Diluted magnetic $A_{1-x}Mn_xB$ semiconductors

V.P. Bryksa1, G.G. Tarasov2, W.T. Masselink2, W. Nolting2, Yu.I. Mazur3 and G.J. Salamo3

1V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, 45, prospect Nauky, 03028 Kyiv, Ukraine
2Humboldt Universitat zu Berlin, Institut fur Physik, 15, Newtonstrasse, 2489 Berlin, Germany
3Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701

Abstract. Novel model of the diluted magnetic semiconductors (DMS) $A_{1-x}Mn_xB$ possessing the metallic conductivity is proposed. Using the coherent potential technique the electron scattering by the randomly distributed Mn centers is taken into account. The exchange scattering of the electron spin by the localized magnetic moment is calculated exactly basing on the spin-polaron limit for the Vonsovskii Hamiltonian.

Keywords: diluted magnetic semiconductors, ferromagnetism, coherent potential, exchange interaction.

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1. Introduction

It is known that the atoms of transition metals generate deep levels within the energy gap of II-VI, III-V semiconductors [1, 2]. The statements related to the problem of deep levels in wide-gap semiconductors doped with the transition metal atoms of low concentration ($x < 0.01$) can be summarized as follows: i) The transition metal atom occurs as the substitution defect in the cationic sub-lattice of semiconductor; ii) Unfilled atomic $d$-orbital of transition elements is occupied following the Hund’s rules for a free atom and is clamped to the vacuum level of semiconductor rather than to the top of the valence band or to the bottom of the conduction band. The deep levels in semiconductors are generated following the scheme of resonant crystal field or broken bonds [1]; iii) Peculiarities of electron spectra in magnetically doped semiconductors can not be explained basing on the solution of two-band model in the tight-binding approximation [1]. The latter problem being essentially the many-body one requires taking into account, along with the crystal field, the Coulomb coupling of electrons and the covalence of binding between the transition element atom and the matrix as well. In general, narrow-gap magnetically doped semiconductors do not follow the behavior of the wide-gap semiconductors containing magnetic atoms [1]. Nevertheless, one can assume that the atom levels of transition elements are also clamped to the vacuum level in narrow-gap semiconductors [3].

Traditionally, it has been considered that the microscopic description of Mn effect in wide-gap semiconductors can be performed using the Vonsovskii Hamiltonian with two exchange constants $\alpha$ and $\beta$ in the mean field approximation. Thus, one has in the case of exchange interaction between the spin of conduction band electron and the localized magnetic moment of the Mn ion

$$H_\text{exch}^c = \alpha \sum_i \langle \sigma_i \rangle \sigma_i \alpha_i^+ a_i^\dagger \rightarrow \alpha \langle \sigma_i \rangle \sigma_i^c,$$

whereas in the case of the valence band hole this coupling takes the form [4–6]

$$H_\text{exch}^h = \beta \sum_i \langle \sigma_i \rangle \sigma_i \beta_i^+ b_i^\dagger \rightarrow \beta \langle \sigma_i \rangle \sigma_i^h.$$

Usually, the $\alpha, \beta$ parameters being derived from magneto-optical or magneto-transport experiments reveal a strong scatter both by values and signs even for the most investigated wide-gap semiconductors. Moreover, in the case of narrow-gap semiconductors demonstrating the metallic properties, it is problematically to determine these microscopic parameters from experiments [7, 8]. In the limiting case of metal, there exists only one band and only one parameter remains to describe the exchange interaction between collectivized carriers and localized spins. Thus, the problem becomes the Kondo problem. The magnetic properties of Mn doped semiconductors are predicted to be diamagnetic at high temperatures, whereas at low temperatures the Van Fleck paramagnetism caused by the transition metal ions is expected under such approach [2]. It should be noticed that the Vonsovskii Hamiltonian, being widely used for the description of the magnetic semiconductors [4], the materials demonstrating the metal-insulator transition [9],
and the magnets with the semi-metallic properties [10], is valid in the case of diluted magnetic semiconductors under the condition of randomly distributed transition ions over the cationic sub-lattice of the semiconductors.

Recently, the Ga$_{1-x}$Mn$_x$As and In$_{1-x}$Mn$_x$As semiconductors with high molar percentage of Mn ($x > 0.01$) have been studied [11, 12]. The growth conditions allow Mn ions to be randomly distributed over the cationic sub-lattice and MnAs clusters do not arise inside the bulk Ga$_{1-x}$Mn$_x$As due to the condition of $x < x_c = 0.13$, where $x_c$ is the percolation limit for the creation of the finite percolation clusters in the face-centered cubic cationic sub-lattice. It has been shown that these semiconductors turn out in the magnetically ordered state like the ferromagnetic phase at the temperatures $T < T_c$ and in the magnetic field [11–13]. Such state can be easily manipulated allowing the spintronic application [14]. Changing the wide-gap semiconductors Ga$_{1-x}$Mn$_x$As by the narrow-gap In$_{1-x}$Mn$_x$Sb compounds possessing larger lattice constant it is possible to get the homogeneous semiconductors of the higher Mn doping. The In$_{1-x}$Mn$_x$Sb semiconductor with $x = 0.02, 0.028$ has been successfully synthesized [15].

The ferromagnetic ordering in the A$_{1-x}$Mn$_xB$ DMS at $x < x_c$ can not be referred to a typical phenomenon of magnetic systems. Indeed, it has been shown [16–18] that in the DMS the double exchange is the mechanism responsible for the ferromagnetic ordering rather than the RKKY mechanism in the case of the metallic conductivity, as it is stated in Ref. [11, 12]. In spite of low Mn concentrations ($x < x_c$) in strongly diluted magnetic semiconductors (SDMS), these latter belong to the magnetic systems, the type of Heisenberg magnetic semiconductors (EuO, EuS, EuSe, EuTe, Ca$_{1-x}$La$_x$MnO$_3$) [4] or the Heusler alloys possessing the structure C1b (PtMnSb, NiMnSb, CrO$_2$, MnSb, MnAs) [19–21]. It is known that ferromagnetism and antiferromagnetism coexist in the Heisenberg magnetic semiconductors [4] resulting in the inhomogeneous magnetic ordering, which can explain a non-monotonic temperature dependence of the resistance [4, 11, 12]. Thus, on the one hand, the problem of metastable magnetic properties of DMS arises. On the other hand, it is known that even the diamagnetic properties of the narrow-gap DMS are inhomogeneous [22]. The departure from the Fermi-behavior of free electrons is observed in the magnetic semiconductors of high conductivity also [19]. This property is proved for the $t$–$J$ model serving an example of the strongly correlated electron system [23]. All the experimental findings mentioned above are of great importance for understanding of SDMS properties.

