Physica 138B (1986) 129–140
North-Holland, Amsterdam

A SELF-CONSISTENT THEORY OF THE MAGNETIC POLARON

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Received 5 November 1984
Revised manuscript received 10 March 1985

A finite temperature self-consistent theory of the magnetic polaron in the s–f model of ferromagnetic semiconductors is developed. The calculations are based on the novel approach of the thermodynamic two-time Green's function methods. This approach consists of the introduction of the "irreducible" Green's functions (IGF) and derivation of the exact Dyson equation and exact self-energy operator. It is shown that IGF method gives a unified and natural approach for a calculation of the magnetic polaron states by taking explicitly into account the damping effects and finite lifetime.

1. Introduction

In the last decade a great deal of effort has been made to understand the physical properties of magnetic semiconductors. The properties of itinerant electrons and the relationship between the magnetic and electrical properties of these substances are at present of great interest [1, 2]. Discussions of the true spectrum of the magnetic semiconductors have recently been undertaken in connection with the magnetic polaron problem [3–7]. The formation of bound polaron-like states due to the effective attraction of the electron and magnon is a very interesting many-body problem. It is possible for the case of the antiferromagnetic coupling of the electron spin to the lattice (magnetic subsystem). Investigations of the magnetic polarons permit us to clarify the nature of the true carriers at low temperatures of the magnetic semiconductors. Under various regimes the bare carriers can be greatly renormalized and the relevant true carriers must be considered. This has been supported from the experimental point of view [8, 9].

The properties of the magnetic polaron states have been investigated at zero temperature in papers [3–5]. Recently a much more detailed theory of the magnetic polaron at $T = 0$ has been given by Shastry and Mattis [6]. In ref. 6 the Green's function for a single electron has been calculated including both spin-conserving and spin-flip processes. Crucial differences between bound- and scattering state contributions to the electron spectral weight have been highlighted. Unfortunately, the damping effects and finite lifetimes have not been taken into account. The only mechanism for the damping of the polaron bound states which has been considered is the decay of a magnetic polaron into an unbound

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electron with spin-flip and magnon. By energy considerations this becomes possible when the magnetic polaron state merges only with the electron–magnon continuum.

The states of the current carriers in ferromagnetic semiconductors have been investigated for an arbitrary value of s–f exchange parameter I in the spin-wave region by a variational procedure in ref. 7. These authors have criticized the present methods of calculation of the one-electron Green's function for the s–f model and claim that an adequate description requires cumbersome and untransparent decoupling procedures.

The purpose of this paper is to discuss further the magnetic polaron problem and develop an unified and complete self-consistent finite-temperature theory by taking into account the damping effects and finite lifetime. For this aim we use the novel irreducible Green's function (IGF) method developed by Plakida for the self-consistent phonon theory [10] and the Heisenberg ferromagnet [11] and by Kuzemsky for the Hubbard model [12]. The IGF method completely describes the quasiparticle inelastic scattering processes in a many-body system and finds quasiparticle spectra with damping in a very general way. From a technical point of view the IGF method is a special kind of the projection-operator approach in the theory of two-time Green's functions [13]. By introducing "irreducible" parts of the GF (or the "irreducible" parts of the operators, from which the GF is constructed) the equation of motion for the GF can be exactly transformed in a Dyson equation with an exact representation of the self-energy operator which is represented by higher-order Green's functions. To calculate the self-energy operator in a self-consistent way, we have to express it approximately by lower-order Green's functions. The IGF method has recently been applied in a number of solid-state problems [14]. Marvakov et al. [15] have recently generalized this method to the calculation of elementary excitations with damping for the s–f model. In [15] the scattering regime has only been considered. The present paper is devoted to developing this approach further to take into account the polaron-like states.

2. Hamiltonian of the s–f model

The total Hamiltonian of the s–f model is given by the following expression [1, 2]:

$$H = H_e + H_{ee} + H_f + H_{s\text{-}f}\,, \tag{1}$$

where H_e is the operator of kinetic energy of itinerant band electrons

$$H_e = \sum_{ij\sigma} t_{ij} a^{\dagger}_{i\sigma} a_{j\sigma} = \sum_{k} \varepsilon_k a^{\dagger}_{k\sigma} a_{k\sigma}\,. \tag{2}$$

Here $\varepsilon_k = N^{-1} \Sigma_{ij} t_{ij} \exp[-\mathrm{i}\boldsymbol{k}(\boldsymbol{R}_i - \boldsymbol{R}_j)]$ is the band energy. Although the itinerant electrons (2) are predominantly d-electrons, they are usually treated as s-electrons for mathematical simplicity. However, the retaining predominant d-character of the itinerant electrons may be very important for describing the magnetic semiconductors as shown by Allan and Edwards [16]. For tight-binding electrons the band energy is given by

$$\varepsilon_k = \sum_{\alpha} t(\boldsymbol{R}_\alpha) \cos(\boldsymbol{k} \cdot \boldsymbol{R}_\alpha)\,. \tag{3}$$

H_{ee} describes the Coulomb interaction of itinerant d-like electrons

$$H_{ee} = \frac{U}{2N} \sum_{kpq\sigma} a^{\dagger}_{k+q,\sigma} a_{k\sigma} a^{\dagger}_{p-q,-\sigma} a_{p,-\sigma}\,. \tag{4}$$

Here U is the Hubbard–Coulomb correlation integral. In the case of a pure semiconductor at low temperatures the "conduction" electron band is empty, and the Coulomb term (4) therefore is not so important. H_f describes the localized moments which are treated by the Heisenberg model

$$H_f = -\tfrac{1}{2}\sum_{ij} J_{ij}\boldsymbol{S}_i \cdot \boldsymbol{S}_j = -\tfrac{1}{2}\sum_{q} J_q \boldsymbol{S}_q \cdot \boldsymbol{S}_{-q}. \tag{5}$$

