The self-consistent theory of elementary excitations in systems with many-branch quasiparticle spectra (ferromagnetic semiconductors)

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Abstract. A unified self-consistent theory of the mutual influence of the electronic and spin subsystems in the s–f model approximation for ferromagnetic semiconductors is developed. The calculations are based on the novel approach of the two-time Green function method. It consists in the introduction of irreducible Green functions (IGF) and the derivation of the exact Dyson equation and the exact self-energy operator. It is shown that the IGF method gives a unified and natural approach for the calculation of the elementary excitation spectrum and damping. The full electronic and magnetic quasiparticle spectra of the s–f model are derived by taking explicitly into account magnon–magnon, electron–magnon and electron–electron scattering processes. The recent Babcenco and Cottam results follow from this theory in the lowest-order approximation.

1. Introduction

In this paper we present a unified and complete self-consistent consideration of the mutual influence of the electron and the spin subsystems in ferromagnetic semi-conductors by taking explicitly into account damping effects and finite lifetimes. A great deal of effort has been made to gain an understanding of the physics of magnetic semiconductors. An important problem is to make clear the relationship between their magnetic and electrical properties. The corresponding theoretical model is known in literature as the s–f model (Krisement 1976, Nolting 1979a).

The s–f model has been intensively discussed in many previous papers on ferro-magnetic semiconductors. Nolting (1978, 1979b) and Nolting and Oles (1980a, b, c, d) calculated the electronic excitation spectrum of a ferromagnetic semiconductor in the strong-coupling limit using an improved moment method. Sinkkonen (1979) developed an intermediate-coupling theory of the s–f model in terms of the functional-derivative method. Nolting and Oles (1981a, b) calculated the magnon spectrum, quasiparticle density of states and edge shifts of doped ferromagnetic semiconductors. The exact nature of the conduction band states was investigated in a very elegant way by Allan and Edwards (1982). They retained the predominant d character of the conduction electrons and found the most important effect of the electron–magnon interaction on the electronic states at $T = 0$. Recently, a significant contribution to the explanation of the observed

electron spin polarisation in the magnetic semiconductor EuS has been made by Edwards (1983) who clarified the true situation in this compound.

A very detailed investigation of the magnetic excitation spectra in the s–f model approximation has been developed by Babcenco and Cottam (1981). These authors give a more detailed description than Woolsey and White (1970), including an optical branch of the magnon spectrum and a Stoner-like continuum of excitations as well as the usual acoustic magnons. Unfortunately the damping effects and the finite lifetimes were not taken into account. The only damping mechanism that has been considered is the decay of a magnon into an electron–hole pair with a spin flip.

The purpose of our paper is to develop a complete self-consistent theory of electronic and magnetic elementary excitations in ferromagnetic semiconductors by taking explicitly into account magnon–magnon, electron–electron and electron–magnon inelastic scattering processes. For this purpose we use the novel irreducible Green functions (IGF) method developed by Plakida (1971, 1973), for the self-consistent phonon theory and for the Heisenberg ferromagnet, and by Kuzemsky (1978), for the Hubbard model. The IGF method allows one completely to describe the quasiparticle inelastic scattering processes in a many-body system and to find quasiparticle spectra with damping in a very general way. From the technical point of view the IGF method is a special kind of projection operator approach in the theory of two-time Green functions (Ichiyanagi 1972).

If one introduces irreducible parts of the Green functions (or irreducible parts of the operators from which the GF is constructed) the equation of motion for the GF can be exactly transformed into Dyson equation. The representation of the self-energy operator in terms of high-order GF is exact too. In order to perform the self-consistent calculation of the self-energy operator we have to express it approximately in terms of low-order GF. Recently, the IGF method has been applied in a number of solid state problems (see Kuzemsky *et al* 1983). Christoph *et al* (1982) used this method for the calculation of elementary excitation spectra in the generalised RKKY model of magnetism, which shows that all branches should be taken into account in performing damping calculations.

The paper is organised as follows: in the next section we introduce the s–f Hamiltonian. In § 3 we derive the exact Dyson equation for one-electron GF by means of the IGF method. The self-consistent approximative formalism for the calculation of the electron self-energy operator is presented in § 4. In § 5 we derive the exact Dyson equation for the spin subsystem. The self-energy operator for this case is calculated in § 6. In § 7 we present our conclusions and possibilities for further development. In the Appendix we give a simple but useful analysis of our truncation procedure on the basis of the moment conservation treatment.

2. The Hamiltonian of the s–f model

The total Hamiltonian of the s–f model is represented by the following sum (Krisement 1976, Nolting 1979a):

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

The kinetic energy operator H_e of the itinerant band electrons is given by the expression

$$H_e = \sum_{ij\sigma} t_{ij} a_{i\sigma}^+ a_{j\sigma} = \sum_{k\sigma} \varepsilon_k a_{k\sigma}^+ a_{k\sigma} \tag{2}$$

where

$$\varepsilon_k = N^{-1} \sum_{ij} t_{ij} \exp[-i k \cdot (R_i - R_j)]$$

is the band energy. Although the itinerant electrons are predominantly d electrons they are usually treated as s electrons for mathematical simplicity. However, retaining the predominant d character of the itinerant electrons may be very important for describing the heavy rare-earth metals and magnetic semiconductors (Cooke 1979, Christoph *et al* 1982, Allan and Edwards 1982). For tight-binding electrons in the lattice with an inversion centre the band energy reads

$$\varepsilon_k = \sum_n t(R_n) \cos(k \cdot R_n). \tag{3}$$

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

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

where U is the Hubbard correlation energy. In the case of a pure semiconductor at low temperatures the conduction electron band is empty and the Coulomb term (4) is therefore not so important. A partial occupation of the band leads to an increase in the role of the Coulomb correlation.

The localised moments with the Hamiltonian H_f are treated in terms of the Heisenberg model:

$$H_f = -\tfrac{1}{2} \sum_{ij} J_{ij} S_i \cdot S_j = -\tfrac{1}{2} \sum_q J_q S_q \cdot S_{-q}. \tag{5}$$

These two subsystems are coupled by a local spin–spin exchange interaction H_{s-f}

$$
\begin{aligned}
H_{s-f} &= -2I \sum_{i\sigma\sigma'} (S_i \cdot \sigma)_{\sigma\sigma'} a_{i\sigma'}^+ a_{i\sigma'} \\
&= -IN^{-1/2} \sum_{kq} \{ S_{-q}^+ a_{k\downarrow}^+ a_{k+q\uparrow} + S_{-q}^- a_{k\uparrow}^+ a_{k+q\uparrow} \\
&\quad + S_{-q}^z (a_{k\uparrow}^+ a_{k+q\uparrow} - a_{k\downarrow}^+ a_{k+q\downarrow}) \}
\end{aligned} \tag{6}
$$

where operator (6) describes the RKKY iteraction of the localised spins of the 4f shell with the spin density of the itinerant electrons. In general the exchange integral $I(k, k+q)$ depends on the quasimomentum (Freeman 1972). (A generalisation for the non-local case can be made directly.)