There exist various theoretical schemes in SDMS study. One of them resembles the computer modeling for strongly frustrated spin glasses [24, 25]. Such approach is based on the random distribution of transition metal over the cationic sub-lattice of the semiconductor and predicts significant deviation from “3/2 law” for the temperature dependence of magnetization, if the temperature tends to zero. The approximation of mean field or the approximation of a virtual crystal is widely used [26, 27]. Here, after the configuration averaging in DMS the search of the electron Green’s functions reduces to the similar problem of the magnetic semiconductor with the mean splitting performed following the Bogolyubov-Tyblikov procedure [28]. Both the disorder and the possibility of the inhomogeneous magnetism are ignored. The contribution of the disorder can be taken into account using the technique of the coherent potential [29–31]. The technique proved to be a powerful tool in the study of magnetic systems of high conductivity; however it is of importance to account correctly for the electron correlations and the dynamic character of scattering. The dynamic mean field (DMF) technique [32] allows the investigation of the strongly correlated systems and the SDMS as well. This technique broadens the resources of the coherent potential method [18, 33]. The standard technique of the Fermi-systems is also used for the study of the correlated carriers in SDMS [34, 35]. However, it is difficult to solve the self-consistent problem for the magnetic subsystem together with the problem of the electron-hole spectrum in the semiconductor.

The ab-initio calculations are considered to be use to get the information about the electron spectrum in the A$_{1-x}$Mn$_xB$ DMS [18, 20, 21]. Nevertheless, the uniqueness of the results as well as their certainty has to be particularly analyzed in such calculations. Therefore, the analytical schemes like that [33] developed for the investigation of the A$_{1-x}$Mn$_xB$ DMS with a metallic type conductivity are of extreme importance. These materials are considered as an example of strongly correlated electron systems [32] combining the electrical and magnetic properties [11–18]. Section II contains the Hamiltonian of A$_{1-x}$Mn$_xB$ DMS and the description of the coherent potential technique [33] allowing the self-consistent approach to the solution of the problem outlined above. In order to take into account the spin-exchange scattering of the electrons by the localized magnetic moment, it is proposed to project the Vonsovskii Hamiltonian in its spin-polaron form [4] onto the effective impurity Anderson model, and then to use the technique of the motion equations for finding the electron propagators separating the irreducible parts of the Green function (Section 3). The spin Green functions are determined to be used further to calculate temperature and magnetic field dependences of the magnetization (Section 4). The concluding remarks to the developed model clarifying the behavior of DMS with the metallic conductivity are presented in Section V.

2. Spin-polaron Hamiltonian for the A$_{1-x}$Mn$_xB$ semiconductors with the metallic conductivity

Following [33] we introduce the Hamiltonian like the Vonsovskii Hamiltonian:

\[
H = H_w + H_M + \alpha \sum_{\langle i,j \rangle} (\vec{\sigma}_i \cdot \vec{\sigma}_j) a^+_i a_j, \quad (1)
\]

\[
H_w = -t \sum_{\langle i,j \rangle} a^+_i a_j, \quad \text{and} \quad (2)
\]

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\[ H_M = \hbar \sum_j S_j^z, \]  
\[ (3) \]

where \( H_W \) is the Hamiltonian of free electrons in the conduction band, \( H_M \) describes the energy of localized magnetic moments in the magnetic field, \( i \) is the transfer parameter defining the width \( W \) of the conduction band, \( \hbar = ghB \), \( g \) is the gyro-magnetic factor, \( \mu_B \) is the Bohr magneton, and \( H \) is the external magnetic field effecting the localized magnetic moment of Mn ion.

For \( A_{1-x}M_{x}B \) DMS calculating their electron and thermodynamic properties, it is necessary to take into account the random distribution of Mn component over AB sub-lattice, if \( x < x_c \). Therefore, besides thermo-dynamic averaging, the averaging over the configurations has to be performed exploiting the cumulant expansions \( [33] \). The chaotic distribution of the magnetic component also complicates the analysis of the atomic boundary of the magnetic sub-system of the semiconductors. The electron spin can not be considered as a true quantum number, while due to the scattering of an electron by the localized magnetic moment of the Mn ion the spin can be changed depending on the sign of the parameter.

Let us exploit the coherent potential scheme basing on the Hamiltonian \((1)\) \([33]\):

\[ < \sigma \rangle (\omega) := \frac{1}{N} \sum_k \frac{\langle \varepsilon \sigma (\omega) \rangle}{\varepsilon_k - \varepsilon_k}, \]  
\[ (4) \]

\[ J_\sigma (\omega) = \left[ \Xi \sigma (\omega) \right]^{-1} \left[ < \sigma \rangle (\omega) \right]^{-1}, \]
\[ (5) \]

\[ \Xi \sigma (\omega) = \frac{(1 - \chi) D_{M}^A (\omega) + x D_{M}^B (\omega) - D_{M}^A (\omega) D_{M}^B (\omega) J_\sigma (\omega)}{1 - (1 - \chi) D_{M}^A (\omega) + x D_{M}^B (\omega) J_\sigma (\omega)} \]  
\[ (6) \]