The two subsystems (band electrons and localized spins) are coupled by a local spin–spin exchange interaction

$$\begin{aligned} H_{sf} &= -2I\sum_{i\sigma\sigma'} (\boldsymbol{S}_i \cdot \boldsymbol{\sigma})_{\sigma\sigma'} a^{\dagger}_{i\sigma} a_{i\sigma'} \\ &= -\frac{I}{\sqrt{N}}\sum_{kq}\{S^{+}_{-q} a^{\dagger}_{k\downarrow} a_{k+q\uparrow} + S^{-}_{-q} a^{\dagger}_{k\uparrow} a_{k+q\downarrow} + S^{z}_{-q}(a^{\dagger}_{k\uparrow} a_{k+q\uparrow} - a^{\dagger}_{k\downarrow} a_{k+q\downarrow})\}. \end{aligned} \tag{6}$$

This term leads to the formation of the bound polaron-like states due to the effective attraction of the electron and magnon in the case of antiferromagnetic coupling ($I < 0$).

3. Dyson equation for bound state Green's function

For the calculation of the electronic quasiparticle spectrum of the described model (1) one must consider the equation of motion for the one-electron GF

$$G_{k\sigma}(t) = \langle\langle a_{k\sigma}(t) a^{\dagger}_{k\sigma}\rangle\rangle. \tag{7}$$

In ref. 15 a self-consistent calculation of the GF (7) has been performed, where the bound states have not been taken into account. To do this, one needs the full generalized Green's function

$$\hat{G}_{k\sigma} = \begin{Vmatrix} \langle\langle a_{k\sigma} \mid a^{\dagger}_{k\sigma}\rangle\rangle & \langle\langle a_{k\sigma} \mid C^{\dagger}_{k\sigma}\rangle\rangle \\ \langle\langle C_{k\sigma} \mid a^{\dagger}_{k\sigma}\rangle\rangle & \langle\langle C_{k\sigma} \mid C^{\dagger}_{k\sigma}\rangle\rangle \end{Vmatrix}. \tag{8}$$

To explain the structure of this GF, let us consider first the equation of motion for the Fourier transform of the GF (7)

$$\omega G_{k\sigma}(\omega) = 1 + \varepsilon_k G_{k\sigma}(\omega) - \frac{I}{\sqrt{N}}\sum_{q}\{\langle\langle S^{-\sigma}_{-q} a_{k+q,-\sigma} \mid a^{\dagger}_{k\sigma}\rangle\rangle + z_{\sigma}\langle\langle S^{z}_{-q} a_{k+q,\sigma} \mid a^{\dagger}_{k\sigma}\rangle\rangle\}, \tag{9}$$

where $z_{\sigma} = 1(-1)$ if $\sigma = \uparrow(\downarrow)$ or $+(-)$. Following [10–15] we introduce by definition the irreducible operator in the right-hand side of eq. (7)

$$(S^{z}_{-q})^{ir} = S^{z}_{-q} - \langle S^{z}_{0}\rangle \delta_{q,0} \tag{10}$$

in which the mean-field contribution is removed. Then the equation of motion (7) can be exactly transformed to the following form:

$$(\omega - \varepsilon^{0}_{k\sigma})\langle\langle a_{k\sigma} \mid a^{\dagger}_{k\sigma}\rangle\rangle + \frac{I}{\sqrt{N}}\langle\langle C_{k\sigma} \mid a^{\dagger}_{k\sigma}\rangle\rangle = 1. \tag{11}$$

Here

$$\varepsilon^0_{k\sigma} = \varepsilon_k - z_\sigma \frac{I\langle S^z_0\rangle}{\sqrt{N}}, \tag{12}$$

$$C_{k\sigma} = \sum_q \{S^{-\sigma}_{-q} a_{k+q,-\sigma} + z_\sigma (S^z_{-q})^{\mathrm{ir}} a_{k+q,\sigma}\} = \alpha_{k\sigma} + \beta_{k\sigma}. \tag{13}$$

In the lattice representation the operator $C_{k\sigma}$ reads

$$C_{i\sigma} = S^{-\sigma}_i a_{i,-\sigma} + z_\sigma (S^z_i)^{\mathrm{ir}} a_{i\sigma}. \tag{14}$$

To study magnetic polaron problem, both the Green's function $\langle\langle a_{k\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle$ and $\langle\langle C_{k\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle$ entered into eq. (8) have to be evaluated in the same way. This is the crucial point of the whole problem. In terms of the variational procedure this means the proper choice of the relevant set of wave functions (cf. [7]).

To calculate $\langle\langle C_{k\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle$ and $\langle\langle C_{k\sigma} \mid C^\dagger_{k\sigma}\rangle\rangle$, let us consider the equation of motion (due to the first-time differentiation) for $\langle\langle S^{-\sigma}_{-q} a_{k+q,-\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle$. In this paper, for the sake of simplicity, we consider only a low electron concentration limit and neglect the U term. A generalization to the finite electron concentration case can be done directly. Thus, we obtain

$$(\omega - \varepsilon^0_{k+q,-\sigma})\langle\langle S^{-\sigma}_{-q} a_{k+q,-\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle = -\frac{I}{\sqrt{N}}\langle\langle S^{-\sigma}_{-q} C_{k+q,-\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle$$

$$- z_\sigma \frac{1}{\sqrt{N}} \sum_p J_p \langle\langle (S^{-\sigma}_{-(p+q)} S^z_p - S^{-\sigma}_p S^z_{-(p+q)}) a_{k+q,-\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle. \tag{15}$$