3. The Dyson equation for the one-electron Green function

For calculation of the electronic quasiparticle spectrum of the described model with Hamiltonian (1) let us consider the equation of motion for the one-electron GF (Zubarev 1960):

$$G_{k\sigma}(t - t') = -i\theta(t - t') \langle [a_{k\sigma}(t), a_{k\sigma}^+(t')]_+ \rangle = \langle\langle_{k\sigma}(t) | a_{k\sigma}^+(t') \rangle\rangle. \tag{7}$$

Performing first time (t) differentiation of (7) for the Fourier transform $G_{k\sigma}(\omega)$ we get

the equation

$$(\omega - \varepsilon_k)G_{k\sigma}(\omega) = 1 + \frac{U}{N}\sum_{pq} \langle\!\langle a^+_{p+q,-\sigma}a_{p,-\sigma}a_{k+q,\sigma}|a^+_{k\sigma}\rangle\!\rangle_\omega$$

$$- IN^{-1/2}\sum_q (\langle\!\langle S^{-\sigma}_{-q}a_{k+q,-\sigma}|a^+_{k\sigma}\rangle\!\rangle_\omega + z_\sigma\langle\!\langle S^z_{-q}a_{k+q,\sigma}|a^+_{k\sigma}\rangle\!\rangle_\omega) \tag{8}$$

where

$$S^{-\sigma}_{-q} = \begin{cases} S^-_{-q} & \text{if } \sigma = + \text{ or } \uparrow \\ S^+_{-q} & \text{if } \sigma = - \text{ or } \downarrow \end{cases} \qquad z_\sigma = \begin{cases} +1 & \text{if } \sigma = + \text{ or } \uparrow \\ -1 & \text{if } \sigma = - \text{ or } \downarrow \end{cases}.$$

Following Plakida (1971) and Kuzemsky (1978) one can introduce the irreducible GF

$$\langle\!\langle (S^z_{-q}a_{k+q,\sigma})^{\text{ir}}|a^+_{k\sigma}\rangle\!\rangle = \langle\!\langle S^z_{-q}a_{k+q,\sigma}|a^+_{k\sigma}\rangle\!\rangle - \delta_{q,0}\langle S^z_{-q}\rangle\langle\!\langle a_{k+q,\sigma}|a^+_{k\sigma}\rangle\!\rangle$$

$$\langle\!\langle (a^+_{p+q,-\sigma}a_{p,-\sigma}a_{k+q,\sigma})^{\text{ir}}|a^+_{k\sigma}\rangle\!\rangle = \langle\!\langle a^+_{p+q,-\sigma}a_{p,-\sigma}a_{k+q,\sigma}|a^+_{k\sigma}\rangle\!\rangle$$

$$- \delta_{q,0}\langle a^+_{p+q,-\sigma}a_{p,-\sigma}\rangle\langle\!\langle a_{k\sigma}|a^+_{k\sigma}\rangle\!\rangle \tag{9}$$

in which the mean-field contributions are removed. The choice of the IGFs is determined by the conditions

$$\langle[(S^z_{-q}a_{k+q,\sigma})^{\text{ir}}, a^+_{k\sigma}]_+\rangle = 0 \tag{10a}$$

$$\langle[(a^+_{p+q,-\sigma}a_{p,-\sigma}a_{k+q,\sigma})^{\text{ir}}, a^+_{k\sigma}]_+\rangle = 0. \tag{10b}$$

The IGFs are defined so that they cannot be reduced to the low-order ones by any kind of decoupling. This reducing procedure leads to extracting all relevant (for the problem under consideration) mean-field renormalisations and putting them into the 'zero-order' (generalised mean-field) GF. For example, in the case of weak electron correlation it will be enough to define a very simple mean-field extraction in the second part of (9), i.e. $\langle a^+_{k\sigma}a_{k\sigma}\rangle$. In the general case the mean-field renormalisations can have very non-trivial structure, and a special projection procedure should be developed for the higher-order GFs as is done for the cases of the Heisenberg ferromagnet (Plakida 1973), the Hubbard model in the strong-correlation limit (Kuzemsky 1978) and the magnetic polaron problem at finite temperatures and an arbitrary values of the s–f exchange.

In order to calculate the IGFs $\langle\!\langle (A(t))^{\text{ir}}|B(t')\rangle\!\rangle$ in expressions (9) we have to write the equations of motion after differentiation with respect to the second time variable t'. Then conditions (10) remove the inhomogeneous terms in these equations. If one introduces irreducible parts for the right-hand side operators by analogy with expressions (9) and (10), the equation of motion (8) can be exactly rewritten in the following form:

$$G_{k\sigma}(\omega) = G^0_{k\sigma}(\omega) + G^0_{k\sigma}(\omega)P_{k\sigma}(\omega)G^0_{k\sigma}(\omega) \tag{11}$$

where the mean-field GF $G^0_{k\sigma}(\omega)$ reads

$$G^0_{k\sigma}(\omega) = (\omega - \varepsilon^0_{k\sigma})^{-1}. \tag{12}$$

Here $\varepsilon^0_{k\sigma}$ is

$$\varepsilon^0_{k\sigma} = \varepsilon_k - z_\sigma IN^{-1/2}\langle S^z_0\rangle + (U/N)n_{-\sigma}.$$

The scattering operator $P_{k\sigma}(\omega)$ is given by expression

$$P_{k\sigma}(\omega) = P^{\text{ee}}_{k\sigma}(\omega) + P^{\text{e-m}}_{k\sigma}(\omega) \tag{13}$$

and

$$P_{k\sigma}^{\text{ee}}(\omega) = \frac{U^2}{N^2} \sum_{pq} \sum_{p'q'} \langle\langle (a_{p+q,-\sigma}^+ a_{p,-\sigma} a_{k+q,\sigma})^{\text{ir}} | (a_{p+q',-\sigma}^+ a_{p',-\sigma} a_{k-q',\sigma}^+)^{\text{ir}} \rangle\rangle \tag{14a}$$

$$P_{k\sigma}^{\text{e-m}}(\omega) = \frac{\text{i}^2}{N} \sum_{qq'} \{ \langle\langle (S_{-q}^z a_{k+q,-\sigma})^{\text{ir}} | (S_{q'}^z a_{k+q',\sigma}^+)^{\text{ir}} \rangle\rangle$$

$$+ \langle\langle S_{-q}^{-\sigma} a_{k+q,-\sigma} | S_{q'}^\sigma a_{k+q',\sigma}^+ \rangle\rangle \} \tag{14b}$$

where the intersubsystem contributions are dropped, i.e.

$$\langle\langle (a_{p+q,-\sigma}^+ a_{p,-\sigma} a_{k+q,\sigma})^{\text{ir}} | (S_{q'}^z a_{k+q',\sigma}^+)^{\text{ir}} + S_{q'}^\sigma a_{k-q',-\sigma}^+ \rangle\rangle$$

is equal to zero because of our simple projection procedure assumed in this paper.