The Green function of all the crystal \( \langle G \sigma (\omega) \rangle \) (Eqn. \((4)\)) is expressed through the microscopic Green function \( \langle G \sigma (\omega) \rangle \). The coherent potential \( J_\sigma (\omega) \) is given by the equation \((5)\) in terms of the \( \langle G \sigma (\omega) \rangle \) function and the self-energy part averaged over the configurations \( \Xi \sigma (\omega) \). In its turn, the \( \Xi \sigma (\omega) \) function (Eqn. \((6)\)) is defined by the local scattering of the electron spin at both the non-magnetic \( D_{M}^A (\omega) \) and magnetic \( D_{M}^B (\omega) \) atoms of the \( i \)-th lattice site. Equations \((4-6)\) have been derived averaging the diagrams of the Hubbard-I approximation. However, the explicit form of the local functions \( D_{M}^A (\omega) \) and \( D_{M}^B (\omega) \) can be found by projecting the Hamiltonian \((1)\) onto the effective Hamiltonian like to the Anderson type \([33]\) following the DMF scheme \([32]\).

For \( A_{1-x}M_{x}B \) DMS, the idea of the spin-polaron Hamiltonian \([4]\) can be utilized provided for the existence of the states with the parallel directions of the localized spin \( S_i \) and the electron spin possessing the energy \( \epsilon_i^f = \epsilon_d - \alpha S / 2 \) (pseudo-spin \( \uparrow \)) and the anti-parallel spins with the energy \( \epsilon_i^a = \epsilon_d + \alpha (S + 1) / 2 \) (pseudo-spin \( \downarrow \)). Using the spin operators \( S_i^+ \) and \( S_i^- \) the electron wave functions \([4]\) are introduced as follows:

\[ \psi_{\alpha \beta} = \psi_{\alpha \beta}^\pm \]  
\[ (7) \]

\[ A_{\alpha}^+(S_{\alpha}^+) = \frac{1}{\sqrt{2S + 1}} \left[ \frac{S + S_{\alpha}^+}{S + S_{\alpha}^+ + 1} + \frac{a_{\alpha}^+ a_{\alpha}^- S_{\alpha}^+}{S + S_{\alpha}^+ + 1} \right] \]

The \( \delta(S_{\alpha}^+, S_{\alpha}^-) \) denotes the state of the magnetic sub-system at the \( i \)-th site in the case of the electron presence, \( S_{\alpha}^+ \) is the spin projection, if the electron is absent, \( S_{\alpha}^- \) is the spin projection, if the electron is present, and \( |0\rangle \) is the ground state of the electron sub-system.

The wave functions \((7)\) are the eigen-functions of the exchange part of the Hamiltonian \((1)\) and can be considered as the wave functions of the atomic limit for the Vonsovskii Hamiltonian \([39]\). These functions are suitable for the expansion of the wave function of the Hamiltonian \((1)\), thus allowing to turn to the spin-polaron limit of the Hamiltonian \((1)\) that can be written for the case of large \( S \) as follows \([4, 33]\):

\[ H = H_0 + H_{h o p}, \]
\[ (8) \]

\[ H_0 = \epsilon_A \sum_{i \sigma} n_{i \sigma} + \left( \epsilon_d - \alpha S / 2 \right) \sum_{i \sigma} (n_{i \sigma} - 1) + \left[ \epsilon_d + \alpha (S + 1) / 2 \right] \sum_{i \sigma = \uparrow \downarrow} + H_M \]
\[ (9) \]

\[ H_{h o p} = H_{h o p}^{+} + H_{h o p}^{-} = \gamma \sum_{\langle i \rangle \sigma} \left[ \left( \epsilon_{\sigma} + \frac{S_i^+ + S_{i+\Delta}^+}{2} + S_i^- + S_{i+\Delta}^- \right) \right]^{(2)} \left[ \epsilon_{\sigma} - 1 \right]^{(1)} + \left( S_i^+ + S_{i+\Delta}^+ \right) \]
\[ (10) \]

Writing down the equations \((8-10)\), it has been taken into account that in case of the electron located at the site of the magnetic ion in the lattice (index \( 2 \) in the operators of creation \( a_{\sigma}^+ \) or annihilation \( a_{\sigma}^- \)) its spin behaves itself.
as a pseudo-spin (localized magnetic moment + electron spin), whereas in case of the electron located at the non-magnetic ion site in the lattice (index 1 in the operators $a_{i\sigma}^{(1)}$ and $a_{i\sigma}^{(-1)}$) the pseudo-spin transforms into the electron spin, which is reflected in the part $H_{i,j}^{xy}$ of the Hamiltonian (10).

In order to utilize the equations (4–6) determining the coherent potential, the Hamiltonian (8) has to be projected onto the Hamiltonian of the Anderson type following the procedure developed in Ref. [33, 42] and assuming that the electron being in the conduction band moves over the non-magnetic ions in the $A_{1-x}Mn_xB$ system with $x < x_c$.

Thus,

$$ H_W \rightarrow H_W = -V \sum_{i,\sigma} \left( a_{i\sigma}^{(1)} \xi_i^{+} + \xi_{i\sigma} a_{i\sigma}^{(-1)} \right) , $$

(11)

where $\xi_i^{+}$ and $\xi_{i\sigma}$ are the Fermi operators of the electron creation and annihilation, respectively, beyond the $i$-th site with the spin $\sigma$. These operators are connected with the coherent potential [33, 42] through the equation

$$ J_\sigma (\omega) = 2\pi V^2 \ll \xi_{i\sigma}^+ \gg_{\omega} \cdot $$

(12)

The commutation relations for the operators entering the Hamiltonians (8-11) are:

$$ \{a_{i\sigma}^{(1)}, a_{j\sigma}^{(-1)}\} = \delta_{ij} \delta_{\sigma\sigma'}, \quad \{a_{i\sigma}^{(1)}, a_{i\sigma}^{(-1)}\} = \delta_{ij} \delta_{\sigma'\sigma} = 0, $$

$$ \{\xi_{i\sigma}^+, a_{i\sigma}^{(1)}\} = 0, \quad \{\xi_{i\sigma}, a_{i\sigma}^{(-1)}\} = 0, $$

