi_{k\sigma}^I = \frac{I^2}{N} \sum_q \int \int \frac{d\omega_1 d\omega_2}{\omega - \omega_1 - \omega_2} F_1(\omega_1, \omega_2)$$

$$\times \left\{ \frac{1}{(\omega_{kq}^b)^2} \left(\frac{-1}{\pi} Im\langle\langle S_{-q}^{-\sigma} | S_q^\sigma \rangle\rangle_{\omega_1} \right) \left(\frac{-1}{\pi} Im\langle\langle C_{k+q-\sigma} | C_{k+q-\sigma}^\dagger \rangle\rangle_{\omega_2} \right) \right.$$

$$\left. + \frac{1}{(\Omega_{kq})^2} \left(\frac{-1}{\pi} Im\langle\langle (S_{-q}^z)^{ir} | (S_q^z)^{ir} \rangle\rangle_{\omega_1} \right) \left(\frac{-1}{\pi} Im\langle\langle C_{k+q\sigma} | C_{k+q\sigma}^\dagger \rangle\rangle_{\omega_2} \right) \right\}$$

$$\tag{139}$$

$$\Pi_{k\sigma}^J = \frac{1}{N} \sum_{qq'} (J_{q'} - J_{q-q'})^2 \int \int \int \frac{d\omega_1 d\omega_2 d\omega_3}{\omega - \omega_1 - \omega_2 - \omega_3}$$

$$\times F_2(\omega_1, \omega_2, \omega_3) \frac{1}{(\omega_{kq}^b)^2} \left(\frac{-1}{\pi} Im\langle\langle (S_{-q'}^z)^{ir} | (S_{q'}^z)^{ir} \rangle\rangle_{\omega_1} \right)$$

$$\times \left(\frac{-1}{\pi} Im\langle\langle S_{-(q-q')}^{-\sigma} | S_{q-q'}^\sigma \rangle\rangle_{\omega_2} \right) \left(\frac{-1}{\pi} Im\langle\langle a_{k+q-\sigma} | a_{k+q-\sigma}^\dagger \rangle\rangle_{\omega_3} \right). \tag{140}$$

Equations (124), (125), (139), and (140) constitute a closed self-consistent system of equations for the single-electron GF of the s–d model in the bound state regime. This system of equations is much more complicated than the corresponding system of equations for the scattering states. We can see that to the extent that the spin and fermion degrees of freedom can be factorized as in Eq. (131), the self-energy operator can be expressed in terms of the initial GFs self-consistently. It is clear that this representation does not depend on any assumption about the explicit form of the spin and fermion GFs in the r.h.s. of Eqs. (139) and (140).

Let us first consider the so-called *"static"* limit. The thorough discussion of this approximation was carried out in Ref. 27. We just show below that a more general form of this approximation follows directly from our formulae. The contributions of the GFs, Eqs. (133) and (134), are then

$$\langle\langle A_p | A_q^\dagger \rangle\rangle^p \simeq \frac{I^2}{N} \delta_{q,p} \int \int \frac{d\omega_1 d\omega_2}{\omega - \omega_1 - \omega_2} F_1(\omega_1, \omega_2) \tag{141}$$

$$\left(\frac{-1}{\pi}Im\langle\langle S_{-q}^{-\sigma}|S_q^\sigma\rangle\rangle_{\omega_1}\right)\left(\frac{-1}{\pi}Im\langle\langle C_{k+q-\sigma}|C_{k+q-\sigma}^\dagger\rangle\rangle_{\omega_2}\right)$$

$$+\delta_{q,p}\frac{1}{N}\sum_{q'}(J_{q'}-J_{q-q'})^2\langle(S_{q'}^z)^{ir}(S_{-q'}^z)^{ir}\rangle\int\int\frac{d\omega_1 d\omega_2}{\omega-\omega_1-\omega_2}F_1(\omega_1,\omega_2)$$

