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

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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 α and β 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

$$H_{exch}^e = \alpha \sum_i (\vec{S}_i \vec{\sigma})_{\sigma\sigma'} a_{i\sigma}^+ a_{i\sigma'} \rightarrow \alpha \langle \vec{S}_i \rangle \vec{\sigma}^e,$$

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

$$H_{exch}^h = \beta \sum_i (\vec{S}_i \vec{\sigma})_{\sigma\sigma'} b_{i\sigma}^+ b_{i\sigma'} \rightarrow \beta \langle \vec{S}_i \rangle \vec{\sigma}^h.$$

Usually, the α , β 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 $Ga_{1-x}Mn_xAs$ and $In_{1-x}Mn_xAs$ 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 $Ga_{1-x}Mn_xAs$ due to the condition of $x < x_c \approx 0.13$, 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 $Ga_{1-x}Mn_xAs$ by the narrow-gap $In_{1-x}Mn_xSb$ compounds possessing larger lattice constant it is possible to get the homogeneous semiconductors of the higher Mn doping. The $In_{1-x}Mn_xSb$ 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, $Ca_{1-x}La_xMnO_3$) [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-Tyablikov 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]. This 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 of 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 problem, 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:

$$H = H_W + H_M + \alpha \sum_{\langle i,j \rangle} (\vec{S}_i \vec{\sigma}_j)_{\sigma\sigma'} a_{i\sigma}^+ a_{j\sigma'}, \quad (1)$$

$$H_W = -t \sum_{\langle i,j \rangle, \sigma} a_{i\sigma}^+ a_{j\sigma}, \quad \text{and} \quad (2)$$

$$H_M = h \sum_j S_j^z, \quad (3)$$

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, t is the transfer parameter defining the width W of the conduction band, $h = g\mu_B H^z$, g is the gyro-magnetic factor, μ_B is the Bohr magneton, and H is the external magnetic field effecting the localized magnetic moment of Mn ion.

For $A_{1-x}Mn_xB$ 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]:

$$\langle G_i^\sigma(\omega) \rangle = \frac{1}{N} \sum_k \langle G_k^\sigma(\omega) \rangle = \frac{1}{N} \sum_k \frac{1}{[\Xi_i^\sigma(\omega)]^{-1} - t_k}, \quad (4)$$

$$J_\sigma(\omega) = [\Xi_i^\sigma(\omega)]^{-1} - \langle G_i^\sigma(\omega) \rangle^{-1}, \quad (5)$$

$$\begin{aligned} \Xi_i^\sigma(\omega) &= \\ &= \frac{(1-x)D_{i\sigma}^A(\omega) + xD_{i\sigma}^{Mn}(\omega) - D_{i\sigma}^A(\omega)D_{i\sigma}^{Mn}(\omega)J_\sigma(\omega)}{1 - ((1-x)D_{i\sigma}^A(\omega) + xD_{i\sigma}^{Mn}(\omega))J_\sigma(\omega)}. \end{aligned} \quad (6)$$

The Green function of all the crystal $\langle G_i^\sigma(\omega) \rangle$ (Eqn. (4)) is expressed through the microscopic Green function $\langle G_k^\sigma(\omega) \rangle$. The coherent potential $J_\sigma(\omega)$ is given by the equation (5) in terms of the $\langle G_i^\sigma(\omega) \rangle$ function and the self-energy part averaged over the configurations $\Xi_i^\sigma(\omega)$. In its turn, the $\Xi_i^\sigma(\omega)$ function (Eqn. (6)) is defined by the local scattering of the electron spin at both the non-magnetic $D_{i\sigma}^A(\omega)$ and magnetic $D_{i\sigma}^{Mn}(\omega)$ 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 $D_{i\sigma}^A(\omega)$ and $D_{i\sigma}^{Mn}(\omega)$ can be found by projecting the Hamiltonian (1) onto the effective Hamiltonian like to the Anderson type [33] following the DMF scheme [32].

For $A_{1-x}Mn_xB$ 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 \vec{S}_i and the electron spin possessing the energy $\varepsilon_d^\uparrow = \varepsilon_d - \alpha S / 2$ (pseudo-spin \uparrow) and the anti-parallel spins with the energy $\varepsilon_d^\downarrow = \varepsilon_d + \alpha(S + 1) / 2$ (pseudo-spin \downarrow). Us-

ing the spin operators $S_i^{+,-}$ and S_i^z the electron wave functions [4] are introduced as follows:

$$\psi_{im}^\pm \equiv \psi_i^\pm(S_{i0}^z) = A_{i\pm}^\pm(S_{i0}^z)\delta(S_{i0}^z, S_i^z)|0\rangle, \quad (7)$$

where

$$A_{i+}^\pm(S_{i0}^z) = \frac{1}{\sqrt{2S+1}} \left\{ \sqrt{S+S_{i0}^z+1} a_{i\uparrow}^\pm + \frac{a_{i\downarrow}^\pm S_i^\pm}{\sqrt{S+S_{i0}^z+1}} \right\}, \text{ and}$$

$$A_{i-}^\pm(S_{i0}^z) = \frac{1}{\sqrt{2S+1}} \left\{ \sqrt{S+S_{i0}^z} a_{i\downarrow}^\pm - \frac{a_{i\uparrow}^\pm S_i^\mp}{\sqrt{S+S_{i0}^z}} \right\}.$$