Then it is convenient to define the following set of the irreducible operators:

$$(S^\sigma_{-p} S^{-\sigma}_{-q})^{\mathrm{ir}} = S^\sigma_{-p} S^{-\sigma}_{-q} - \langle S^\sigma_q S^{-\sigma}_{-q}\rangle \delta_{p,-q}, \tag{16a}$$

$$(S^{-\sigma}_{-(p+q)} S^z_p - S^{-\sigma}_p S^z_{-(p+q)})^{\mathrm{ir}} = S^{-\sigma}_{-(p+q)} S^z_p - S^{-\sigma}_p S^z_{-(p+q)} - \{\langle S^z_0\rangle(\delta_{p,0} - \delta_{p,-q}) + (A_{-p} - A_{-(p+q)})\} S^{-\sigma}_{-q}, \tag{16b}$$

where

$$A_q = \frac{2K^{zz}_q + K^{-+}_q}{2\langle S^z_0\rangle} = \frac{2\langle (S^z_{-q})^{\mathrm{ir}} (S^z_q)^{\mathrm{ir}}\rangle + \langle S^-_{-q} S^+_q\rangle}{2\langle S^z_c\rangle}. \tag{16c}$$

Note that before introducing the irreducible operators (16) one has to extract from $\langle\langle S^{-\sigma}_{-q} C_{k+q,-\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle$ the terms proportional to the initial Green's function $\langle\langle S^{-\sigma}_{-q} a_{k+q,-\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle$ using the spin commutation relation. It must be represented by introducing the spin-operators ordering rule in the calculations.

After a simple algebra eq. (15) can be written in the following form:

$$(1 - I\Lambda_{k\sigma}(\omega))\langle\langle \alpha_{k\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle + \frac{I}{\sqrt{N}} \phi(k) \langle\langle a_{k\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle$$

$$= \sum_q \left\{ \frac{\langle\langle A_{k,q} \mid a^\dagger_{k\sigma}\rangle\rangle}{\omega + z_\sigma \omega_q - \varepsilon^0_{k+q,-\sigma}} + \frac{2I\Lambda_{k\sigma}(\omega)\langle\langle B_{k,q} \mid a^\dagger_{k\sigma}\rangle\rangle}{\omega - \varepsilon^0_{k+q,\sigma}} \right\}, \tag{17}$$

where

$$\phi(k)=\sum_q\left\{\frac{\langle S^{-\sigma}_{-q}S^{\sigma}_{q}\rangle}{\omega+z_\sigma\omega_q-\varepsilon^0_{k+q,-\sigma}}+\frac{2I\Lambda_{k\sigma}(\omega)\langle(S^z_{-q})^{\mathrm{ir}}(S^z_q)^{\mathrm{ir}}\rangle}{\omega-\varepsilon^0_{k+q,\sigma}}\right\}, \tag{17a}$$

$$\Lambda_{k\sigma}(\omega)=\frac{1}{N}\sum_q(\omega+z_\sigma\omega_q-\varepsilon^0_{k+q,-\sigma})^{-1}, \tag{17b}$$

$$\omega_q=\frac{1}{\sqrt{N}}\langle S^z_0\rangle(J_0-J_q)+\frac{1}{\sqrt{N}}\sum_p(J_p-J_{p-q})\frac{2K^{zz}_p+K^{-+}_p}{2\langle S^z_0\rangle}. \tag{17c}$$

Here ω_q denotes the magnon energy in the generalized mean-field approximation [11]. The higher-order operators $A_{k,q}$ and $B_{k,q}$ have the form (cf. [15])

$$A_{k,q}=-\frac{I}{\sqrt{N}}C_{k+q,-\sigma}S^{-\sigma}_{-q}-z_\sigma\frac{1}{\sqrt{N}}\sum_p J_p(S^{-\sigma}_{-(q+p)}S^z_p-S^{-\sigma}_pS^z_{-(q+p)})^{\mathrm{ir}}a_{k+q,-\sigma}, \tag{18a}$$

$$B_{k,q}=-z_\sigma\frac{I}{\sqrt{N}}(S^z_{-q})^{\mathrm{ir}}C_{k+q,\sigma}. \tag{18b}$$

The irreducible operators (10), (16a) and (16b) have been introduced so that the operators $A_{k,q}$ and $B_{k,q}$ satisfy the conditions

$$\langle[A_{k,q},a^\dagger_{k\sigma}]_+\rangle=\langle[A_{k,q},C^\dagger_{k\sigma}]_+\rangle\equiv 0, \tag{19}$$
$$\langle[B_{k,q},a^\dagger_{k\sigma}]_+\rangle=\langle[B_{k,q},C^\dagger_{k\sigma}]_+\rangle\equiv 0.$$

We now consider the GF $\langle\langle(S^z_{-q})^{\mathrm{ir}}a_{k+q,\sigma}\mid a^\dagger_{k\sigma}\rangle\rangle$. Similarly to eq. (17) we have

$$\langle\langle\beta_{k\sigma}\mid a^+_{k\alpha}\rangle\rangle+\frac{I}{\sqrt{N}}\sum_q\frac{\langle(S^z_{-q})^{\mathrm{ir}}(S^z_q)^{\mathrm{ir}}\rangle}{\omega-\varepsilon^0_{k+q,\sigma}}\langle\langle a_{k\sigma}\mid a^+_{k\sigma}\rangle\rangle=\sum_q\frac{\langle\langle B_{k,q}\mid a^+_{k\sigma}\rangle\rangle}{\omega-\varepsilon^0_{k+q,\sigma}}. \tag{20}$$