From the Dyson equation

$$G_{k\sigma}(\omega) = G_{k\sigma}^0(\omega) + G_{k\sigma}^0(\omega) M_{k\sigma}(\omega) G_{k\sigma}(\omega) \tag{15}$$

we get the following equation for $M_{k\sigma}(\omega)$:

$$P_{k\sigma}(\omega) = M_{k\sigma}(\omega) + M_{k\sigma}(\omega) G_{k\sigma}^0(\omega) P_{k\sigma}(\omega) \tag{16}$$

from which it follows that we can say, in complete analogy to the diagrammatic technique, that the self-energy operator $M_{k\sigma}(\omega)$ is defined as a proper (connected) part of the scattering operator $P_{k\sigma}(\omega)$:

$$M_{k\sigma}(\omega) = (P_{k\sigma}(\omega))^{\text{c}}. \tag{17}$$

It should be emphasised that for the retarded (and advanced) GFs the proper part has only a symbolic character. However, one can use the causal instead of retarded GF at any step in the calculations because the equation of motion has the same form for all three (retarded, advanced and causal) GFs.

In a certain sense there is a possibility of controlling, in diagrammatic language, the relevant decoupling procedure in further approximative self-energy calculations. Thus, in contrast to the standard equation-of-motion approach the decoupling is only introduced in the self-energy operator. A concrete calculation will be given in the next section.

4. A self-consistent approximative calculation of the electron self-energy operator

To find useful explicit expressions for $M_{k\sigma}(\omega)$ we have to evaluate the high-order GFs in equations (16) and (17). The electron–electron part (16) has been previously found by Kuzemsky (1978) by considering the electron correlation effects in Hubbard model in the band limit. In the pair approximation for $M_{k\sigma}^{\text{ee}}(\omega)$ he obtained

$$M_{k\sigma}^{\text{ee}}(\omega) = \frac{U^2}{N^2} \sum_{pq} \int_{-\infty}^{+\infty} \frac{\text{d}\omega_1 \,\text{d}\omega_2 \,\text{d}\omega_3}{\omega + \omega_1 - \omega_2 - \omega_3} [n(\omega_1)(1 - n(\omega_2) - n(\omega_3))$$

$$+ n(\omega_2)n(\omega_3)] g_{p+q,-\sigma}(\omega_1) g_{k+p,\sigma}(\omega_2) g_{p,-\sigma}(\omega_3) \tag{18}$$

where

$$g_{k\sigma}(\omega) = -(1/\pi) \operatorname{Im} G_{k\sigma}(\omega + \text{i}\varepsilon) = (1/2\pi)(\text{e}^{\beta\omega} + 1) A_{k\sigma}(\omega). \tag{19}$$

Let us consider now the spin–electron inelastic scattering. It is convenient to write

down $M_{k\sigma}^{\rm em}(\omega)$ in the form

$$
\begin{aligned}
M_{k\sigma}^{\rm e-m}(\omega) = M_{k\sigma}^{\alpha\beta}(\omega) &= \frac{I^2}{N} \sum_{qq'} \langle\!\langle S_{-q}^\alpha a_{k+q,\sigma} | S_{q'}^\beta a_{k+q',\sigma}^+ \rangle\!\rangle^{({\rm ir,c})} \\
&= \frac{I^2}{N} \sum_{qq'} \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{{\rm d}\omega'}{\omega - \omega'} \, ({\rm e}^{\beta\omega'} + 1) \\
&\quad \times \int_{-\infty}^{+\infty} {\rm d}t \, {\rm e}^{{\rm i}\omega' t} \langle S_{q'}^\beta a_{k+q',\sigma}^+ S_{-q}^\alpha(t) a_{k+q,\sigma}(t) \rangle^{({\rm ir,c})}.
\end{aligned}
\tag{20}
$$

If one uses the following decoupling procedure:

$$
\langle S_{q'}^\beta a_{k+q',\sigma}^+ S_{-q}^\alpha(t) a_{k+q,\sigma}(t) \rangle^{({\rm ir,c})} \simeq \langle S_{q'}^\beta S_{-q}^\alpha(t) \rangle \langle a_{k+q',\sigma}^+ a_{k+q,\sigma}(t) \rangle
\tag{21}
$$

the corresponding approximative expression for $M_{k\sigma}^{\rm e-m}(\omega)$ neglects the vertex correlations, i.e. the correlations between propagations of the electrons and the magnetic excitations. In another paper we will consider the magnetic polaron problem where such correlations are very important. Taking into account the spectral theorem (Zubarev 1960) we obtain from equations (20) and (21)

$$
\begin{aligned}
M_{k\sigma}^{\rm e-m}(\omega) = \frac{I^2}{N} \sum_q \int_{-\infty}^{+\infty} {\rm d}\omega_1 \, {\rm d}\omega_2 \, \frac{1 + \nu(\omega_1) - n(\omega_2)}{\omega - \omega_1 + \omega_2} \, & \big(m_q^{\sigma,-\sigma}(\omega_1) g_{k-q,-\sigma}(\omega_2) \\
& + m_q^{zz}(\omega_1) g_{k-q,\sigma}(\omega_2) \big)
\end{aligned}
\tag{22}
$$

where the following symbols are introduced:

$$
\begin{aligned}
m_q^{\alpha\beta}(\omega) &= (1/\pi) \, {\rm Im} \, \langle\!\langle S_q^\alpha | S_{-q}^\beta \rangle\!\rangle = (1/2\pi)({\rm e}^{\beta\omega} - 1) K_q^{\alpha\beta}(\omega) \\
K_q^{\alpha\beta}(t) &= \langle S_{-q}^\beta S_q^\alpha(t) \rangle.
\end{aligned}
\tag{23}
$$

Here $\nu(\omega)$ and $n(\omega)$ denote the Bose and the Fermi distribution function, respectively.

Equations (11), (18) and (22) form a closed self-consistent system of equations for the one-electron GF of a ferromagnetic semiconductor. There the electron–electron scattering is accounted for in the pair approximation and the spin–electron scattering is described by neglecting the vertex correlations. In principle we can substitute in the RHS of the equations (18) and (22) any relevant initial GF and find a solution by repeated integration.