(13)

$$ S_i^{2+} + S_i^{2-} = 2\delta_{ij} S_i^{2}, \quad \left[ S_i^{2+} S_i^{2-} + S_i^{2} S_i^{2+}ight] + (S_i^{2+})^2 = S(S+1), $$

If one assumes that the relations between the local parts of the Green functions derived basing on the Vonsovskii Hamiltonian (1) have the form of

$$ D^{A}_i (\omega) = \ll a_{i\sigma}^{(1)} | a_{i\sigma}^{(-1)} \gg_{\omega} = \ll a_{i\sigma}^{(-1)} | a_{i\sigma}^{(1)} \gg_{\omega} = 0, $$

(14)

the self-consistent scheme for finding the electron Green functions built using the equations (4–6, 12, 14) becomes completely closed.

Passing on to the great canonical distribution, the chemical potential $\mu$ determined solely by the mean number of the electrons $n_{i}^{(1)}$ at the non-magnetic site in case of the $A_{1-x}Mn_xB$ crystals with $x < x_c$ is defined traditionally through relations

$$ n_{i}^{(1)} = \sum_\sigma n_{i\sigma}^{(1)} = $$

$$ = \sum_\sigma \int_{-\infty}^{\infty} d\omega \frac{1}{2\pi} e^{\mu(\omega-\mu)} \ll 2\text{Im} \langle \langle a_{i\sigma}^{(1)} | a_{i\sigma}^{(-1)} \rangle \gg_{\omega+i\epsilon} \rangle \rightarrow 0, $$

(15)

$$ n_{i}^{(2)} = \sum_\sigma n_{i\sigma}^{(2)} = $$

$$ = \sum_\sigma \int_{-\infty}^{\infty} d\omega \frac{1}{2\pi} e^{\mu(\omega)} \ll 2\text{Im} \langle \langle a_{i\sigma}^{(2)} | a_{i\sigma}^{(-2)} \rangle \gg_{\omega+i\epsilon} \rangle \rightarrow 0. $$

3. Formulation of the effective single node electron task

Let us write the equations of motion for the operators $a_{i\sigma}^{(1,2)}$ using the effective Hamiltonian (8):

$$ \hat{E}_{i\sigma}^{(1)}, \hat{H} = \hat{E}_{i\sigma}^{A} a_{i\sigma}^{(1)} + \gamma \sum_\Delta \left\{ \left[ S_i^+ + S_i^{-} / 2 \right] a_{i\sigma}^{(2)} + \right. $$

$$ + \left. S_{i+\Delta} a_{i+\Delta,\sigma}^{(2)} \right\} - V_{\xi i\sigma} \cdot $$

$$ \hat{E}_{i\sigma}^{(2)}, \hat{H} = (\epsilon_d - \alpha \left[ S + \pi \right] / 2) a_{i\sigma}^{(1)} + $$

$$ + \gamma \sum_\Delta \left\{ \left[ S_i^+ + S_i^{-} / 2 + S_{i+\Delta}^+ S_{i+\Delta}^+ \right] a_{i\sigma}^{(2)} + \right. $$

$$ + \left. \left[ S + \pi + S_{i+\Delta} / 2 \right] a_{i+\Delta,\sigma}^{(2)} \right\}. $$

(16)

The notions $\pi_{i\sigma} = \{0 : \sigma = \uparrow \}, \{1 : \sigma = \downarrow \}$ are introduced in the commutation relations (13). The general expressions for the Green functions ($\hbar = 1$) built on the $A, B$ operators are as follows

$$ \omega < \hat{A}_{i} \hat{B} >_{\omega} = \frac{1}{2\pi} \ll \hat{A}_{i} \hat{B} \gg_{\omega}, $$

(17)

$$ \omega < \hat{A}_{i} \hat{B} >_{\omega} = \frac{1}{2\pi} \ll \hat{A}_{i} \hat{B} \gg_{\omega} = \ll \hat{A}_{i} \hat{B} \gg_{\omega}. $$

Using (17), the equations for the Green functions $\ll a_{i\sigma}^{(1)} | a_{i\sigma}^{(1)} \gg_{\omega}, \ll a_{i\sigma}^{(2)} | a_{i\sigma}^{(2)} \gg_{\omega}$ can be written as

$$ (\omega - \epsilon_{A}) \ll a_{i\sigma}^{(1)} | a_{i\sigma}^{(1)} \gg_{\omega} = \frac{1}{2\pi} < a_{i\sigma}^{(1)}, a_{i\sigma}^{(-1)} > + $$

$$ + \gamma \sum_\Delta \ll \left[ S + \pi + S_{i+\Delta} / 2 \right] a_{i+\Delta,\sigma}^{(2)} | a_{i\sigma}^{(1)} \gg_{\omega} + $$

$$ + \gamma \sum_\Delta \ll S_{i+\Delta} a_{i+\Delta,\sigma}^{(2)} | a_{i\sigma}^{(1)} \gg_{\omega} - \ll \xi_{i\sigma}^{-1} | a_{i\sigma}^{(1)} \gg_{\omega}, $$

$$ \omega + \alpha \pi / 2 \ll a_{i\sigma}^{(2)} | a_{i\sigma}^{(1)} \gg_{\omega} = \frac{1}{2\pi} \ll \left[ S + \pi + S_{i+\Delta} / 2 \right] a_{i+\Delta,\sigma}^{(2)} | a_{i\sigma}^{(1)} \gg_{\omega} + $$

$$ + \gamma \sum_\Delta \ll \left[ S + \pi + S_{i+\Delta} / 2 \right] a_{i+\Delta,\sigma}^{(2)} | a_{i\sigma}^{(1)} \gg_{\omega} + $$

$$ + \ll \left[ S_{i+\Delta} - S_{i} \right] a_{i\sigma}^{(2)} | a_{i\sigma}^{(-1)} \gg_{\omega} - $$