Then from eqs. (17) and (20) we obtain

$$\frac{I}{\sqrt{N}}\psi_{k\sigma}(\omega)\langle\langle a_{k\sigma}\mid a^\dagger_{k\sigma}\rangle\rangle+\langle\langle C_{k\sigma}\mid a^\dagger_{k\sigma}\rangle\rangle$$
$$=\sum_q\left\{\frac{\langle\langle A_{k,q}\mid a^\dagger_{k\sigma}\rangle\rangle}{[1-I\Lambda_{k\sigma}(\omega)](\omega+z_\sigma\omega_q-\varepsilon^0_{k+q,-\sigma})}+\frac{[1+I\Lambda_{k\sigma}(\omega)]\langle\langle B_{k,q}\mid a^\dagger_{k\sigma}\rangle\rangle}{[1-I\Lambda_{k\sigma}(\omega)](\omega-\varepsilon^0_{k+q,\sigma})}\right\}, \tag{21}$$

where

$$\psi_{k\sigma}(\omega)=\sum_q\left\{\frac{\langle S^{-\sigma}_{-q}S^{\sigma}_{q}\rangle}{[1-I\Lambda_{k\sigma}(\omega)](\omega+z_\sigma\omega_q-\varepsilon^0_{k+q,-\sigma})}+\frac{[I+I\Lambda_{k\sigma}(\omega)]\langle(S^z_{-q})^{\mathrm{ir}}(S^z_q)^{\mathrm{ir}}\rangle}{[1-I\Lambda_{k\sigma}(\omega)](\omega-\varepsilon^0_{k+q,\sigma})}\right\}. \tag{22}$$

Analogously one can write the equation for GF $\langle\langle C_{k\sigma}\mid C^\dagger_{k\sigma}\rangle\rangle$. So, the equations of motion (9), (17), (19), (21) can be summarized in the matrix form (cf. [15])

$$\hat{\Omega}\hat{G}_{k\sigma} = \hat{I} + \sum_{p} \hat{\phi}_p \hat{G}_1 . \tag{23}$$

Here

$$\hat{\Omega} = \begin{Vmatrix} \omega - \varepsilon^0_{k\sigma} & I/\sqrt{N} \\ (I/\sqrt{N})\psi_{k\sigma}(\omega) & 1 \end{Vmatrix}, \qquad \hat{I} = \begin{Vmatrix} 1 & 0 \\ 0 & \psi_{k\sigma}(\omega) \end{Vmatrix}, \tag{24}$$

$$\hat{\phi}_p = \begin{Vmatrix} 0 & 0 \\ 1/\omega_{k,p} & 1/\Omega_{k,p} \end{Vmatrix}, \qquad \hat{G}_1 = \begin{Vmatrix} \langle\langle A_{k,p} \mid a^\dagger_{k\sigma}\rangle\rangle & \langle\langle A_{k,p} \mid C^\dagger_{k\sigma}\rangle\rangle \\ \langle\langle B_{k,p} \mid a^\dagger_{k\sigma}\rangle\rangle & \langle\langle B_{k,p} \mid C^\dagger_{k\sigma}\rangle\rangle \end{Vmatrix} \tag{25}$$

with the notation

$$\omega_{k,q} = [1 - I\Lambda_{k\sigma}(\omega)](\omega + z_o\omega_q - \varepsilon^0_{k+q,-\sigma}), \tag{26a}$$

$$\Omega_{k,q} = [1 - I\Lambda_{k\sigma}(\omega)](\omega - \varepsilon^0_{k+q,\sigma})/[1 + I\Lambda_{k\sigma}(\omega)] . \tag{26b}$$

Comparing eq. (24) with the results of paper [15] one can see that $\psi_{k\sigma}(\omega)$ play the role of the generalized "susceptibility" of the spin–electron bound states instead of a simple electron susceptibility $\chi_0(k, \omega)$ in the scattering-state regime

$$\chi_0(k, \omega) = \frac{1}{N}\sum_{q} \frac{n_{k+q\downarrow} - n_{q\uparrow}}{\omega + \varepsilon_q - \varepsilon_{k+q} - \Delta} . \tag{27}$$

To obtain a Dyson equation, we have to use the second-time t' differentiation for the matrix GF $\hat{G}_1$ and then to introduce the "right" irreducible parts as discussed above for "left" operators. Thus, we obtain the exact equation

$$\hat{G}_{k\sigma} = \hat{G}^0_{k\sigma} + \hat{G}^0_{k\sigma}\hat{P}_{k\sigma}\hat{G}^0_{k\sigma} , \tag{28}$$

where the generalized mean-field Green's function $\hat{G}^0_{k\sigma}(\omega)$ reads

$$\hat{G}^0_{k\sigma}(\omega) = \hat{\Omega}^{-1}\hat{I} . \tag{29}$$

The scattering operator $\hat{P}_{k\sigma}(\omega)$ is given by the expression

$$\hat{P}_{k\sigma}(\omega) = \hat{I}^{-1}\Big\{\sum_{pq} \hat{\phi}_p \hat{P}(p, q)\hat{\phi}^\dagger_q\Big\}\hat{I}^{-1} , \tag{30}$$

where

$$\hat{P}(p, q) = \begin{Vmatrix} \langle\langle A_{k,p} \mid A^\dagger_{k,q}\rangle\rangle & \langle\langle A_{k,p} \mid B^\dagger_{k,q}\rangle\rangle \\ \langle\langle B_{k,p} \mid A^\dagger_{k,q}\rangle\rangle & \langle\langle B_{k,p} \mid B^\dagger_{k,q}\rangle\rangle \end{Vmatrix} . \tag{31}$$