For first step in the iteration we choose the following simple one-pole expression:

$$
g_{k\sigma}(\omega) = \delta(\omega - \varepsilon_{k\sigma}).
\tag{24}
$$

Then from the equations (18) and (22) we obtain

$$
\begin{aligned}
M_{k\sigma}^{\rm ee}(\omega) &= \frac{U^2}{N^2} \sum_{pq} \frac{n_{p+q,-\sigma}(1 - n_{k+p,\sigma} - n_{q,-\sigma}) + n_{k+p,\sigma} n_{q,-\sigma}}{\omega - \varepsilon_{p+q,-\sigma} - \varepsilon_{k+p,\sigma} + \varepsilon_{q,-\sigma}} \\
&= \frac{U^2}{N^2} \sum_{pq} \frac{N_{kpq}}{\omega - \Omega_{kpq}}
\end{aligned}
\tag{25}
$$

$$
\begin{aligned}
M_{k\sigma}^{\rm e-m}(\omega) = \frac{I^2}{N} \sum_q \int_{-\infty}^{+\infty} {\rm d}\omega_1 \, \bigg(& \frac{1 + \nu(\omega_1) - n_{k-q,-\sigma}}{\omega - \omega_1 - \varepsilon_{k-q,-\sigma}} \, m_q^{\sigma,-\sigma}(\omega_1) \\
& + \frac{1 + \nu(\omega_1) - n_{k-q,\sigma}}{\omega - \omega_1 - \varepsilon_{k-q,\sigma}} \, m_q^{zz}(\omega_1) \bigg).
\end{aligned}
\tag{26}
$$

The expression (25) was found by Kuzemsky (1978). It describes electron–electron pair scattering in the paramagnetic state of the electron subsystem. The expression (26) contains some results found by Krisement (1976), Nolting (1977), Kuivalainen *et al* (1979), Sinkkonen (1979) and Woolsey and White (1970). In order to obtain the results of Woolsey and White (1970) it is necessary to neglect $m_q^{zz}(\omega)$ (which is reasonable at low temperatures) and to use as a first iteration the expression

$$-(1/\pi) \operatorname{Im} \langle\!\langle S_q^\alpha | S_{-q}^{-\sigma} \rangle\!\rangle = z_\sigma(2\langle S_0^z \rangle / N^{1/2}) \delta(\omega - z_\sigma \omega_q) \tag{27}$$

where $\omega(q) = Dq^2$ is the magnon energy. Then we obtain the Woolsey and White (1970) perturbative result:

$$M_{k\uparrow}^{\text{e–m}}(\omega) = \frac{2\langle S_0^z \rangle I^2}{N^{3/2}} \sum_q \frac{n_{k+q,\downarrow} + \nu_q}{\omega - \varepsilon_{k+q,\downarrow} + \omega_q} \tag{28a}$$

$$M_{k\downarrow}^{\text{e–m}} = \frac{2\langle S_0^z \rangle I^2}{N^{3/2}} \sum_q \frac{1 - n_{k-q,\uparrow} + \nu_q}{\omega - \varepsilon_{k-q,\uparrow} - \omega_q}. \tag{28b}$$

In the state limit for $K_q^{\alpha\beta}(t) \simeq K_q^{\alpha\beta}(0)$ one can immediately obtain the Sinkkonen (1979) result

$$M_{k\sigma}^{\text{e–m}}(\omega) = \frac{I^2}{N} \sum_q \int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega'}{\omega - \omega'} [K_q^{\sigma,-\sigma} g_{k-q,-\sigma}(\omega') + K_q^{zz} g_{k-q,\sigma}(\omega')] \tag{29}$$

from which the Kuivalainen *et al* (1979) result can be found as a special case.

The renormalised electron energy appears as a self-consistent solution of the equation

$$\omega - \varepsilon_{k\sigma}^0 - \operatorname{Re} M_{k\sigma}(\omega) = 0 \tag{30}$$

together with equations (18) and (22) or with equations (25) and (26). In this way the energy shifts of the electrons can be calculated from the set of non-linear integral equations (30), (25) and (26). So the electron linewidth is given by

$$\Gamma_{k\sigma}(\omega) = 1/\tau = -\operatorname{Im} M_{k\sigma}(\omega + \mathrm{i}\varepsilon)$$

$$\tilde{\Gamma}_{k\sigma} = \operatorname{Im} M_{k\sigma}(\varepsilon_{k\sigma}) / (1 - \partial \operatorname{Re} M_{k\sigma}(\omega)/\partial\omega |_{\omega = \varepsilon_{k\sigma}}) \tag{31}$$

and the one-electron density of states is defined as

$$D_\sigma(\omega) = \frac{1}{\pi N} \sum_k \frac{\Gamma_{k\sigma}(\omega)}{(\omega - \varepsilon_{k\sigma})^2 + \Gamma_{k\sigma}^2(\omega)} \tag{32}$$

(cf Allan and Edwards 1982). On the basis of equations (31) and (32) we can consider modified (due to electron–electron correlation effect) expressions for the electron effective mass, electron mobility and electron specific heat obtained by Woolsey and White (1970).

5. The Dyson equation for the spin Green functions

To study the magnetic excitation spectrum of the localised spin subsystem we need the GF

$$R(t - t') = -\mathrm{i}\theta(t - t')\langle[S_k^+(t), S_{-k}^-(t')]_-\rangle = \langle\!\langle S_k^+(t) | S_{-k}^-(t') \rangle\!\rangle. \tag{33}$$

Christoph *et al* (1982), however, show that for the many-branch quasiparticle excitation spectrum it is necessary to evaluate the matrix GF (cf Babcenco and Cottam 1981)

$$\hat{R}(t) = \begin{Vmatrix} \langle\langle S_k^+ \mid S_{-k}^- \rangle\rangle & \langle\langle S_k^+ \mid \sigma_{-k}^- \rangle\rangle \\ \langle\langle \sigma_k^+ \mid S_{-k}^- \rangle\rangle & \langle\langle \sigma_k^+ \mid \sigma_{-k}^- \rangle\rangle \end{Vmatrix} \tag{34}$$

where

$$\sigma_k^+ = \sum_q a_{q\uparrow}^+ a_{k+q\downarrow} \qquad \sigma_{-k}^- = (\sigma_k^+)^+ = \sum_q a_{k+q\downarrow}^+ a_{q\uparrow}.$$

By differentiation of the GF $\langle\langle S_k^+ \mid B \rangle\rangle$ with respect to the first time t and introducing the IGF following Plakida (1973) and Christoph *et al* (1982) it is convenient to introduce the irreducible operators

$$\left. \begin{aligned} (S_q^z)^{\text{ir}} &= S_q^z - \langle S_0^z \rangle \delta_{q,o} \\ (S_{k-q}^+ (S_q^z)^{\text{ir}} - S_q^+ (S_{k-q}^z)^{\text{ir}})^{\text{ir}} &= S_{k-q}^+ (S_q^z)^{\text{ir}} - S_q^+ (S_{k-q}^z)^{\text{ir}} - (A_q - A_{k-q}) S_k^+ \end{aligned} \right\} \tag{35}$$

$$A_q = (2K_q^{zz} + K_q^{-+})/2\langle S_0^z \rangle \tag{36}$$

we find the equation of motion

$$\Omega_1 \langle\langle S_k^+ \mid B \rangle\rangle_\omega + \Omega_2 \langle\langle \sigma_k^+ \mid B \rangle\rangle_\omega = \begin{Bmatrix} (N^{1/2}/I)\Omega_2 \\ 0 \end{Bmatrix} + \langle\langle A \mid B \rangle\rangle_\omega. \tag{37}$$

