Electronic Spectrum of a Magnetic Semiconductor in the *s-f* Exchange Model Approximation

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The electronic spectrum of a magnetic semiconductor has been analysed in the *s-f* exchange model approximation using the irreducible Green function method. An analytic expression of the electronic self-energy operator has been obtained and it may be used to find a self-consistent procedure in separate specific cases. The electronic spectrum of a wide-band magnetic semiconductor has been studied in detail.

I. The magnetic semiconductor is an example of a physical system whose properties are defined by the interaction between two electronic subsystems. The current carriers (the "*s*-electrons") interact with the magnetic moments of the partially filled *f*- (d-) atomic shells. The magnetic alignement affects the movement of the currents carriers by re-normalizing their energy spectrum and these carriers on their turn affect the magnetic alignement.

The typical magnetic semiconductors (the europium chalcogenides for example) may be considered within the *s-f*-exchange model approximation [1—3] with the Hamiltonian

$$H = H_s + H_f + H_{sf} \tag{1}$$

where H_s is the kinetic energy operator for the band electrons

$$H_s = \sum_{k\sigma} t(k)\, a^+_{k\sigma} a_{k\sigma}. \tag{2}$$

H_f describes the behaviour of the localized magnetic moments within the Heisenberg approximation.

$$H_f = -\frac{1}{4} \sum_q J(-q)\,]S^+_q S^-_{-q} + S^-_q S^+_{-q} + 2S^z_q S^z_{-q}], \tag{3}$$

and H_{sf} defines the spin-spin interaction between the two subsystems

$$H_{\delta f} = \frac{I}{\sqrt{N}} \sum_{k,q} \{S^+_{-q} a^+_{k\downarrow} a_{k+q\uparrow} + S^-_{-q} a^+_{k\uparrow}\, a_{k+q\downarrow} + S^z_{-q} (a^+_{k\uparrow} a_{k+q\uparrow} - a^+_{k\downarrow} a_{k+q\downarrow})\} \tag{4}$$

(all notations in formulae (2)—(4) have their generally accepted meaning).

The total Hamiltonian H represents the simplest starting point for the theoretical consideration of the magnetic semiconductors. Despite that, the problem is a many-body one and it cannot be solved exactly. Additional simplifying assumptions are needed for that purpose. Thus, at low temperatures the magnetic subsystem may be considered in the spin-wave approximation and the effect of electron-magnon interaction on the electron bands may be accounted for in various ratios between the Hamiltonian parameters [4—6]. At higher temperatures, when the spin-wave approximation is no longer valid, the magnetic sublattice may be considered as a static system and its effect on the

conduction electrons is defined by an effective field which is proportional to the magnetization and the static spin-correlation functions [7, 8]. In fact, such a simplification is possible since the magnetic excitation energies are low with respect to the electronic energies [2]. A detailed review of the results obtained thus far and the methods used is contained in the references [1—3].

The *s-f* exchange interaction affects substantially the electronic spectrum of the magnetic semiconductor at temperatures lower than the temperature of magnetic phase transition. The re-normalized conduction electron energies are temperature dependent and the electronic states have a finite life time [8]. These effects are most suitably accounted for by the Green function method [9]. The purpose of the present work is to find the electronic quasi-particle spectrum re-normalized by the *s-f* exchange in a wide temperature range and to account explicitly for the contribution of damping of the electronic states when calculating the various characteristics of the magnetic semiconductor. By the variant of the irreducible Green function method [10, 11] a closed expression has been obtained for the electron selfenergy operator at arbitrary H parameter values. This representation provides a possibility to find a self-consistent procedure when obtaining various approximate expressions in the separate specific cases.

2. The single-particle properties of the band electron system are defined by the anticommutating Green function

$$G_{k\sigma}(t)=\langle\langle a_{k\sigma}(t)\mid a^{+}_{k\sigma}\rangle\rangle,$$

where k *is* the electron wave vector and σ is the z-th component of its spin Its Fourier transform $G_{k\sigma}(E)$ satisfies the equation

$$(5)\quad EG_{k\sigma}(E)=1+t(k)G_{k\sigma}(E)-\frac{I}{\sqrt{N}}\sum_{q}\{\langle\langle S^{-\sigma}_{-q}a_{k+q,-\sigma}\mid a^{+}_{k\sigma}\rangle\rangle+Z_{\sigma}\langle\langle S^{z}_{-q}a_{k+q,\sigma}\mid a^{+}_{k\sigma}\rangle\rangle\}$$

where $Z_{\sigma}=1(-1)$ if $\sigma=\uparrow(\downarrow)$ or $+(-)$.