From the Dyson equation

$$\hat{G}_{k\sigma}(\omega) = \hat{G}^0_{k\sigma}(\omega) + \hat{G}^0_{k\sigma}(\omega)\hat{M}_{k\sigma}(\omega)\hat{G}_{k\sigma}(\omega) , \tag{32}$$

we get the following equation for the self-energy operator $\hat{M}_{k\sigma}(\omega)$:

$$\hat{P}_{k\sigma}(\omega) = \hat{M}_{k\sigma}(\omega) + \hat{M}_{k\sigma}(\omega)\hat{G}^0_{k\sigma}(\omega)\hat{P}_{k\sigma}(\omega), \tag{33}$$

from which it follows that we can speak in a complete analogy to the diagramatic technique that the $\hat{M}_{k\sigma}$ is defined as a proper (connected) part of the scattering operator $\hat{P}_{k\sigma}$:

$$\hat{M}_{k\sigma}(\omega) = \{\hat{P}_{k\sigma}(\omega)\}^c. \tag{34}$$

It should be emphasized that for the retarded (and advanced) GF's the proper part has only a symbolic character. But one can use the causal instead of retarded GF at any step of calculations due to the same form of the equation of motion for all three (retarded, advanced, and causal) GF's. In some sense there is such a possibility to control, in the diagramatic language, the relevant decoupling procedure in further approximative self-energy calculations. $\hat{M}_{k\sigma}(\omega)$ has the following exact representation

$$\hat{M}_{k\sigma}(\omega) = \begin{Vmatrix} 0 & 0 \\ 0 & \Pi_{k\sigma}(\omega)/\psi_{k\sigma}(\omega) \end{Vmatrix}, \tag{35}$$

where $\Pi_{k\sigma}(\omega)$ denotes

$$\Pi_{k\sigma}(\omega) = \sum_{pq} \left\{ \frac{\langle\langle A_{k,p} \mid A^\dagger_{k,q}\rangle\rangle^c}{\omega_{k,p}\omega_{k,q}} + \frac{\langle\langle A_{k,p} \mid B^\dagger_{k,q}\rangle\rangle^c}{\omega_{k,p}\Omega_{k,q}} + \frac{\langle\langle B_{k,p} \mid A^\dagger_{k,q}\rangle\rangle^c}{\Omega_{k,p}\omega_{k,q}} + \frac{\langle\langle B_{k,p} \mid B^\dagger_{k,q}\rangle\rangle^c}{\Omega_{k,p}\Omega_{k,q}} \right\}. \tag{36}$$

Hence, the determination of the full GF $\hat{G}_{k\sigma}$ has been reduced to the determination of the mean-field GF $\hat{G}^0_{k\sigma}$ and the self-energy operator $\hat{M}_{k\sigma}$.

4. Excitation spectrum of the magnetic polaron

The mean-field matrix GF $\hat{G}^0_{k\sigma}(\omega)$ has the explicit form

$$\hat{G}^0_{k\sigma}(\omega) = \frac{1}{\det\hat{\Omega}} \begin{Vmatrix} 1 & -\dfrac{I}{\sqrt{N}}\psi_{k\sigma}(\omega) \\ -\dfrac{I}{\sqrt{N}}\psi_{k\sigma}(\omega) & (\omega - \varepsilon^0_{k\sigma})\psi_{k\sigma}(\omega) \end{Vmatrix}. \tag{37}$$

Here $\det\hat{\Omega}$ reads

$$\det\hat{\Omega} = \omega - \varepsilon^0_{k\sigma} - (I^2/N)\psi_{k\sigma}(\omega). \tag{38}$$

Let us consider only GF$\langle\langle a_{k\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle$. It can be rewritten in the following form:

$$\langle\langle a_{k\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle = \{[\langle\langle a_{k\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle^0]^{-1} - \Sigma_\sigma(\boldsymbol{k}, \omega)\}^{-1}, \tag{39}$$

where $(\langle\langle a_{k\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle^0)^{-1} = \det\hat{\Omega}$ and the self-energy corrections are given by

$$\Sigma_\sigma(k,\omega)=\frac{I^2}{N}\frac{\Pi_{k\sigma}(\omega)}{1-\psi^{-1}_{k\sigma}(\omega)\Pi_{k\sigma}(\omega)}. \tag{40}$$

As it follows from eq. (38), the generalized mean-field GF $\langle\langle a_{k\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle^0$ has a very nontrivial structure which is quite different from the standard scattering-state regime form:

$$\langle\langle a_{k\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle = \{(\langle\langle a_{k\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle^0)^{-1} - M^{\rm em}_{k\sigma}\}^{-1}, \tag{41}$$

where

$$\langle\langle a_{k\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle^0 = (\omega-\varepsilon^0_{k\sigma})^{-1},$$

$$M^{\rm em}_{k\sigma}(\omega)=\frac{I^2}{N}\sum_{qq'}\{\langle\langle S^{-\sigma}_{-q}a_{k+q,-\sigma} \mid S^\sigma_{q'}a^\dagger_{k+q',-\sigma}\rangle\rangle^{\rm c} + \langle\langle (S^z_{-q}a_{k+q,\sigma})^{\rm ir} \mid (S^z_{q'}a^\dagger_{k+q',\sigma})^{\rm ir}\rangle\rangle^{\rm c}\}. \tag{42}$$

For the bound polaron-like electron–magnon states the mean-field renormalizations are quite different from the Hartree–Fock renormalizations. In general, the quasiparticle energies are determined by the equation

$$E_{k\sigma}=\varepsilon^0_{k\sigma}+(I^2/N)\psi_{k\sigma}(E_{k\sigma}) \tag{43}$$

and the energy spectrum $E_{k\sigma}$ consists of two bands for any electron spin projection. At the atomic limit ($\varepsilon_k=0$) and $\omega_q\to 0$ we obtain the exact analytical representation given in paper [7]

$$\langle\langle a_{k\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle^0|_{\rm at}=\frac{S+z_\sigma S_z+1}{2S+1}(\omega+IS)^{-1}+\frac{S-z_\sigma S_z}{2S+1}(\omega-I(S+1))^{-1}, \tag{44}$$

where S and $S_z=\langle S^z_0\rangle/\sqrt{N}$ are the spin-value and magnetization, respectively. Moreover, our generalized mean-field solution is exactly reduced to the Shastry–Mattis [6] result for $T=0$,

$$\langle\langle a_{k\sigma} \mid a^\dagger_{k\sigma}\rangle\rangle^0|_{\rm SM}=\left\{\omega-\varepsilon^0_{k\sigma}-\delta_{\sigma\downarrow}2I^2S\frac{\Lambda_{k\sigma}(\omega)}{[1-\Lambda_{k\sigma}(\omega)]}\right\}^{-1}. \tag{45}$$