Here

$$\Omega_1 = \omega - \frac{\langle S_0^z \rangle}{N^{1/2}} (J_0 - J_k) - N^{-1/2} \sum_q (J_q - J_{q-k}) \frac{2K_q^{zz} + K_q^{-+}}{2\langle S_0^z \rangle}$$
$$- \frac{I}{N} (n_\uparrow - n_\downarrow) \tag{38}$$

$$\Omega_2 = 2\langle S_0^z \rangle I/N \tag{39}$$

and B denotes the operators S_{-k}^- or σ_{-k}^-. The many-particle operator A reads

$$A = \frac{1}{N} \sum_q (S_{k-q}^+ (S_q^z)^{\text{ir}} - S_q^+ (S_{k-q}^z)^{\text{ir}})^{\text{ir}} + \frac{I}{N} \sum_{pq} \{ S_{k-q}^+ (a_{p\uparrow}^+ a_{p+q\uparrow} - a_{p\downarrow}^+ a_{p+q\downarrow})^{\text{ir}}$$
$$- 2(S_{k-q}^z)^{\text{ir}} a_{p\uparrow}^+ a_{p+q\downarrow} \} \tag{40}$$

and it satisfies the conditions

$$\langle [A, S_{-k}^-]_- \rangle = \langle [A, \sigma_k^-]_- \rangle = 0.$$

Now we consider the GF $\langle\langle \sigma_k^+ \mid B \rangle\rangle$. Similarly to equation (37), we have

$$-N^{1/2} \chi_0^{\text{df}} \langle\langle S_k^+ \mid B \rangle\rangle_\omega + (1 - U\chi_0^{\text{df}}) \langle\langle \sigma_k^+ \mid B \rangle\rangle_\omega = \begin{Bmatrix} 0 \\ -N\chi_0^{\text{df}} \end{Bmatrix} + \sum_p \frac{1}{\omega_{p,k}} \langle\langle B_p \mid B \rangle\rangle_\omega \tag{41}$$

where

$$\omega_{p,k} = \omega + \varepsilon_p - \varepsilon_{p+k} - \Delta \tag{42a}$$

$$\Delta = 2\langle S_0^z \rangle I/N^{1/2} + (U/N)(n_\uparrow - n_\downarrow) \tag{42b}$$

$$\chi_0^{\text{df}} = \frac{1}{N} \sum_p \frac{n_{p+k\downarrow} - n_{p\uparrow}}{\omega_{p,k}}. \tag{42c}$$

The irreducible operator B_p is defined by

$$B_p = -\frac{I}{N^{1/2}} \sum_{qq'} [S^+_{-q'}(a^+_{p\uparrow} a_{q+q'\uparrow} \delta_{q,p+k} - a^+_{q\downarrow} a_{p+k\downarrow} \delta_{p,q+q'})^{ir}$$

$$- (S^z_{-q'})^{ir}(a^+_{p\uparrow} a_{q+q'\downarrow} \delta_{q,p+k} - a^+_{q\uparrow} a_{p+k\downarrow} \delta_{p,q+q'})]$$

$$+ \frac{U}{N} \sum_{qq'} (a^+_{p\uparrow} a^+_{q+q\uparrow} a_{q\uparrow} a_{p+k+q'\downarrow} - a^+_{p+q'\uparrow} a^+_{q-q'\downarrow} a_{q\downarrow} a_{p+k\downarrow})^{ir} \tag{43}$$

and the equations of motion (37) and (41) can be summarised in the matrix form

$$\hat{\Omega}\hat{R} = \hat{I} + \sum_p \hat{\varphi}_p \hat{R}^{(1)}_p. \tag{44}$$

Here

$$\hat{\Omega} = \begin{Vmatrix} \Omega_1 & \Omega_2 \\ -IN^{1/2}\chi^{df}_0 & 1 - U\chi^{df}_0 \end{Vmatrix} \qquad \hat{I} = \begin{Vmatrix} (N^{1/2}/I)\Omega_2 & 0 \\ 0 & -N\chi^{df}_0 \end{Vmatrix} \tag{45}$$

$$\hat{\varphi}_p = \begin{Vmatrix} 1/N & 0 \\ 0 & 1/\omega_{p,k} \end{Vmatrix} \qquad \hat{R}^{(1)}_p = \begin{Vmatrix} \langle\langle A|S^-_{-k}\rangle\rangle & \langle\langle A|\sigma^-_{-k}\rangle\rangle \\ \langle\langle B_p|S^-_{-k}\rangle\rangle & \langle\langle B_p|\sigma^-_{-k}\rangle\rangle \end{Vmatrix}. \tag{46}$$

In order to obtain a Dyson equation we have to use the equation of motion for the matrix GF $\hat{R}^{(1)}(t)$ and introduce the irreducible parts as discussed above. Thus we get

$$\hat{R} = \hat{R}^{(0)} + \hat{R}^{(0)}\hat{P}\hat{R}^{(0)} \tag{47}$$

$$\hat{P} = \hat{I}^{-1}\left(\sum_{pq} \hat{\varphi}_p \hat{P}(p,q)\hat{\varphi}_q\right)\hat{I}^{-1} \qquad \hat{R}^{(0)} = \hat{\Omega}^{-1}\hat{I} \tag{48}$$

and

$$\hat{P}(p,q) = \begin{Vmatrix} \langle\langle A|A^+\rangle\rangle & \langle\langle A|B^+_q\rangle\rangle \\ \langle\langle B_p|A^+\rangle\rangle & \langle\langle B_p|B^+_q\rangle\rangle \end{Vmatrix}. \tag{49}$$

Using the definition (13) the equation (47) can be transformed into the exact Dyson equation

$$\hat{R} = \hat{R}^{(0)} + \hat{R}^{(0)}\hat{\Pi}\hat{R} \tag{50}$$

with the self-energy operator $\hat{\Pi}$ given as

$$\hat{\Pi} = \{\hat{P}\}^c. \tag{51}$$

The solution of equation (50) can be written in the form

$$\hat{R} = [(\hat{R}^{(0)})^{-1} - \hat{\Pi}]^{-1}. \tag{52}$$

Hence the determination of $\hat{R}$ has been reduced to the determination of the mean-field GF $\hat{R}^{(0)}$ and the self-energy operator $\hat{\Pi}$.

In the explicit form the mean-field GF $\hat{R}^{(0)}$ is expressed by

$$\hat{R}^{(0)} = \frac{1}{\det \hat{\Omega}} \begin{Vmatrix} (1 - U\chi^{df}_0)(N^{1/2}/I)\Omega_2 & N\chi^{df}_0\Omega_2 \\ N\chi^{df}_0\Omega_2 & -N\chi^{df}_0\Omega_1 \end{Vmatrix} \tag{53}$$

where

$$\det \hat{\Omega} = (1 - U\chi^{df}_0)\Omega_1 + N^{1/2}I\chi^{df}_0\Omega_2. \tag{54}$$

Then for the localised spin GF $\langle\!\langle S_k^+ | S_{-k}^-\rangle\!\rangle_\omega^{(0)}$ we find

$$\langle\!\langle S_k^+ | S_{-k}^-\rangle\!\rangle_\omega^{(0)} = \frac{2\langle S_0^z\rangle}{N^{1/2}} \left(\omega - \frac{\langle S_0^z\rangle}{N^{1/2}} (J_0 - J_k) - \frac{1}{N^{1/2}} \sum_q (J_q - J_{q-k}) \frac{2K_q^{zz} + K_q^{-+}}{2\langle S_0^z\rangle} \right.$$

$$\left. - \frac{I}{N} (n_\uparrow - n_\downarrow) + 2\frac{I^2}{N^{1/2}} \langle S_0^z\rangle \chi_0^{df}(1 - U\chi_0^{df})^{-1} \right)^{-1}. \tag{55}$$

As follows from expression (55), the two interacting subsystems (localised spins and itinerant electrons) are described in the generalised Hartree–Fock approximation, which can be considered as a good starting point for studying wide-band ferromagnetic semiconductors. The magnetic excitation spectrum following from the GF (55) consists of three branches: the acoustical spin waves, the optical spin waves and the Stoner-like continuum of excitations. Our considerations generalise the first-order theory given by Babcenco and Cottam (1981) (cf Bartel 1973, Christoph *et al* 1982).