The irreducible (ir) Green functions will be introduced in the right side of eqn. (5) by the relation

$$(6)\qquad (S^{z}_{-q})^{\mathrm{ir}}=S^{z}_{-q}-\langle S^{z}_{0}\rangle\delta_{q,0}\,.$$

Thus, eqn. (5) may be written in the form

$$(7)\quad [E-\varepsilon^{\mathrm{MF}}_{k\sigma}]G_{k\sigma}(E)=1-\frac{I}{\sqrt{N}}\sum_{q}\{\langle\langle S^{-\sigma}_{-q}a_{k+q,-\sigma}\mid a^{+}_{k\sigma}\rangle\rangle+Z_{\sigma}\langle\langle (S^{z}_{-q})^{\mathrm{ir}}a_{k+q,\sigma}\mid a^{+}_{k\sigma}\rangle\rangle,$$

where

$$(8)\qquad \varepsilon^{\mathrm{MF}}_{k\sigma}=t(k)-Z_{\sigma}\frac{I}{\sqrt{N}}\langle\langle S^{z}_{0}\rangle.$$

Relation (6) shows that the irreducible Green functions do not contain the mean field re-nomalizations. This provides a possibility to re-formulate the standard procedure of the two-time temperature Green functions [9], to write the Dyson equation and to obtain an exact analytical representation of the self-enegy operator. Then, the approximate solutions for the Green function will be written as definite approximations for the self-energy operator [10, 11].

The equations for the higher-order Green functions on the right side of equality (7) can be written in a similar manner:

$$(9)\quad [E-\varepsilon^{\mathrm{MF}}_{k\sigma}]\langle\langle A\mid a^{+}_{k\sigma}\rangle\rangle=-\frac{I}{\sqrt{N}}\sum_{q'}\{\langle\langle A\mid S^{\sigma}_{q'}a^{+}_{k+q',-\sigma}\rangle\rangle+Z_{\sigma}\langle\langle A\mid (S^{z}_{q'})^{\mathrm{ir}}a^{+}_{k+q,\sigma}\rangle\rangle\},$$

where

$$A=\left\{\begin{array}{l} S_{-q}^{-\sigma}\, a_{k+q,\,-\sigma} \\ (S_{-q}^{z})^{\mathrm{ir}}\ \ a_{k+q,\,\sigma} \end{array}\right\}.$$

It follows from (7) and (9) that $G_{k\sigma}(E)$ satisfies the equation

$$G_{k\sigma}(E)=G_{k\sigma}^{\mathrm{MF}}(E)+G_{k\sigma}^{\mathrm{MF}}(E)P_{k\sigma}(E)G_{k\sigma}^{\mathrm{MF}}(E). \tag{10}$$

The zero-order Green function

$$G_{k\sigma}^{\mathrm{MF}}(E)=(E-\varepsilon_{k\sigma}^{\mathrm{MF}})^{-1}$$

takes into account the mean molecular field acting by the localized spin on the condition electrons and the scattering operator $P_{k\sigma}(E)$ is related to the self-energy operator $M_{k\sigma}(E)$ through the equation

$$P_{k\sigma}(E)=M_{k\sigma}(E)+M_{k\sigma}(E)G_{k\sigma}^{\mathrm{MF}}(E)P_{k\sigma}(E),$$

which, together with the Dyson equation for $G_{k\sigma}(E)$

$$G_{k\sigma}(E)=G_{k\sigma}^{\mathrm{MF}}(E)+G_{k\sigma}^{\mathrm{MF}}(E)M_{k\sigma}(E)G_{k\sigma}(E) \tag{11}$$

produces following expression of $M_{k\sigma}(E)$:

$$M_{k\sigma}(E)=\frac{I^2}{N}\sum_{qq'}\{\langle\langle S_{-q}^{-\sigma}a_{k+q,-\sigma}|\, S_{q'}^{\sigma}a_{k+q',\,-\sigma}^{+}\rangle\rangle^{(\mathrm{P})}+\langle\langle (S_{-a}^{z})^{\mathrm{ir}}a_{k+q,\,\sigma}\,|\,(S_{q'}^{z})^{\mathrm{ir}}a_{k+q',\,\sigma}^{+}\rangle\rangle^{(\mathrm{P}}$$

$$+Z_{\sigma}[\langle\langle S_{-q}^{-\sigma}a_{k+q-\sigma}|\,(S_{q'}^{z})^{\mathrm{ir}}\,a_{k+q',\sigma}^{+}\rangle\rangle^{(\mathrm{P})}+\langle\langle (S_{-q}^{z})^{\mathrm{ir}}\,a_{k+q,\,\sigma}\,|\,S_{q'}^{\sigma}a_{k+q',-\sigma}^{+}\rangle\rangle^{(\mathrm{P})}]\}, \tag{12}$$

e. $M_{k\sigma}$ corresponds to the "proper part" of the scattering operator $P_{k\sigma}$.

The equality (12) defines an exact representation of the self-energy operator $M_{k\sigma}$ by the higher-order Green functions taking into account the various correlation effects between the two electronic subsystems of the magnetic semiconductor. For this reason a similar treatment has to be done also for the localized spin system which may provide suitable self-consistent solutions. For the Fourier transform of the "transverse" Green spin function $F_q(E)=\langle\langle S_q^{+}\,|\,S_{-q}^{-}\rangle\rangle$ an equation such as (11) is obtained:

$$F_q(E)=F_q^{\mathrm{MF}}(E)+F_q^{\mathrm{MF}}(E)\,\Pi_q(E)F_q(E), \tag{13}$$

where

$$F_q^{\mathrm{MF}}(E)=\frac{2\langle S_0^z\rangle}{\sqrt{N}}\ \frac{1}{E-\omega(q)}, \tag{14}$$

and

$$\omega(q)=\frac{\langle S_0^z\rangle}{\sqrt{N}}(J_0-J_q)+\frac{1}{\sqrt{N}}\sum_{q'}(J_{q'}-J_{q-q'})\frac{2K_{q'}^{zz}+K_{q'}^{-+}}{2\langle S_0^z\rangle}+\frac{I}{N}(n_{\uparrow}-n_{\downarrow}) \tag{15}$$

and $\Pi_q(E)$ is the self-energy operator whose explicit form in terms of the higher order irreducible Green functions will not be given here. Expressions (14) and (15) define the properties of the localized spin system within the Hartree-Fock approximation. The first two terms in the spin excitation energy $\omega(q)$ originate by the Heisenberg Hamiltonian [10, 12], and the third term takes into account

the molecular field spin-polarized conduction electrons ($n_\uparrow$ and $n_\downarrow$ are the average number of spin-up and spin-down electrons, respectively, and K_q^{zz} and K_q^{-+} are the spin correlators.

3. The self-consistent field definition of the electronic self-energy operator requires its approximate reppresentation by the lower-order Green functions. Since $M_{k\sigma}$ describes the processes of inelastic scattering of the conduction electrons over the localized spins, its approximate representation would be defined by the nature of the physical assumptions about this scattering. We shall consider the approximate representation of the irreducible functions such as $\langle\langle S^\alpha_{-q} a_{k+q,\sigma} \mid S^\beta_q, a_{k+q',\sigma}\rangle\rangle^{(\mathrm{ir})}$. By the spectral theorem [9], we obtain

$$\langle\langle S^\alpha_{-q} a_{k+q,\sigma} \mid S^\beta_q, a^+_{k+q',\sigma}\rangle\rangle^{(\mathrm{ir})} = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{dE'}{E-E'}(e^{\tilde{\beta}E'}+1)$$

(16)

$$\times \int_{-\infty}^{+\infty} dt\, e^{iE't}\langle S^\beta_q, a^+_{k+q',\sigma} S^\alpha_{-q}(t) a_{k+q,\sigma}(t)\rangle^{\mathrm{ir}}.$$