The magnetic polaron states are formed only for antiferromagnetic s–f coupling ($I<0$) when there is a lowering of the band electron energy due to the effective attraction of the electron and magnon. At $T=0$ the excitation spectrum of the magnetic polaron problem has been investigated in a great detail [3–6]. In general, one needs numerical calculations of the excitation spectrum (43). For this aim the explicit form of the correlations functions $\langle S^{-\sigma}_{-q}S^\sigma_q\rangle$ and $\langle (S^z_{-q})^{\rm ir}(S^z_q)^{\rm ir}\rangle$ must be taken into account [17, 18].

Let us consider two limiting cases where analytical calculations are possible:

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

$$E_{k\downarrow}\simeq\varepsilon_k+I\frac{S(S+S_z+1)+S_z(S-S_z+1)}{2S}+\frac{1}{N}\sum_q\left\{-I\frac{\varepsilon_{k-q}-\varepsilon_k+2I(S-S_z)}{\varepsilon_{k-q}-\varepsilon_k-2IS_z}\right\}\frac{\langle S^+_qS^-_{-q}\rangle}{2S}, \tag{46a}$$

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

$$E_{k\downarrow}\simeq I(S+1)+\frac{2(S+1)(S+S_z)}{(2S+1)(S+S_z+1)}\varepsilon_k+\frac{1}{N}\sum_q\frac{\varepsilon_{k-q}-\varepsilon_k}{2S+1}\frac{\langle S^+_qS^-_{-q}\rangle}{S+S_z+1}, \tag{46b}$$

where we removed the longitudinal spin correlations for the sake of simplicity. Here W is the bandwidth in the limit $I = 0$. Now we consider the low-temperature (spin-wave) limit in eqs. (46) in which it may be reasonable to assume that $S_z \approx S$ and $\langle S_q^+ S_{-q}^- \rangle \approx 2S(1 + \nu_q)$. Here $\nu_q = [\exp(\beta\omega_q) - 1]^{-1}$. Thus, we obtain (cf. [7, 19])

$$E_{k\downarrow} = \varepsilon_k + IS + \frac{2I^2S}{N}\sum_q \frac{1}{\varepsilon_k - \varepsilon_{k-q} + 2IS} + \frac{1}{N}\sum_q \left\{ -I\frac{\varepsilon_{k-q} - \varepsilon_k}{\varepsilon_{k-q} - \varepsilon_k - 2IS}\right\}\nu_q, \qquad \text{for } |I|S \ll W, \tag{47a}$$

$$E_{k\downarrow} = I(S+1) + \frac{2S}{2S+1}\varepsilon_k + \frac{1}{N}\sum_q \frac{2S}{2S+1}\left(\frac{\varepsilon_{k-q} - \varepsilon_k}{2S+1}\right)\nu_q, \qquad \text{for } |I| \gg W. \tag{47b}$$

Using expressions (47) one can estimate the binding energy of the polaron-like state which can be defined as

$$\varepsilon_B = \varepsilon^0_{k\downarrow} - E_{k\downarrow} \tag{48a}$$

because in the H–F approximation the spin-down band is given by the expression $\varepsilon^0_{k\downarrow} = \varepsilon_k + IS$. We obtain

$$\varepsilon_B = \varepsilon^0_{B1} - \frac{1}{N}\sum_q \left\{ -I\frac{\varepsilon_{k-q} - \varepsilon_k}{\varepsilon_{k-q} - \varepsilon_k - 2IS}\right\}\nu_q, \qquad \text{for } |I|S \ll W \tag{49a}$$

and

$$\varepsilon_B = \varepsilon^0_{B2} - \frac{1}{N}\sum_q \frac{2S}{2S+1}\left(\frac{\varepsilon_{k-q} - \varepsilon_k}{2S+1}\right)\nu_q, \qquad \text{for } |I|S \gg W, \tag{49b}$$

where

$$\varepsilon^0_{B1} = \frac{2I^2S}{N}\sum_q \frac{1}{\varepsilon_{k-q} - \varepsilon_k - 2IS} \simeq \frac{|I|S}{W}|I|,$$
$$\varepsilon^0_{B2} = -I + \frac{\varepsilon_k}{2S+1} \simeq |I|. \tag{50}$$

The temperature dependence of the energy spectrum in the spin-wave region is given by the usual $T^{5/2}$ behaviour. In a general case one takes into account a more exact form of the correlation function $\langle S_q^+ S_{-q}^- \rangle$, for example, the famous VLP result [17].

5. Damping of polaron states

To find explicit useful expressions for the self-energy operator $\Sigma_\sigma(k, \omega)$ (40), suitable approximations to evaluate the higher-order GF's in (36) should be used. To calculate the self-energy in a self-consistent way, we have to approximate it by the lower-order GF's. Let us consider GF's appearing in (36). It is convenient to write down $\langle\langle A_{k,p} \mid A^\dagger_{k,q}\rangle\rangle^c$ in the form

$$\langle\langle A_{k,p} \mid A^{\dagger}_{k,q}\rangle\rangle^{c} = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{d\omega'}{\omega-\omega'}(e^{\beta\omega'}+1)\int dt\, e^{i\omega' t}\langle A^{\dagger}_{k,q}A_{k,p}(t)\rangle^{c}. \tag{51}$$