(18)

Since the Green functions are of the single node character onto the self-returning paths [23, 33], one can distinguish the irreducible parts from the self-energy parts of the electron Green functions when constructing the Dyson equations [39-42]. In order to perform this operation, the commutators (16) are rewritten as

$$ \hat{E}_{i\sigma}^{(1)}, \hat{H} = \hat{E}_{i\sigma}^{A} a_{i\sigma}^{(1)} + \alpha_{i\sigma}^{(1)} a_{i\sigma}^{(1)} + \alpha_{i\sigma}^{(2)} a_{i\sigma}^{(2)} + Z_{i\sigma}^{(1)}, $$

$$ \hat{E}_{i\sigma}^{(2)}, \hat{H} = \hat{E}_{i\sigma}^{A} a_{i\sigma}^{(2)} + a_{i\sigma}^{(2)} a_{i\sigma}^{(1)} + \alpha_{i\sigma}^{(2)} a_{i\sigma}^{(1)} + Z_{i\sigma}^{(2)}. $$

(19)

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where the coefficients $a^{(1,2)}_{1\sigma}$ are determined from the orthogonality conditions for the anti-commutators of the electron operators and the irreducible parts $Z^{(1,2)}_{i\sigma}$ at the different lattice sites:

$$\left\{G^{(1,2)}_{i\sigma} + Z^{(1,2)}_{i\sigma}\right\} = 0 \quad \text{and} \quad \left\{G^{(1,2)}_{i\sigma} + Z^{(1,2)}_{i\sigma}\right\} = 0 .$$  \hspace{1cm} (20)

Then the explicit expressions of the coefficients $a^{(1,2)}_{1\sigma}$ under the condition (20) are given by

$$a^{(1)}_{1\sigma} = 0,$$

$$a^{(2)}_{1\sigma} = \gamma(S + \pi_{\sigma} + <S^z> / 2),$$

and

$$a^{(2)}_{2\sigma} = \gamma(S + \pi_{\sigma} + <S^z> ).$$

Here it is assumed that the magnetic ordering is homogeneous and does not depend on the lattice site,

$$\left\{S^z + \Delta\right\} = \left\{S^z\right\}, \quad \left\{S^\sigma + \Delta\right\} = \left\{S^\sigma\right\} = \left\{S^\sigma\right\}. \hspace{1cm} (22)

The equations of motion for each Green’s function of the expression (18) with the right-side operator $a^{(1)}_{1\sigma}$ can be written using the second relation (17). Similar expressions are written for determination of the functions $<< a^{(1)}_{1\sigma} | a^{(2)}_{1\sigma} >>$ and $<< a^{(2)}_{2\sigma} | a^{(2)}_{2\sigma} >>$.

All found functions can be unified by the matrix form as follows:

$$\begin{pmatrix}
\omega - \epsilon_A - a^{(1)}_{1\sigma} & -a^{(2)}_{1\sigma} \\
-a^{(2)}_{1\sigma} & \omega - \epsilon_d - a^{(2)}_{2\sigma}
\end{pmatrix}
\begin{pmatrix}
\hat{G}_{1\sigma} \\
\hat{G}_{2\sigma}
\end{pmatrix}
= \begin{pmatrix}
1/2\pi & 0 \\
0 & 1/2\pi
\end{pmatrix}
+ \begin{pmatrix}
<< Z^{(1)}_{i\sigma} | Z^{(1)}_{i\sigma} >> & << Z^{(1)}_{i\sigma} | Z^{(2)}_{i\sigma} >> \\
<< Z^{(2)}_{i\sigma} | Z^{(1)}_{i\sigma} >> & << Z^{(2)}_{i\sigma} | Z^{(2)}_{i\sigma} >>
\end{pmatrix}
\times
\begin{pmatrix}
\omega - \epsilon_A - a^{(1)}_{1\sigma} & -a^{(1)}_{2\sigma} \\
-a^{(1)}_{2\sigma} & \omega - \epsilon_d - a^{(2)}_{2\sigma}
\end{pmatrix}^{-1} .
\hspace{1cm} (23)

This can be rewritten in the form of matrix equation of scattering:

$$\hat{G}_{1\sigma} = \hat{G}_{0\sigma} + \hat{G}_{0\sigma} \hat{P}_{\sigma} \hat{G}_{0\sigma} , \hspace{1cm} (24)$$

where

$$\hat{G}_{0\sigma} = \frac{1}{2\pi}
\begin{pmatrix}
\omega - \epsilon_A - a^{(1)}_{1\sigma} & -a^{(2)}_{1\sigma} \\
-a^{(2)}_{1\sigma} & \omega - \epsilon_d - a^{(2)}_{2\sigma}
\end{pmatrix}
\frac{\omega - \epsilon_d - a^{(2)}_{2\sigma}}{(\omega - \epsilon_A - a^{(1)}_{1\sigma})(\omega - \epsilon_d - a^{(2)}_{2\sigma}) - a^{(1)}_{2\sigma}a^{(2)}_{1\sigma}},
\begin{pmatrix}
\omega - \epsilon_A - a^{(2)}_{1\sigma} & -a^{(1)}_{2\sigma} \\
-a^{(1)}_{2\sigma} & \omega - \epsilon_d - a^{(2)}_{2\sigma}
\end{pmatrix}^{-1},
\frac{1}{2\pi}
\begin{pmatrix}
\omega - \epsilon_d - a^{(2)}_{1\sigma} & -a^{(1)}_{2\sigma} \\
-a^{(1)}_{2\sigma} & \omega - \epsilon_A - a^{(1)}_{1\sigma}
\end{pmatrix}^{-1}.
\hspace{1cm} (25)