In the limit $k \to 0$, $\omega \to 0$, the GF (55) can be written as

$$\langle\!\langle S_k^+ | S_{-k}^-\rangle\!\rangle_\omega^{(0)} = (2\langle S_0^z\rangle/N^{1/2}) (\omega - \omega(k)) \tag{56}$$

where the acoustical spin wave energies $\omega(k) = D_{ac}k^2$ are determined by the stiffness constant D_{ac}:

$$D_{ac} = \frac{\langle S_0^z\rangle}{2N^{1/2}} \left(\psi_0 + \sum_q \psi_q \frac{2K_q^{zz} + K_q^{-+}}{2\langle S_0^z\rangle} + \frac{N^{1/2}}{2\langle S_0^z\rangle} \frac{1}{N} \sum_q (n_{q\uparrow} + n_{q\downarrow})\tfrac{1}{2}(\hat{k} \cdot \nabla_q)^2 \varepsilon_q \right.$$

$$\left. + \frac{N^{1/2}}{2\langle S_0^z\rangle} \frac{1}{N\Delta} \sum_q (n_{q\downarrow} - n_{q\uparrow})(\hat{k} \cdot \nabla_q \varepsilon_q)^2 \right). \tag{57}$$

Here

$$\psi_q = \sum_n (\hat{k} \cdot R_n)^2 J(|R_n|) \exp(-iq \cdot R_n)$$

and the sum is taken over the lattice sites denoted by R_n; $J(|R_n|)$ is the exchange integral and $\hat{k} = k/k$. The stiffness constant D_{ac} can be expressed in terms of the Hamiltonian parameters if one evaluates the band splitting Δ by self-consistently solving the RPA equation

$$n_\sigma = \sum_k n_{k\sigma} = \sum_k \left[\exp \beta \left(\varepsilon_k + \frac{U}{N} n_{-\sigma} - \frac{I}{N^{1/2}} \langle S_0^z\rangle - \varepsilon_F \right) + 1 \right]^{-1}. \tag{58}$$

6. Spin self-energy operator and the magnon damping

The self-energy operator $\hat{\Pi}$ can be expressed approximately in terms of the low-order GFs. As an example let us consider the calculation of the GF $\langle\!\langle A | A^+\rangle\!\rangle$. Using the spectral theorem and neglecting the high-order correlation effects (vertex corrections) between the magnetic excitations and charge-density fluctuations we obtain

$$\langle\!\langle A | A^+\rangle\!\rangle_\omega^{ir,c} = \frac{1}{N} \sum_q (J_q - J_{k-q})^2$$

$$\times \int_{-\infty}^{+\infty} d\omega_1 \, d\omega_2 \, \frac{1 + \nu(\omega_1) + \nu(\omega_2)}{\omega - \omega_1 - \omega_2} m_{k-q}^{+-}(\omega_1) m_q^{zz}(\omega_2)$$

$$
+ \frac{I^2}{N^2} \sum_{pp'q\sigma} \int_{-\infty}^{+\infty} \mathrm{d}\omega_1\, \mathrm{d}\omega_2\, \frac{\nu(\omega_1)\nu(\omega_2)/\nu(\omega_1 + \omega_2)}{\omega - \omega_1 - \omega_2}
$$

$$
\times\, m_{k-q}^{+-}(\omega_1)\left(-\frac{1}{\pi}\,\mathrm{Im}\langle\!\langle a_{p\sigma}^{+} a_{p+q\sigma} | a_{p'\sigma}^{+} a_{p'-q\sigma}\rangle\!\rangle_{\omega_2}\right)
$$

$$
+ 4\frac{I^2}{N^2} \sum_{pp'q} \int_{-\infty}^{+\infty} \mathrm{d}\omega_1\, \mathrm{d}\omega_2\, \frac{\nu(\omega_1)\nu(\omega_2)/\nu(\omega_1 + \omega_2)}{\omega - \omega_1 - \omega_2}
$$

$$
\times\, m_{k-q}^{zz}(\omega_1)\left(-\frac{1}{\pi}\,\mathrm{Im}\langle\!\langle a_{p\uparrow}^{+} a_{p+q\downarrow} | a_{p'\downarrow}^{+} a_{p'-q\uparrow}\rangle\!\rangle_{\omega_2}\right). \tag{59}
$$

According to the same arguments as given above, the GFs $\langle\!\langle A|B_q^+\rangle\!\rangle_\omega$, $\langle\!\langle B_p|A^+\rangle\!\rangle_\omega$ and $\langle\!\langle B_p|B_q^+\rangle\!\rangle$ can be represented in a similar form. This leads to the self-consistent system of equations for $\hat{R}$ and $\hat{\Pi}$.

For the first iteration we put

$$
-(1/\pi)\,\mathrm{Im}\langle\!\langle S_{k-q}^{+}|S_{-k+q}^{-}\rangle\!\rangle_\omega = (2\langle S_0^z\rangle/N^{1/2})\delta(\omega - \omega_{k-q}) \tag{60}
$$

$$
-(1/\pi)\,\mathrm{Im}\langle\!\langle a_{p\sigma}^{+} a_{p+q\sigma} | a_{p'\sigma}^{+} a_{p'-q\sigma}\rangle\!\rangle_\omega = (n_{p\sigma} - n_{p'\sigma})\delta(\omega + \varepsilon_{p\sigma} - \varepsilon_{p'\sigma})\delta_{p',p+q} \tag{61}
$$

in the RHS of (59) and get (cf Christoph *et al* 1982)

$$
\langle\!\langle A|A^+\rangle\!\rangle_\omega^{\mathrm{ir,c}} = \frac{2\langle S_0^z\rangle}{N^{3/2}} \sum_q (J_q - J_{k-q})^2 \int_{-\infty}^{+\infty} \mathrm{d}\omega'\, \frac{1 + \nu(\omega') + \nu(\omega_{k-q})}{\omega - \omega' - \omega_{k-q}}\, m_q^{zz}(\omega')
$$

$$
+ 2\frac{\langle S_0^z\rangle}{N^{1/2}} \frac{I^2}{N^2} \sum_{pq\sigma} \frac{(1 + \nu(\omega_{k-q}))n_{p+q\sigma}(1 - n_{p\sigma}) - \nu(\omega_{k-q})n_{p\sigma}(1 - n_{p+q\sigma})}{\omega - \omega_{k-q} + \varepsilon_{p+q\sigma} - \varepsilon_{p\sigma}}
$$

$$
+ 4\frac{I^2}{N^2} \sum_{pq} \int_{-\infty}^{+\infty} \mathrm{d}\omega'\, \frac{(1 + \nu(\omega'))n_{p-q\uparrow}(1 - n_{p\downarrow}) - \nu(\omega')n_{p\downarrow}(1 - n_{p+q\uparrow})}{\omega - \omega' + \varepsilon_{p-q\uparrow} - \varepsilon_{p\downarrow}}
$$

$$
\times\, m_{k-q}^{zz}(\omega') \tag{62}
$$

where the first term describes the magnon–magnon inelastic scattering and the others account for the magnon–electron scattering. The concrete calculations need a suitable assumption for the longitudinal spin susceptibility. For this one can use the Cottam (1977) result.