$$\times\left(\frac{-1}{\pi}Im\langle\langle S_{-(q-q')}^{-\sigma}|S_{q-q'}^\sigma\rangle\rangle_{\omega_1}\right)\left(\frac{-1}{\pi}Im\langle\langle a_{k+q-\sigma}|a_{k+q-\sigma}^\dagger\rangle\rangle_{\omega_2}\right)$$

$$\langle\langle B_p|B_q^\dagger\rangle\rangle^p\simeq\frac{I^2}{N}\delta_{q,p}\langle(S_q^z)^{ir}(S_{-q}^z)^{ir}\rangle\int\frac{d\omega_1}{\omega-\omega_1}F_1(\omega_1)$$

$$\times\left(\frac{-1}{\pi}Im\langle\langle C_{k+q\sigma}|C_{k+q\sigma}^\dagger\rangle\rangle_{\omega_1}\right)\tag{142}$$

$$F_1(\omega_1)=(1-f(\omega_1))\,.$$

In the limit of low carrier concentration it is possible to drop the Fermi distribution function in Eqs. (133)–(140). In principle, we can use, in the r.h.s. of Eqs. (135) and (137), any workable first iteration-step form of the GF and find a solution by iteration (see Ref. 87). It is most convenient to choose, as the first iteration step, the following simple one-pole expressions:

$$\frac{-1}{\pi}Im\langle\langle S_{-p}^{-\sigma}a_{k+q+p-\sigma}|S_p^\sigma a_{k+q+p-\sigma}^\dagger\rangle\rangle_\omega$$

$$=\langle S_{-p}^{-\sigma}S_p^\sigma\rangle\delta(\omega+z_\sigma\omega_p-\varepsilon(k+q+p-\sigma))\,,$$

$$\frac{-1}{\pi}Im\langle\langle(S_{-p}^z)^{ir}a_{k+q+p\sigma}|(S_p^z)^{ir}a_{k+q+p\sigma}^\dagger\rangle\rangle_\omega$$

$$=\langle(S_{-p}^z)^{ir}(S_p^z)^{ir}\rangle\delta(\omega-\varepsilon(k+q+p-\sigma))\,,$$

$$\frac{-1}{\pi}\langle\langle S_{-q}^{-\sigma}|S_q^\sigma\rangle\rangle_\omega=-z_\sigma 2\langle S_z\rangle\delta(\omega+z_\sigma\omega_q)\,,$$

$$\frac{-1}{\pi}Im\langle\langle a_{k+q+p-\sigma}|a_{k+q+p-\sigma}^\dagger\rangle\rangle_\omega=\delta(\omega-\varepsilon(k+q-\sigma))\,.\tag{143}$$

Using Eqs. (129)–(136) in (125) we obtain the self-consistent approximate expression for the self-energy operator (the self-consistency means that we express approximately the self-energy operator in terms of the initial GF, and, in principle, one can obtain the required solution by a suitable iteration procedure)

$$\Sigma_{k\sigma}(\omega)\simeq\frac{2I^2\langle S_0^z\rangle}{N^{3/2}}\sum_{qp}\frac{\delta_{\sigma\downarrow}+N(\omega_q)}{(\omega_{k,q}^b)^2}\left(\frac{\langle S_p^\sigma S_{-p}^{-\sigma}\rangle}{\omega+z_\sigma(\omega_q-\omega_p)-\varepsilon(k+q-p-\sigma)}\right.$$

$$\left.+\frac{\langle(S_{-p}^z)^{ir}(S_p^z)^{ir}\rangle}{\omega+z_\sigma\omega_q-\varepsilon(k+q+p-\sigma)}\right)$$

$$+ \frac{I^2}{N} \sum_{qp} \int d\omega' \frac{(1 + N(\omega'))}{(\Omega_{k,q})^2} \left(\frac{-1}{\pi} Im \langle\langle (S_q^z)^{ir} | (S_{-q}^z)^{ir} \rangle\rangle_{\omega'} \right)$$