The matrix equation of scattering (24) transforms into the Dyson matrix equation

$$\hat{G}_{\sigma} = \hat{G}_{0\sigma} + \hat{G}_{0\sigma} \hat{M}_{\sigma} \hat{G}_{\sigma} , \hspace{1cm} \hat{M}_{\sigma} = irr \hat{P}_{\sigma} irr \hat{G}_{0\sigma} irr \hat{P}_{\sigma} + ... \hspace{1cm} (26)$$

where

$$\hat{M}_{\sigma} = irr \hat{P}_{\sigma} irr \hat{G}_{0\sigma} irr \hat{P}_{\sigma} + ... \hspace{1cm} (26)$$

The explicit form of the irreducible parts representing the first order approximation for the (see Appendix) is given by

$$\text{irr} \quad \langle \langle Z^{(1)}_{i\sigma} | Z^{(1)}_{i\sigma} \rangle \rangle \quad \text{irr} \quad \langle \langle Z^{(1)}_{i\sigma} | Z^{(2)}_{i\sigma} \rangle \rangle \quad \text{irr} \quad \langle \langle Z^{(2)}_{i\sigma} | Z^{(1)}_{i\sigma} \rangle \rangle \quad \text{irr} \quad \langle \langle Z^{(2)}_{i\sigma} | Z^{(2)}_{i\sigma} \rangle \rangle \hspace{1cm} \Theta_{\sigma}^{22} - J_{\sigma}(\omega) / 2\pi ,$$

where

$$\Theta_{\sigma}^{jk} = \langle \langle a^{(j)}_{1\sigma} | a^{(k)}_{1\sigma} \rangle \rangle \hspace{1cm} \langle \langle a^{(j)}_{2\sigma} | a^{(k)}_{2\sigma} \rangle \rangle \hspace{1cm} \langle \langle a^{(j)}_{2\sigma} | a^{(k)}_{2\sigma} \rangle \rangle \hspace{1cm} \langle \langle a^{(j)}_{2\sigma} | a^{(k)}_{2\sigma} \rangle \rangle \hspace{1cm} \langle \langle a^{(j)}_{2\sigma} | a^{(k)}_{2\sigma} \rangle \rangle .$$

and

$$\langle \langle a^{(j)}_{1\sigma} | a^{(k)}_{1\sigma} \rangle \rangle \hspace{1cm} \langle \langle a^{(j)}_{2\sigma} | a^{(k)}_{2\sigma} \rangle \rangle \hspace{1cm} \langle \langle a^{(j)}_{2\sigma} | a^{(k)}_{2\sigma} \rangle \rangle \hspace{1cm} \langle \langle a^{(j)}_{2\sigma} | a^{(k)}_{2\sigma} \rangle \rangle .$$
spin Green functions. We present the method to find such averages through the calculation of the electron functions (27–29), which casts doubt on the validity of the results. Here we take the derivatives of the Brillouin function [31, 34, 35, 37], which is hardly suitable for the analytical treatment, but allows the perfect numerical analysis.

The irreducible electron functions (27–29) contain averages of the localized magnetic moments like 

$$
\langle S^z \rangle, \langle S^\sigma \rangle, \langle S^+ S^- \rangle, \langle S^+ S^z \rangle, \langle S^- S^z \rangle.
$$

Self-consistent finding of these averages is of importance for the correct solution of the sets (4–6) and (27–29), and for the ascertainment of the phase transition nature [11–15] in DMS [28]. Usually in the calculation of the electron spectrum of magnetic semiconductors, these averages are taken as derivatives of the Brillouin function [31, 34, 35, 37], which casts doubt on the validity of the results.

Here we present the method to find such averages through the spin Green functions $$\langle S^+_i \mid S^-_j \rangle > \omega$$ and $$\langle S^+_i \mid S^+_j \rangle > \omega$$ following the Bogolyubov-Tyablikov scheme.

4. Formulation of the effective single node spin task

Let us write the equations of motion for the Bose-like spin operators $$S^\sigma_i$$ and $$S^\sigma$$:

$$
[S^\sigma_i, H] = \sum_{\Delta} \left[ S^+_{i-\Delta} a_{i, \Delta}^{(2)+} + S^-_{i+\Delta} a_{i, -\Delta}^{(2)+} + S^+_{i, \Delta} a_{i-\Delta}^{(2)+} + S^-_{i, -\Delta} a_{i+\Delta}^{(2)+} + S^+_{i+\Delta} a_{i, \Delta}^{(2)} + S^-_{i-\Delta} a_{i-\Delta}^{(2)} + S^+_{i, \Delta} a_{i, -\Delta}^{(2)} + S^-_{i, -\Delta} a_{i, \Delta}^{(2)} \right]
$$

(31)

where the notions are introduced as follows:

$$
S^\sigma_i, H = \sigma h S_i^\sigma - \sigma \sum_{\Delta} \left[ \frac{\omega_{\sigma}}{2} \left( a_{i, \Delta}^{(2)+} + a_{i, \Delta}^{(2)+} + a_{i-\Delta}^{(2)+} + a_{i-\Delta}^{(2)+} + a_{i, \Delta}^{(2)} + a_{i, -\Delta}^{(2)} + a_{i-\Delta}^{(2)} + a_{i-\Delta}^{(2)} + a_{i, \Delta}^{(2)} + a_{i, -\Delta}^{(2)} + a_{i-\Delta}^{(2)} + a_{i-\Delta}^{(2)} \right) +
$$

$$
+ \left[ S^+_{i, \Delta} a_{i-\Delta}^{(2)+} + S^-_{i, \Delta} a_{i-\Delta}^{(2)+} + S^+_{i, -\Delta} a_{i+\Delta}^{(2)+} + S^-_{i, -\Delta} a_{i+\Delta}^{(2)+} \right]
$$

(32)

By analogy to the electron irreducible parts (19), deduced from the equations of motion (18) the irreducible spin parts for the equations of motion (32) are introduced:

$$
\left[ S^+_i, H \right] = h S_i^+ + \beta_1^{(1)} S_i^+ + \beta_2^{(2)} S_i^+ + \tilde{Y}^{(1)}
$$

(33)

and

$$
\left[ S^-_i, H \right] = S_i^- + \beta_1^{(2)} S_i^- + \beta_2^{(2)} S_i^- + \tilde{Y}^{(2)}.
$$

From the requirement of equality of the averages taken for the commutators of the irreducible parts $$\tilde{Y}^{(1,2)}$$ and the spin operators $$S_i^+, S_i^-$$:

$$
\left[ S^-_i, \tilde{Y}^{(1,2)} \right] = 0 \quad \text{and} \quad \left[ S^-_i, \tilde{Y}^{(1,2)} \right] = 0,
$$

(34)

one finds $$\beta_1^{(1,2)} = \beta_2^{(1,2)} = 0$$.