In order to calculate the damping of the magnetic excitations in the ferromagnetic semiconductor it is necessary to take into account all matrix elements of the self-energy operator $\hat{\Pi} = |\Pi_{ij}|$:

$$
\Pi_{11} = (I^2/N\Omega_2^2)\langle\!\langle A|A^+\rangle\!\rangle_\omega^{\mathrm{ir,c}} \tag{63}
$$

$$
\Pi_{12} = \Pi_{21}^* = -\frac{1}{N^{3/2}\chi_0^{\mathrm{df}}\Omega_2} \sum_q \frac{1}{\omega_{q,k}} \langle\!\langle A|B^+\rangle\!\rangle_\omega^{\mathrm{ir,c}} \tag{64}
$$

$$
\Pi_{22} = \frac{1}{N^2(\chi_0^{\mathrm{df}})^2} \sum_{pq} \frac{1}{\omega_{p,k}\omega_{q,k}} \langle\!\langle B_p|B_q^+\rangle\!\rangle_\omega^{\mathrm{ir,c}}. \tag{65}
$$

Then the matrix GF R becomes

$$
\hat{R} = [(\hat{R}^{(0)})^{-1} - \hat{\Pi}]^{-1}
$$

$$
= \frac{1}{\det[(\hat{R}^{(0)})^{-1} - \hat{\Pi}]} \left\| \begin{array}{cc} \dfrac{\langle\!\langle S_k^+|S_{-k}^-\rangle\!\rangle_\omega}{\det \hat{R}^{(0)}} - \Pi_{22} & -\left(\dfrac{\langle\!\langle S_k^+|\sigma_{-k}^-\rangle\!\rangle_\omega}{\det \hat{R}^{(0)}} + \Pi_{12}\right) \\[2ex] -\left(\dfrac{\langle\!\langle \sigma_k^+|S_{-k}^-\rangle\!\rangle_\omega}{\det \hat{R}^{(0)}} + \Pi_{21}\right) & \dfrac{\langle\!\langle \sigma_k^+|\sigma_{-k}^-\rangle\!\rangle_\omega}{\det \hat{R}^{(0)}} - \Pi_{11} \end{array} \right\| \tag{66}
$$

and the spin GF gets the form

$$
\langle\!\langle S_k^+|S_{-k}^-\rangle\!\rangle_\omega = [(\langle\!\langle S_k^+|S_{-k}^-\rangle\!\rangle_\omega^0)^{-1} - \Sigma(k, \omega)]^{-1} \tag{67}
$$

where $\Sigma(k, \omega)$ is given by

$$
\Sigma(k, \omega) = \Pi_{11} - (I/N^{1/2} \det \hat{R}^{(0)} - \Pi_{12})(I/N^{1/2} \det \hat{R}^{(0)} - \Pi_2)
$$
$$
\times [(1 - U\chi_0^{df})/N\chi_0^{df} \det \hat{R}^{(0)} + \Pi_{22}]^{-1}
$$
$$
\times I^2 \chi_0^{df}/(1 - U\chi_0^{df}) \det \hat{R}^{(0)}. \tag{68}
$$

The GF (67) contains acoustical and optical magnon excitations as well as a Stoner-like continuum of excitations damped by magnon–magnon, electron–electron and electron–magnon inelastic scattering processes. For brevity we only present the calculation of the acoustical magnon damping. For small k and ω the linear terms in Π_{ij} are essential and we find

$$
\langle\!\langle S_k^+|S_{-k}^-\rangle\!\rangle_\omega = (2\langle S_0^z\rangle/N^{1/2})[\omega - \omega_k - (2\langle S_0^z\rangle/N^{1/2})\Sigma(k, \omega)]^{-1} \tag{69}
$$

$$
\Sigma(k, \omega) = \Pi_{11} + (\Pi_{12} + \Pi_{21})N^{1/2}I\chi_0^{df}/(1 - U\chi_0^{df})
$$
$$
+ [NI^2(\chi_0^{df})^2/(1 - U\chi_0^{df})^2]\Pi_{22}. \tag{70}
$$

Then the spectral density of the spin wave excitations with wave-vector k reads

$$
-(1/\pi) \operatorname{Im}\langle\!\langle S_k^+|S_{-k}^-\rangle\!\rangle_\omega
$$
$$
= 2N^{-1/2}\langle S_0^z\rangle\Gamma(k, \omega)/[(\omega - \omega_k - \Delta(k, \omega))^2 + \Gamma^2(k, \omega)] \tag{71}
$$

where the expressions

$$
\Delta(k, \omega) = (2\langle S_0^z\rangle/N^{1/2}) \operatorname{Re}\Sigma(k, \omega) \tag{72}
$$

and

$$
\Gamma(k, \omega) = -(2\langle S_0^z\rangle/N^{1/2}) \operatorname{Im}\Sigma(k, \omega) \tag{73}
$$

describe the shift and damping of the acoustical magnons respectively.

Finally we shall estimate the temperature dependence of $\Gamma(k, \omega)$ due to electron–magnon scattering at low temperatures. We have

$$
\operatorname{Im} \Pi_{11} \sim \sum_{pq\sigma} \nu(\omega_{k+q})(n_{p+q\sigma} - n_{p\sigma})\delta(\omega - \omega_{k+q} + \varepsilon_{p+q\sigma} - \varepsilon_{p\sigma}). \tag{74}
$$

If one substitutes

$$
\sum_{pq} \to \frac{V}{(2\pi)^6} \int \mathrm{d}p \int \mathrm{d}q \tag{75}
$$

and expands in powers of q, it follows that

$$\text{Im}\,\Pi_{11} \sim \frac{V^2}{(2\pi)^6}\, 2\pi \int \mathrm{d}\boldsymbol{p} \int_0^{q\max} q^2\, \mathrm{d}q \int \mathrm{d}\cos\theta\, \varphi(n_{p\sigma}, \nu(\omega_q)) \frac{\delta(\cos\theta - \cos\theta_0)}{q|\partial\varepsilon_{p\sigma}/\partial\boldsymbol{p}|}$$

$$\sim \frac{1}{2\beta D_{ac}} \int_0^{\beta\omega\max} \mathrm{d}x\, \frac{1}{e^x - 1} \sim T. \tag{76}$$

The other contributions to $\Sigma(\boldsymbol{k}, \omega)$ can be treated in the same manner. So the electron–magnon low-temperature dependence of $\Gamma(\boldsymbol{k}, \omega)$ is

$$\Gamma(\boldsymbol{k}, \omega) \sim \Gamma_1 T \tag{77}$$

where $\Gamma_1 \to 0$ in the limit $k, \omega \to 0$.