Here $\tilde{\beta}=(k_BT)^{-1}$ where k_B is the Boltzmann constant and T is the absolute temperature. The correlation function in (16) may be decoupled in the following manner:

(17) $$\langle\langle S^\beta_{q'} a^+_{k+q',\sigma} S^\alpha_{-q}(t) a_{k+q,\sigma}(t)\rangle\rangle \simeq \langle S^\beta_q S^\alpha_{-q}(t)\rangle \langle a^+_{k+q,\sigma} a_{k+q,\sigma}(t)\rangle.$$

The approximate representation (17) neglects the correlation between the conduction electrons and the magnetic subsystem excitations and it is legitimate at lower densities of the quasiparticles. Further, from the definition of irreducibility for the operators, it follows that only averages of products from such operators referring to different times contribute since the "single time" averages have already been accounted for by the zero order Green functions. Expressing the correlation functions on the right side of equality (17) using the spectral theorem, we can find within the chosen approximation the contribution of the function $\langle\langle S^\alpha_{-q} a_{k+q,\sigma} \mid S^\beta_q a^+_{k+q',\sigma}\rangle\rangle^{(\mathrm{ir})}$ to the self-energy operator $M_{k\sigma}$:

$$M^{\alpha\beta}_{k\sigma}(E) = \frac{I^2}{N}\sum_{qq'}\langle\langle S^\alpha_{-q} a_{k+q,\sigma} \mid S^\beta_{q'} a^+_{k+q',\sigma}\rangle\rangle^{(\mathrm{ir})}$$

(18) $$= \frac{I^2}{N}\sum_q \int_{-\infty}^{+\infty} dE_1 \int_{-\infty}^{+\infty} dE_2 \frac{1+\nu(E_1)-n(E_2)}{E-E_1-E_2} m^{\alpha\beta}_q(E_1) g_{k+q,\sigma}(E_2),$$

where $m^{\alpha\beta}_q(E)$ and $g_{k\sigma}(E)$ are the one-paricle spectral densities defined through the equalities

$$m^{\alpha\beta}_q(E) = -\frac{1}{\pi}\mathrm{Im}\langle\langle S^\alpha_{-q} \mid S^\beta_{q'}\rangle\rangle, \quad g_{k\sigma}(E) = -\frac{1}{\pi}\mathrm{Im}\langle\langle a_{k\sigma} \mid a^+_{k\sigma}\rangle\rangle,$$

and $\nu(E)$ and $n(E)$ are the corresponding Bose and Fermi type functions, respectively:

$$\nu(E) = (e^{\tilde{\beta}E}-1)^{-1}, \quad n(E) = (e^{\tilde{\beta}E}+1)^{-1}.$$

The resulting representation of the higher-order Greer functions takes into account the dynamic nature of the interaction between the electrons and the localized spins. Another approach is possible when simplifying the functions (16). Let us assume that the process of electron scattering does not produce changes in the energy state of the magnetic subsystem of the semiconductor, i. e. the scattering is elastic. Then the spin correlation function on the right side of equality (17) may be approximated by its value at $t=0$

$$K_q^{\beta\alpha}(t)=\langle S_q^\beta S_{-q}^\alpha(t)\rangle \simeq \langle S_q^\beta S_{-q}^\alpha\rangle = K_q^{\beta\alpha}$$

and

$$M_{k\sigma}^{\alpha\beta}(E)=\frac{I^2}{N}\sum_q K_q^{\beta\alpha}\int_{-\infty}^{+\infty} dE' \frac{g_{k+q,\sigma}(E')}{E-E'}. \tag{19}$$

Finally, for the self-energy operator $M_{k\sigma}$ of the one-particle electronic Green function we may write

$$M_{k\sigma}(E)=\frac{I^2}{N}\sum_q \left\{ K_q^{zz}\int_{-\infty}^{+\infty}\frac{dE'}{E-E'} g_{k+q,\sigma} + \int_{-\infty}^{+\infty} dE_1 \int_{-\infty}^{+\infty} dE_2 \frac{1+\nu(E_1)-n(E_2)}{E-E_1-E_2} m_q^{-\sigma,\sigma}(E_1)\, g_{k+q,-\sigma}(E_2) \right\}. \tag{20}$$

whose structure, taking into account the relations (18) and (19) speaks about the physical nature of the assumptions made.