Then using the equations for the Bose-operators $$\tilde{A}$$ and $$\tilde{B}$$,

$$
\omega << \tilde{A} \mid \tilde{B} >> _\omega = \frac{1}{2\pi} < [\tilde{A}, \tilde{B}] > < [\tilde{A}, \tilde{H}] \mid \tilde{B} >> _\omega,
$$

(35)

the equations of motion (33) can be written as follows:

$$
(\omega - h) < S^+_i \mid S^-_j >> _\omega = 2 < S^+_i > + < Y^{(1)}_i \mid S^-_j >> _\omega,
$$

(36)

$$
\omega < S^-_i \mid S^-_j >> _\omega = < S^-_i > + < Y^{(2)}_i \mid S^-_j >> _\omega.
$$

Constructing the equations for searching the Green functions $$\langle S^+_i \mid S^-_j \rangle > _\omega$$ and $$\langle S^+_i \mid S^+_j \rangle > _\omega$$, and performing the procedure (35) with these functions, one gets the matrix equation

$$
\begin{pmatrix}
\omega - h & 0 \\
0 & \omega
\end{pmatrix}
\begin{pmatrix}
\langle S^+_i \mid S^-_j \rangle > _\omega \\
\langle S^+_i \mid S^+_j \rangle > _\omega
\end{pmatrix}
= \left[ \begin{array}{c}
\frac{1}{2\pi} < 2 < S^-_i \mid S^-_j > > _\omega - < S^-_i > \end{array} \right]
$$

(37)

where the notions are introduced as follows:
\[
\hat{S} = \begin{cases}
&\langle \langle S_i^+ | S_i^- \rangle \rangle \omega, \quad \langle \langle S_i^+ | S_i^- \rangle \rangle \omega, \\
&\langle \langle S_i^2 | S_i^2 \rangle \rangle \omega, \quad \langle \langle S_i^2 | S_i^2 \rangle \rangle \omega, \\
&\langle \langle S_i^2 | S_i^2 \rangle \rangle \omega, \quad \langle \langle S_i^2 | S_i^2 \rangle \rangle \omega,
\end{cases}
\]

\[
\hat{Y} = \begin{cases}
&\langle \langle Y_i^{(1)} | Y_i^{(1)} \rangle \rangle \omega, \quad \langle \langle Y_i^{(1)} | Y_i^{(1)} \rangle \rangle \omega, \\
&\langle \langle Y_i^{(2)} | Y_i^{(2)} \rangle \rangle \omega, \quad \langle \langle Y_i^{(2)} | Y_i^{(2)} \rangle \rangle \omega,
\end{cases}
\]

\[
S_0 = \begin{cases}
0 & \frac{1}{\omega - h} \omega \left( < S_i^2 > / \pi - < S_i^2 > / 2 \pi \right), \\
1 & \frac{1}{\omega - h} \omega \left( < S_i^2 > / \pi - < S_i^2 > / 2 \pi \right), \\
0 & < S_i^2 > / 2 \pi, \\
0 & < S_i^2 > / 2 \pi, 
\end{cases}
\]

\[
A_i = \begin{cases}
\frac{2 < S_i^2 >}{\omega - h} - < S_i^2 >, \\
\frac{2 < S_i^2 >}{\omega - h} - < S_i^2 >, \\
0 & < S_i^2 > / 2 \pi, \\
0 & < S_i^2 > / 2 \pi,
\end{cases}
\]

\[
\hat{A}_2 = \frac{\omega^2 < S_i^2 >}{(\omega - h)\omega < S_i^2 >} \times
\]

\[
\left( (\omega - h)^2 < S_i^2 > - 2(\omega - h)\omega < S_i^2 > \right)
\]

Let us write the matrix equation of scattering for the spin Bose-like operators,

\[
\hat{S} = \hat{S}_0 + \hat{S}_0 A_i \hat{Y}_2 \hat{S}_0.
\]

Transform the equation (39) into the Dyson equation

\[
\hat{S} = \hat{S}_0 + \hat{S}_0 D \hat{S},
\]

with the mass operator in the form

\[
D = \hat{A}_1^{-1} \hat{Y} \hat{A}_1 + \hat{A}_2^{-1} \hat{Y} \hat{A}_2 + \hat{S}_0 \hat{A}_1^{-1} \hat{Y} \hat{A}_2 \hat{S}_0 + \ldots
\]

Using the technique described in Appendix, the explicit form for the irreducible matrix elements of the spin part of the \( \hat{Y} \) can be presented as:

\[
\langle \langle Y_i^{(1)} | Y_i^{(1)} \rangle \rangle \omega = \frac{1}{2} \hat{S}_0^{\omega} + \hat{S}_0^{\omega} + \hat{A}_1^{-1} \hat{Y} \hat{A}_1 \hat{S}_0 \hat{A}_1^{-1} \hat{Y} \hat{A}_2 \hat{S}_0 + \ldots
\]

The theoretical treatment of \( A_{1-x}Mn_xB \) DMS basing on the self-consistent analysis of the electron and magnetic properties of DMS possessing the metallic type conductivity is developed. On the one hand, the chaotic distribution of Mn ions over the semiconductor lattice is taken into account by building a coherent potential, on the other hand, the local task of electron spin scattering by the localized magnetic moment is solved exactly.