7. Conclusions

The Hamiltonian of the s–f model, as given in the text, is the simplest theoretical model for studying magnetically ordered semiconductors. In this paper we use the IGF method as a unified and self-consistent formalism for the full description of the electronic and magnetic spectra of wide-band semiconductors including electron–magnon, electron–electron and magnon–magnon scattering processes. The importance of the results presented is certainly not in the application to any concrete substance—their interest is of a more fundamental nature. They contain a complete picture of the quasiparticle inelastic scattering in systems with many-branch spectra of excitations and can be applied to other models. Let us point out also that the s–f model with an additional Hubbard interaction term can be useful for some transition and rare-earth metals and their compounds (cf Christoph *et al* 1982). The formalism developed in this paper can be extended to antiferromagnetic semiconductors and applied to the magnetic polaron problem.

Appendix

Let us write the one-electron spectral density (19) in the form (Kuzemsky 1978)

$$g_{k\sigma}(\omega) = (1/\pi)\Gamma_{k\sigma}(\omega)/[(\omega - \varepsilon_{k\sigma})^2 + \Gamma_{k\sigma}^2(\omega)] \simeq (1 - a_{k\sigma})\delta(\omega - \varepsilon_{k\sigma})$$

$$+ (1/\pi)\Gamma_{k\sigma}(\omega)/(\omega - \varepsilon_{k\sigma})^2 \tag{A1}$$

where the unknown constant $a_{k\sigma}$ is defined by the condition

$$\int_{-\infty}^{+\infty} g_{k\sigma}(\omega)\, \mathrm{d}\omega = 1. \tag{A2}$$

Then within this approximation for the average electron occupation numbers we get

$$n_\sigma = \frac{1}{N} \sum_k n(\varepsilon_{k\sigma}) + \frac{I^2}{N^2} \sum_{kq} \frac{n(\varepsilon_{k+q\sigma}^0) - n(\varepsilon_{k\sigma})}{(\varepsilon_{k+q\sigma}^0 - \varepsilon_{k\sigma})^2} K_q^{zz}$$

$$+ \frac{I^2}{N^2} \sum_{kq} \frac{n(\varepsilon_{k+q,-\sigma}^0 - z_\sigma\omega_q) - n(\varepsilon_{k\sigma})}{(\varepsilon_{k+q,-\sigma}^0 - z_\sigma\omega_q - \varepsilon_{k\sigma})^2}$$

$$\times \left(K_q^{-\sigma,\sigma} - {}_\sigma\frac{2\langle S_0^z\rangle}{N^{1/2}} n(\varepsilon_{k+q,-\sigma}^0 + z_\sigma\omega_{q'}) \right). \tag{A3}$$

As follows from equation (A3), they are determined in a self-consistent way. The first term in the RHS describes the effects of renormalising the particle energies and the subsequent terms account for the particle scattering by the fluctuations of the magnetic moment in the second order of I and explicitly include the damping of the electronic states. Equation (A1) conserves the first four moments in the second order of I and in the low-concentration limit we have

$$M^{(0)} = \int_{-\infty}^{-\infty} g_{k\sigma}(\omega)\, d\omega = 1 \tag{A4}$$

$$M^{(1)} = \int_{-\infty}^{+\infty} \omega g_{k\sigma}(\omega)\, d\omega = \varepsilon_{k\sigma}^0, \tag{A5}$$

$$M^{(2)} = \int_{-\infty}^{+\infty} \omega^2 g_{k\sigma}(\omega)\, d\omega$$

$$= (\varepsilon_{k\sigma}^0)^2 + \frac{I^2}{N}\sum_q \left(K_q^{zz} + K_q^{-+} + \frac{2\langle S_0^z\rangle}{N^{1/2}}(\delta_{\sigma\downarrow} + z_0 n(\varepsilon_{k+q,\sigma}^0)) \right)$$

$$= (\varepsilon_{k\sigma}^0)^2 + I^2(S - z_0\langle S^z\rangle)(S + z_\sigma\langle S^z\rangle + 1) = (\varepsilon_{k\sigma}^0)^2 + I^2(D_2 + D_{1\sigma}) \tag{A6}$$

$$M^{(3)} = \int_{-\infty}^{+\infty} \omega^3 g_{k\sigma}(\omega)\, d\omega = (\varepsilon_{k\sigma}^0)^3 + I^2 \left(2\varepsilon_k D_\sigma + \frac{1}{N}\sum_q \varepsilon_{k+q}(K_q^{zz} + K_q^{-\sigma,\sigma}) \right)$$

$$+ I^3[2z_\sigma\langle S^z\rangle(\langle S^z\rangle^2 - R_0 - \tfrac{1}{2}D_{1\sigma}) - z_0\langle S^z\rangle D_2] \tag{A7}$$

$$M^{(4)} = \int_{-\infty}^{+\infty} \omega^4 g_{k\sigma}(\omega)\, d\omega = (\varepsilon_{k\sigma}^0)^4 + I^2 \left(3\varepsilon_k^2 D_\sigma + 2\varepsilon_k \frac{1}{N}\sum_q \varepsilon_{k+q}(k_q^{zz} + k_{q'}^{-\sigma,\sigma}) \right.$$

$$\left. + \frac{1}{N}\sum_q \varepsilon_{k+q}^2(K_q^{zz} + K_q^{-\sigma,\sigma}) \right) - I^3 \left(4z_0\varepsilon_k\langle S^z\rangle D_\sigma + z_\sigma \frac{2\langle S^z\rangle}{N} \right.$$

$$\times \sum_q \varepsilon_{k+q}(K_q^{zz} + K_q^{-\sigma,\sigma})$$

$$\left. + z_\sigma \frac{2\langle S^z\rangle}{N}\sum_q \varepsilon_{k+q}(K_q^{zz} - K_q^{-\sigma,\sigma}) \right) + 4I^4\langle S^z\rangle^2 D_\sigma \tag{A8}$$

where

$$K_q^{-\sigma,\sigma} = (2\langle S_0^z\rangle/N^{1/2})(\delta_{\sigma\downarrow} + \nu(\omega_q)) \qquad \langle S^z\rangle = N^{-1/2}\langle S_0^z\rangle \qquad D_2 = S^2 - \langle S^z\rangle^2$$

$$D_{1\sigma} = S - z_\sigma\langle S^z\rangle \qquad R_o = \langle (S^z)^2\rangle \qquad D_\sigma = \frac{1}{N}\sum_q (K_q^{zz} + K_q^{-\sigma,\sigma}).$$

Thus the first four moments calculated with the spectral density (A1) coincide with the exact moments in the second order of I in the low-concentration limit.

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