When determining the electronic spectrum, the characteristics of the magnetic subsystem K_q^{zz} and $m_q^{-\sigma,\sigma}(E)$ may be chosen in a suitable way. Then, equations (11) and (20) form a closed system for the one electron Green function $G_{k\sigma}(E)$. By setting the spectral density $g_{k\sigma}(E)$ in the right side of equality (20), $G_{k\sigma}(E)$ may be found and the result obtained may be used in the following, more accurate, representation of $g_{k\sigma}(E)$.

4. In comparison with other works, let us consider the case of a wide-band ferromagnetic semiconductor for which a well-defined small parameter is present $IS/W \ll 1$ (W is the conduction band width, defined by $t(k)$, I is the exchange integral and S is the spin localized at the crystal lattice sites). Then, as a reasonable initial approximation for one particle spectral density $g_{k\sigma}(E)$, the following pole representation may be used:

$$g_{k\sigma}(E)=\delta(E-\varepsilon_{k\sigma}^{\mathrm{MF}}) \tag{21}$$

where $\varepsilon_{k\sigma}^{\mathrm{MF}}$ is defined by the expression (8). Setting $m_q^{-\sigma,\sigma}(E)$ in the Hartree Fock approximation (14)

$$m_q^{-\sigma,\sigma}(E)=Z_{-\sigma}\frac{2\langle S_0^z\rangle}{\sqrt{N}}\delta[E-Z_{-\sigma}\omega(q)] \tag{22}$$

the static spin transverse correlators are defined by the equation

$$K_q^{-\sigma,\sigma}=\frac{2\langle S_0^z\rangle}{\sqrt{N}}[\delta_{\sigma\downarrow}-\nu(\omega(q)] \tag{23}$$

and substituting the expressions (21)—(23) into eqn (20) we obtain the self-energy operator in the following form:

$$M_{k\sigma}(E)=\frac{I^2}{N}\sum_q{}'\left[\frac{K_q^{zz}}{E-\varepsilon^{MF}_{k+q,\sigma}}+\frac{K_q^{-\sigma,\sigma}+2\frac{\langle S_0^z\rangle}{\sqrt{N}}n\left[\varepsilon^{MF}_{k+q,-\sigma}-Z_\sigma\omega(q)\right]}{E+Z_\sigma\omega(q)-\varepsilon^{MF}_{k+q,-\sigma}}\right] \tag{24}$$

In expression (24) the first term describes the contribution of the band electron scattering processes without change in the electron spin and the second term accounts for the spin flip processes. It is further seen that within the approximation used, the self-energy operator $M_{k\sigma}$ dependes on the number of electrons only when the dynamic nature of the *s-f* exchange is accounted for and just at temperatures lower than the critical one, when $\langle S_0^z\rangle\neq 0$. Representation (24) thus generalizes the results obtained in refs. [4, 7, 13].

The real part of the self-energy operator defines the electronic spectrum, $E_{k\sigma}$ re-normalized by the *s-f* exchange. This spectrum is given as a solution of the equation

$$E_{k\sigma}=\varepsilon^{MF}_{k\sigma}+\mathrm{Re}\,M_{k\sigma}(E),$$

and its imaginary part $\Gamma_{k\sigma}(E)$ defines the damping of the electronic states and affects the density of states. Following [14], let us write the one-particle spectral density $g_{k\sigma}(E)$ in the following way

$$g_{k\sigma}(E)=-\frac{1}{\pi}\,\mathrm{Im}\,G_{k\sigma}(E)=\frac{1}{\pi}\,\frac{\Gamma_{k\sigma}(E)}{(E-E_{k\sigma})^2+\Gamma^2_{k\sigma}(E)}$$

$$\approx(1-a_{k\sigma})\delta(E-E_{k\sigma})+\frac{1}{\pi}\frac{\Gamma_{k\sigma}E}{(E-E_{k\sigma})^2} \tag{25}$$