Then we obtain

$$\langle A^{\dagger}_{k,q}A_{k,p}(t)\rangle^{c} = \frac{I^2}{N}\langle S^{\sigma}_{q}C^{\dagger}_{k+q,-\sigma}C_{k+p,-\sigma}(t)S^{-\sigma}_{-p}(t)\rangle + \langle a^{\dagger}_{k+q,-\sigma}F^{\dagger}_{-q,-\sigma}F_{-p,-\sigma}(t)a_{k+p,-\sigma}(t)\rangle. \tag{52}$$

We use the following decoupling procedure:

$$\begin{aligned}
&\langle S^{\sigma}_{q}C^{\dagger}_{k+q,-\sigma}C_{k+p,-\sigma}(t)S^{-\sigma}_{-p}(t)\rangle \approx \delta_{q,p}\langle S^{\sigma}_{q}S^{-\sigma}_{-q}(t)\rangle\langle C^{\dagger}_{k+q,-\sigma}C_{k+q,-\sigma}(t)\rangle,\\
&\langle a^{\dagger}_{k+q,-\sigma}F^{\dagger}_{-q,-\sigma}F_{-p,-\sigma}(t)a_{k+p,-\sigma}(t)\rangle \approx \delta_{q,p}\langle F^{\dagger}_{-q,-\sigma}F_{-q,-\sigma}(t)\rangle\langle a^{\dagger}_{k+q,-\sigma}a_{k+q,-\sigma}(t)\rangle.
\end{aligned} \tag{53}$$

Here

$$\langle F^{\dagger}_{-q,-\sigma}F_{-q,-\sigma}(t)\rangle = \frac{1}{N}\sum_{pp'}J_pJ_{p'}\langle[(S^{z}_{-p})^{ir}S^{\sigma}_{q+p} - (S^{z}_{-(q+p)})^{ir}S^{\sigma}_{-p}]^{ir}[S^{-\sigma}_{-(q+p')}(t)(S^{z}_{p'}(t))^{ir} - S^{-\sigma}_{p'}(t)(S^{z}_{-(q+p')}(t))^{ir}]^{ir}\rangle. \tag{54}$$

The approximation (53) results from the neglect of the vertex corrections, i.e., the correlation between propagation of the polarons and the magnetic excitations and the electrons and the magnons, respectively. Taking into account the spectral theorem we obtain from (51)–(53)

$$\begin{aligned}
\langle\langle A_{k,p} \mid A^{\dagger}_{k,q}\rangle\rangle^{c} = {}& \frac{I^2}{N}\delta_{q,p}\int\int\frac{d\omega_1\, d\omega_2(1+\nu(\omega_1))}{\omega-\omega_1-\omega_2}\left\{-\frac{1}{\pi}\mathrm{Im}\langle\langle S^{-\sigma}_{-q} \mid S^{\sigma}_{q}\rangle\rangle_{\omega_1}\right\}\\
&\times\left\{-\frac{1}{\pi}\mathrm{Im}\langle\langle C_{k+q,-\sigma} \mid C^{\dagger}_{k+q,-\sigma}\rangle\rangle_{\omega_1}\right\} + \delta_{p,q}\sum_{q'}(J_{q'}-J_{q-q'})^2\\
&\times\int\int\int\frac{d\omega_1\, d\omega_2\, d\omega_3[1+\nu(\omega_1)][1+\nu(\omega_2)]}{\omega-\omega_1-\omega_2-\omega_3}\left\{-\frac{1}{\pi}\mathrm{Im}\langle\langle(S^{z}_{-q})^{ir}(S^{z}_{q})^{ir}\rangle\rangle_{\omega_1}\right\}\\
&\times\left\{-\frac{1}{\pi}\mathrm{Im}\langle\langle S^{-\sigma}_{-(q-q')} \mid S^{\sigma}_{q-q'}\rangle\rangle_{\omega_2}\right\}\left\{-\frac{1}{\pi}\mathrm{Im}\langle\langle a_{k+q,-\sigma} \mid a^{\dagger}_{k+q,-\sigma}\rangle\rangle_{\omega_3}\right\},
\end{aligned} \tag{55}$$

$$\begin{aligned}
\langle\langle B_{x,p} \mid B^{\dagger}_{k,q}\rangle\rangle^{c} = {}& \delta_{p,q}\frac{I^2}{N}\int\frac{d\omega_1\, d\omega_2[1+\nu(\omega_1)]}{\omega-\omega_1-\omega_2}\left\{-\frac{1}{\pi}\mathrm{Im}\langle\langle(S^{z}_{-q})^{ir}(S^{z}_{q})^{ir}\rangle\rangle_{\omega_1}\right\}\\
&\times\left\{-\frac{1}{\pi}\mathrm{Im}\langle\langle C_{k+q,\sigma} \mid C^{\dagger}_{k+q,\sigma}\rangle\rangle_{\omega_2}\right\}
\end{aligned} \tag{56}$$

and $\langle\langle A_{k,p} \mid B^{\dagger}_{k,q}\rangle\rangle$, $\langle\langle B_{k,p} \mid A^{\dagger}_{k,q}\rangle\rangle$ contributions are removed. In eqs. (55) and (56) we drop the Fermi distribution function due to the low electron concentration approximation. Eqs. (32), (55) and (56) form a closed self-consistent system of equations. In principle, we may substitute into the right-hand side of (55) and (56) any relevant initial Green's functions and solve it by iterations. We choose for the first iteration step the following simple one-pole expressions:

$$
\begin{aligned}
&-\frac{1}{\pi}\operatorname{Im}\langle\langle S^{-\sigma}_{-p}a_{k+q+p,-\sigma} \mid S^{\sigma}_{p}a^{\dagger}_{k+q+p,-\sigma}\rangle\rangle_{\omega} = \langle S^{-\sigma}_{-p}S^{\sigma}_{p}\rangle\delta(\omega + z_{\sigma}\omega_{p} - \varepsilon_{k+q+p,-\sigma}),\\
&-\frac{1}{\pi}\operatorname{Im}\langle\langle (S^{z}_{-p})^{\mathrm{ir}}a_{k+q+p,\sigma} \mid (S^{z}_{p})^{\mathrm{ir}}a^{\dagger}_{k+q+p,\sigma}\rangle\rangle_{\omega} = \langle (S^{z}_{-p})^{\mathrm{ir}}(S^{z}_{p})^{\mathrm{ir}}\rangle\delta(\omega - \varepsilon_{k+q+p,\sigma}),\\
&-\frac{1}{\pi}\operatorname{Im}\langle\langle S^{-\sigma}_{-q} \mid S^{\sigma}_{q}\rangle\rangle_{\omega} = -z_{\sigma}\frac{2\langle S^{z}_{0}\rangle}{\sqrt{N}}\delta(\omega + z_{\sigma}\omega_{q}),\\
&-\frac{1}{\pi}\operatorname{Im}\langle\langle a_{k+q,-\sigma} \mid a^{\dagger}_{k+q,-\sigma}\rangle\rangle = \delta(\omega - \varepsilon_{k+q,-\sigma}).
\end{aligned}
\tag{57}
$$

Then we obtain from (36), (55)–(57)

$$
\begin{aligned}
\Pi_{k\sigma}(\omega) \approx{}& \frac{2\langle S^{z}_{0}\rangle I^{2}}{N^{3/2}}\sum_{q,p}\frac{\delta_{\sigma\downarrow} + \nu(\omega_{q})}{\omega^{2}_{k,q}}\left\{\frac{\langle S^{\sigma}_{p}S^{-\sigma}_{-p}\rangle}{\omega + z_{\sigma}(\omega_{q} - \omega_{p}) - \varepsilon_{k+q-p,\sigma}} + \frac{\langle (S^{z}_{-p})^{\mathrm{ir}}(S^{z}_{p})^{\mathrm{ir}}\rangle}{\omega + z_{\sigma}\omega_{q} - \varepsilon_{k+q-p,-\sigma}}\right\}\\
&+\frac{I^{2}}{N}\sum_{q,p}\int \mathrm{d}\omega'\frac{1 + \nu(\omega')}{\Omega^{2}_{k,q}}\left\{-\frac{1}{\pi}\operatorname{Im}\langle\langle (S^{z}_{-q})^{\mathrm{ir}} \mid (S^{z}_{q})^{\mathrm{ir}}\rangle\rangle_{\omega'}\right\}\\
&\times\left\{\frac{\langle S^{-\sigma}_{-p}S^{\sigma}_{p}\rangle}{\omega - \omega_{1} + z_{\sigma}\omega_{q} - \varepsilon_{k+q+p,-\sigma}} + \frac{\langle (S^{z}_{-p})^{\mathrm{ir}}(S^{z}_{p})^{\mathrm{ir}}\rangle}{\omega - \omega_{1} - \varepsilon_{k+q+p,\sigma}}\right\},
\end{aligned}
\tag{58}
$$

where we write down only the s–f exchange inelastic scattering contributions for brevity. For a concrete calculation in a wide region of temperature we need a suitable approximation for the longitudinal spin susceptibility. For this aim one may use the results of paper [18]. Using the self-energy $\Sigma_{\sigma}(k, \omega)$ we obtain the shift $\Delta_{\sigma}(k, \omega)$ and damping $\Gamma_{\sigma}(k, \omega)$ of the electronic states taking into account magnetic polaron states

$$
\Delta_{\sigma}(k, \omega) = \operatorname{Re}\Sigma_{\sigma}(k, \omega); \qquad \Gamma_{\sigma}(k, \omega) = -\operatorname{Im}\Sigma_{\sigma}(k, \omega). \tag{59}
$$

For example, the s–f exchange inelastic scattering contribution to the damping for the spin-wave region reads

$$
\Pi_{k\downarrow}(\omega) = (2SI)^{2}\frac{1}{N}\sum_{pq}\frac{1}{\omega^{2}_{k,q}}\frac{\nu(\omega_{p})[1 + \nu(\omega_{q})]}{\omega - (\omega_{q} - \omega_{p}) - \varepsilon_{k+q+p\downarrow}}. \tag{60}
$$

As it follows from (60), the damping of magnetic polaron arises from combined processes of absorption and emission of magnons with different energy $(\omega_{q} - \omega_{p})$.

7. Conclusions

In this paper we have shown that the IGF method gives a unified and self-consistent formalism for a complete description of the electronic spectrum including bound polaron-like states and inelastic scattering processes for magnetic semiconductors within the s–f model Hamiltonian. Contrary to the claim made in ref. 7 our one-electron Green's function correctly reproduces the true spectrum of the current carriers in a very natural way because the IGF method permits us to extract all relevant (for the

problem under consideration) mean-field renormalizations and put them into the "zero-order" (generalized mean-field) GF. In a general case the mean-field renormalizations can have a very nontrivial structure as in cases of the Hubbard model in the strong correlation limit [12] and the magnetic polaron problem at finite temperatures and an arbitrary value of s–f exchange. To obtain this nontrivial structure of the mean-field renormalizations correctly, one must construct the full matrix GF built on the complete algebra of relevant operators and develop a special projection procedure for higher-order GF's in accordance with the finding algebra. Moreover, for the first time in our theory we are able to calculate explicitly the full self-energy operator $\Sigma(k, \omega)$ for magnetic polaron problem.

Note that a similar but distinct task is the problem of the bound magnetic polaron in semiconductor [20, 21]. The BMP consists of an impurity electron localized in a shallow donor state accompanied by an inhomogenous local magnetization and it can also be considered by the present method, but it is the object of a subsequent paper.

Acknowledgments

One of the authors (D.I.M.) would like to thank Professor Abdus Salam, International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste.

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