In our previous analysis [33], for the sake of simplicity, the transverse components of the \( S_i^\sigma \) have been neglected when the Vonskovskii Hamiltonian was written in the spin-polaron approximation (8, 9). In the case of
The Bogolyubov-Tyablikov decoupling of the operators gives
\[
\left(1 + \frac{1}{2\Delta} S_{i+\Delta}^z\right) a_{i+\Delta}^{(2)+} (t) (1 + \frac{1}{2\Delta} S_{i+\Delta}^z) a_{i+\Delta}^{(2)} = \left(1 + \frac{1}{2\Delta} S_{i+\Delta}^z\right) a_{i+\Delta}^{(2)+} (t) a_{i+\Delta}^{(2)} \tau. \tag{A.3}
\]

While the localized magnetic moments do not interact immediately, it appears that
\[
S_{i+\Delta}^z(t) = e^{-it\hat{H}_0} S_{i+\Delta}^z e^{it\hat{H}_0} = S_{i+\Delta}^z. \tag{A.4}
\]

Then one gets
\[
A^{irr} = \sum_{\Delta,\Delta'} \left(1 + \frac{1}{2\Delta} S_{i+\Delta}^z\right) \left(1 + \frac{1}{2\Delta'} S_{i+\Delta'}^z\right) a_{i+\Delta}^{(2)+} a_{i+\Delta'}^{(2)} \tau > \omega. \tag{A.5}
\]

It is assumed that the system after the configuration averaging becomes homogeneous one. Using this assumption \(A^{irr}\) expression can be written as
\[
A^{irr} = \left(1 + \frac{1}{2\Delta} S_{i+\Delta}^z\right) a_{i+\Delta}^{(2)+} a_{i+\Delta}^{(2)} \tau > \omega. \tag{A.6}
\]

For the irreducible Green functions like
\[
irr < (1 + \frac{1}{2\Delta} S_{i+\Delta}^z) a_{i+\Delta}^{(2)+} a_{i+\Delta}^{(2)} \tau > \omega. \tag{A.7}
\]

the more complicated result can be derived,
\[
\sum_{\Delta,\Delta'} irr < (1 + \frac{1}{2\Delta} S_{i+\Delta}^z) a_{i+\Delta}^{(2)+} a_{i+\Delta}^{(2)} \tau > \omega = \left(\sum \left(1 + \frac{1}{2\Delta} S_{i+\Delta}^z\right) a_{i+\Delta}^{(2)+} a_{i+\Delta}^{(2)} \tau > \omega = \sum_{\Delta,\Delta'} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \times \left(1 + \frac{1}{2\Delta} S_{i+\Delta}^z\right) a_{i+\Delta}^{(2)+} a_{i+\Delta}^{(2)} \tau > \omega. \tag{A.8}
\]

Following such procedure for all the terms of irreducible parts of the electron Green functions derived from the equations of motion (18, 19), we get expressions for the scattering matrix \(P_{\sigma}\) (24) written in the equations (27–29).

Using the similar technique, the irreducible spin parts entering into the equation (41) are determined. Basing on the spectral theorem for the Fermi operators [38, 41, 42]:
\[
S_{i+\Delta}^z(t) = e^{-it\hat{H}_0} S_{i+\Delta}^z e^{it\hat{H}_0} = e^{-it\hat{H}_0} S_{i+\Delta}^z. \tag{A.9}
\]
Then, performing the Bogolyubov-Tyablikov decoupling, one receives:
\[
\begin{align*}
S_{\uparrow}^2(t) & = \frac{(1-n_\uparrow^0)(n_\uparrow^0)}{2}\left[ e^{\beta(e_{\uparrow}^0-\epsilon_A)} \langle S_{\uparrow}^x S_{\uparrow}^y \rangle \right] + \frac{\beta}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega'} \left[ -2\text{Im} \langle S_{\uparrow}^x S_{\uparrow}^y \rangle \omega' \right] \\
S_{\downarrow}^2(t) & = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega'} \left[ e^{\beta(e_{\downarrow}^0-\epsilon_A)} \langle S_{\downarrow}^x S_{\downarrow}^y \rangle \right] + \frac{\beta}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega'} \left[ -2\text{Im} \langle S_{\downarrow}^x S_{\downarrow}^y \rangle \omega' \right],
\end{align*}
\]
where the following relation is utilized:
\[
a_{\uparrow,\downarrow}(t) = e^{-itH_0}a_{\uparrow,\downarrow}(t)e^{-itH_0} = e^{i\epsilon_{\uparrow,\downarrow}(t)}a_{\uparrow,\downarrow}(t),
\]
\[
(\text{A.11})
\]
Finally, the irreducible spin part $S_{\uparrow\downarrow}$ takes the following form:
\[
\begin{align*}
S_{\uparrow\downarrow}^\uparrow & = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega'} \left[ e^{\beta(e_{\uparrow}^0-\epsilon_A)} \langle S_{\uparrow}^x S_{\uparrow}^y \rangle \right] = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega'} \left[ e^{\beta(e_{\downarrow}^0-\epsilon_A)} \langle S_{\downarrow}^x S_{\downarrow}^y \rangle \right],
\end{align*}
\]
Similarly for the part $S_{\uparrow\downarrow}^\downarrow = \sum_{\Delta,\Delta'} \langle S_{\uparrow}^x S_{\downarrow}^y \rangle \langle S_{\uparrow}^x S_{\downarrow}^y \rangle \rangle_{\omega' \omega}$ one has
\[
\begin{align*}
S_{\uparrow\downarrow}^\downarrow & = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega'} \left[ e^{\beta(e_{\uparrow}^0-\epsilon_A)} \langle S_{\uparrow}^x S_{\downarrow}^y \rangle \right] = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega'} \left[ e^{\beta(e_{\downarrow}^0-\epsilon_A)} \langle S_{\downarrow}^x S_{\uparrow}^y \rangle \right],
\end{align*}
\]
References

V.P. Bryksa et al.: Diluted magnetic A\(_{1-x}\)Mn\(_x\)B semiconductors