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

$$\int_{-\infty}^{+\infty}g_{k\sigma}(E)dE=1.$$

Then, within this approximation for the average occupation numbers for states with spin σ we get

$$n_\sigma=\frac{1}{N}\sum_k n(E_{k\sigma})=\frac{I^2}{N^2}\sum_{k,q}{}'\frac{K_q^{zz}}{(\varepsilon^{MF}_{k+q,\sigma}-E_{k\sigma})^2}\{n(\varepsilon^{MF}_{k+q,\sigma})-n\{E_{k\sigma})\}$$

$$+\frac{I^2}{N^2}\sum_{k,q}{}'\frac{K_q^{-\sigma,\sigma}+Z_\sigma\frac{2\langle S_0^z\rangle}{\sqrt{N}}n\left[\varepsilon^{MF}_{k+q,-\sigma}-Z_\sigma\omega(q)\right]}{(\varepsilon^{MF}_{k+q,-\sigma}-Z_\sigma\omega(q)-E_{k\sigma})^2}\{n[\varepsilon^{MF}_{k+,-\sigma}-Z_\sigma\omega(q)]-n(E_{k\sigma})\}. \tag{26}$$

As follows from eqn (26), the occupation numbers are determined in a self-consistent way. The first term on the right side describes the effects of re-normalizing the particle energies and the subsequent terms account for the particle scattering by the fluctuations of the magnetic moment in second order of I and explicitly account for the damping of the electronic states. The form of

the one particle spectral density obtained in (25) at low temperatures is analogous to the Nolting representation based on considerations of intuitive nature [15]. This form may be used to find analytically the spectral density moments, whose explicit form may be found also in an independent way [8, 16].

Expression (24) may be used to reproduce exactly the first three moments of the single-particle spectral density. As known [8, 16], this result may be carried out by the following two-pole approximation

$$g_{k\sigma}(E)=\frac{S+Z_\sigma\langle S^z\rangle+1}{2S+1}\,\delta(E+IS-t(k))+\frac{S-Z_\sigma\langle S^z\rangle}{2S+1}\,\delta(E-I(S+1)-t(k)),$$

which corresponds to two undamping quasi-particle bands. In our opinion, the description of the electronic spectrum taking into account the damping of the quasi-particle states corresponds more accurately to the physical nature of the phenomena taking place in the wide-band ferromagnetic semiconductor.

References

1. Krisement, O. — J. Magn. Magn. Mater., **3** (1976), 7.
2. Nolting, W. — Phys. Stat. Sol. (b), **96** (1979), 11.
8. Nagaev, E. L. — Physics of Magnetic Semiconductors, Moskow, 1979 (in Russian).
4. Woolsey, R. B., R. M. White. — Phys. Rev. B, **1** (1970), 4474.
5. Sriram Shastry, B., D. C. Mattis. — Phys. Rev. B, **24** (1981), 5340.
6. Allan, S. R., D. M. Edwards. — J. Phys. C, **15** (1982), 2151.
7. Sinkonen, J. — Phys. Rev. B, **19** (1979), 6407.
8. Nolting, W., A. M. Oleś. — Phys. Rev. B, **22** (1980), 6184.
9. Zubarev, D. N. — Usp. Fiz. Nauk, **71** (1960), 71 [Sov. Phys. Usp., **3** (1960), 320].
10. Plakida, N. M. — Phys. Lett. A, **43** (1973), 481.
11. Kuzemsky. A. L. — Theor. Math. Phys., **36** (1978), 208.
12. Mubayi, V., R. V. Lange. — Phys. Rev., **178** (1969), 882.
13. Rys, F., J. S. Helman, W. Baltensberger. — Phys. Kondens, Materie, **6** (1967 105.
14. Tyablikov, S. V. Methods in the Quantum Theory of Magnetism, Moskow, 1975 (in Russian).
15. Nolting, W. — Phys. Stat. Sol. (b), **79** (1977), 573.
16. Čapek, V. — Phys. Stat. Sol. (b), **103** (1981), 107.

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Электронный спектр магнитного полупроводника в приближении обменной *s-f* модели

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(Резюме)

В настоящей работе анализируется электронный спектр магнитного полупроводника в приближении обменной $s-f$ модели путем использования метода неприводимых функций Грина. Получено аналитическое представление электронного массового оператора, что дает возможность построения самосогласованной процедуры в отдельных конкретных случаях. Подробно исследуется электронный спектр широкозонного магнитного полупроводника.