$$\times \left(\frac{\langle S_{-p}^{-\sigma} S_p^{\sigma} \rangle}{\omega - \omega' + z_{\sigma} \omega_q - \varepsilon(k + q + p - \sigma)} + \frac{\langle (S_{-p}^z)^{ir} (S_p^z)^{ir} \rangle}{\omega - \omega' - \varepsilon(k + q + p\sigma)} \right).$$

$$(144)$$

Here we write down for brevity the contribution of the s–d interaction to the inelastic scattering only. For the spin-wave approximation and low temperatures we get

$$\Sigma_{k\downarrow}(\omega) \simeq \frac{(2SI)^2}{N} \sum_{qp} \frac{1}{(\omega_{k,q}^b)^2} \frac{N(\omega_p)(1 + N(\omega_q))}{\omega - (\omega_q - \omega_p) - \varepsilon(k + q - p \downarrow)} . \qquad (145)$$

Using the self-energy $\Sigma_{k\sigma}(\omega)$ it is possible to calculate the energy shift $\Delta_{k\sigma}(\omega) = Re \, \Sigma_{k\sigma}(\omega)$ and damping $\Gamma_{k\sigma}(\omega) = -Im \Sigma_{k\sigma}(\omega)$ of the itinerant carrier in the bound state regime. As it follows from Eq. (145), the damping of the magnetic polaron state arises from the combined processes of absorption and emission of magnons with different energies $(\omega_q - \omega_p)$. Then the real and imaginary part of self-energy give the effective mass, lifetime and mobility of the itinerant charge carriers

$$\frac{m^*}{m} = 1 - \left[Re \frac{\partial \Sigma_{k\sigma}}{\partial \varepsilon(k\sigma)} \right] \Bigg|_{\varepsilon(k\sigma) = \epsilon_F} \qquad (146)$$

$$\varrho = \left(\frac{m}{ne^2} \right) \left(\frac{1}{\tau} \right) ; \quad \frac{1}{\tau} = Im \Sigma_{k\sigma}(\varepsilon(k\sigma))|_{\varepsilon(k\sigma) = \epsilon_F} . \qquad (147)$$

9. Conclusions

In summary, we have presented an analytical approach to treating the charge quasiparticle dynamics of the spin-fermion (s–d) model which provides a basis for description of the physical properties of magnetic and diluted magnetic semiconductors. We have investigated the mutual influence of the s–d and direct exchange effects on interacting systems of itinerant carriers and localized spins. We set out the theory as follows. 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 used. 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. 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 spin-fermion model is important to characterize the true quasiparticle excitations and the role of magnetic correlations. It was shown that the charge and magnetic dynamics of the spin-fermion model can be understood in terms of the 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 generalized mean fields and, second, the explicit self-consistent calculation of the charge and spin-wave quasiparticle spectra and their damping for the two interacting subsystems. This analysis includes the scattering and bound state regimes that determine the essential physics. We demonstrated analytically, by contrasting the scattering and bound state regime that the damping of magnetic polaron is affected by both the *s–d* and direct exchange. Thus, the present consideration is the most complete analysis of the scattering and bound state quasiparticle spectra of the spin-fermion model. 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. Thus, this 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. We have attempted to keep the mathematical complexity within reasonable bounds by restricting the discussion, whenever possible, to the minimal necessary formalization. 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 the bound and scattering quasiparticle states of the correlated lattice fermions and spins. The key to understanding of the formation of magnetic polaron in magnetic semiconductors lies in the right description of the generalized mean fields 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 essential new feature of our treatment is that it takes account the fact that the charge carrier operators $(a^\dagger_{k\sigma}, a_{k\sigma})$ should be treated on the equal footing with the complex

"spin-fermion" operators $(C^{\dagger}_{k\sigma}, C_{k\sigma})$. The solution thus obtained agrees with that obtained in the seminal paper of Shastry and Mattis,[74] where an approach limited to zero temperature was used.

Finally, we wish to emphasize a broader relevance of the results presented here to other complex magnetic materials. The detailed consideration of the state of itinerant charge carriers in DMS along this line will be considered separately.

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