The $\delta(S_{i0}^z, S_i^z)$ denotes the state of the magnetic sub-system at the i -th site in the case of the electron presence, S_{i0}^z is the spin projection, if the electron is absent, S_i^z 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]:

$$H = H_0 + H_{hop}, \quad (8)$$

$$\begin{aligned} H_0 &= \varepsilon_A \sum_{i\sigma} n_{i\sigma}^{(1)} + (\varepsilon_d - \alpha S / 2) \sum_i n_{i\sigma=\uparrow}^{(2)} + \\ &+ [\varepsilon_d + \alpha(S+1) / 2] \sum_i n_{i\sigma=\downarrow}^{(2)} + H_M \end{aligned} \quad (9)$$

$$\begin{aligned} H_{hop} &= H_{t^2/S} + H_W = \\ &= \gamma \sum_{(i\Delta)} \left\{ [S + (S_i^z + S_{i+\Delta}^z) / 2 + S_i^+ S_{i+\Delta}^-] a_{i\sigma=\uparrow}^{(2)+} a_{i+\Delta\sigma=\downarrow}^{(2)} + \right. \\ &+ (S + S_i^z / 2) a_{i\sigma=\uparrow}^{(2)+} a_{i+\Delta\sigma=\uparrow}^{(1)} + (S + S_{i+\Delta}^z / 2) a_{i\sigma=\uparrow}^{(1)+} a_{i\sigma=\uparrow}^{(2)} + \\ &+ [S + 1 + (S_i^z + S_{i+\Delta}^z) / 2 + S_i^- S_{i+\Delta}^+] a_{i\sigma=\downarrow}^{(2)+} a_{i+\Delta\sigma=\downarrow}^{(2)} + \\ &+ (S + 1 + S_i^z / 2) a_{i\sigma=\downarrow}^{(2)+} a_{i+\Delta\sigma=\downarrow}^{(1)} + \\ &+ (S + 1 + S_{i+\Delta}^z / 2) a_{i\sigma=\downarrow}^{(1)+} a_{i+\Delta\sigma=\downarrow}^{(2)} + \\ &+ (S_{i+\Delta}^+ - S_i^+) a_{i\sigma=\downarrow}^{(2)+} a_{i+\Delta\sigma=\uparrow}^{(2)} + S_{i+\Delta}^+ a_{i\sigma=\downarrow}^{(1)+} a_{i+\Delta\sigma=\uparrow}^{(2)} - \\ &- S_i^+ a_{i\sigma=\downarrow}^{(2)+} a_{i+\Delta\sigma=\uparrow}^{(1)} + (S_{i+\Delta}^- - S_i^-) a_{i\sigma=\uparrow}^{(2)+} a_{i+\Delta\sigma=\downarrow}^{(2)} + \\ &+ S_{i+\Delta}^- a_{i\sigma=\uparrow}^{(1)+} a_{i+\Delta\sigma=\downarrow}^{(2)} - S_i^- a_{i\sigma=\uparrow}^{(2)+} a_{i+\Delta\sigma=\downarrow}^{(1)} \left. \right\} + H_W \\ \gamma &= \frac{t}{2S+1} \end{aligned} \quad (10)$$

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 $a_{i\sigma}^{(2)+}$ or annihilation $a_{i\sigma}^{(2)}$) 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 $H_{i^2/S}$ 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,

$$H_W \rightarrow H'_W = -V \sum_{i,\sigma} (a_{i\sigma}^{(1)} \xi_{i\sigma}^+ + \xi_{i\sigma} a_{i\sigma}^{(1)+}), \quad (11)$$

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

$$J_\sigma(\omega) = 2\pi V^2 \ll \xi_{i\sigma} | \xi_{i\sigma}^+ \gg_\omega. \quad (12)$$

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

$$\begin{cases} \{a_{i\sigma}^{(2)}; a_{j\sigma'}^{(2)+}\} = \delta_{ij} \delta_{\sigma\sigma'}, & \{a_{i\sigma}^{(1)}; a_{j\sigma'}^{(1)+}\} = \delta_{ij} \delta_{\sigma\sigma'}, \\ \{a_{i\sigma}^{(2)}; a_{j\sigma'}^{(1)+}\} = 0, & \{\xi_{i\sigma}; a_{i\sigma}^{(1,2)+}\} = 0, \end{cases} \quad (13)$$

$$\begin{cases} [S_i^+; S_j^-] = 2\delta_{ij} S_i^z, & [S_i^\pm; S_j^\pm] = \mp \delta_{ij} S_i^\pm, \\ \frac{1}{2}(S_i^+ S_i^- + S_i^- S_i^+) + (S_i^z)^2 = S(S+1), \end{cases}$$

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

$$D_{i\sigma}^A(\omega) = \ll a_{i\sigma}^{(1)} | a_{i\sigma}^{(1)+} \gg_\omega \text{ and} \quad (14)$$

$$D_{i\sigma}^{Mn}(\omega) = \ll a_{i\sigma}^{(2)} | a_{i\sigma}^{(2)+} \gg_\omega,$$

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 μ determined solely by the mean number of the electrons $n^{(1)}$ at the non-magnetic site in case of the $A_{1-x}Mn_xB$ crystals with is defined traditionally through relations

$$\begin{aligned} n^{(1)} &= \sum_\sigma n_\sigma^{(1)} = \\ &= \sum_\sigma \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{e^{\beta(\omega-\mu)} + 1} \left[-2 \operatorname{Im}(\ll a_{i\sigma}^{(1)} | a_{i\sigma}^{(1)+} \gg_{\omega+i\varepsilon}) \right]_{\varepsilon \rightarrow 0}, \end{aligned} \quad (15)$$

$$\begin{aligned} n^{(2)} &= \sum_\sigma n_\sigma^{(2)} = \\ &= \sum_\sigma \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{e^{\beta\omega} + 1} \left[-2 \operatorname{Im}(\ll a_{i\sigma}^{(2)} | a_{i\sigma}^{(2)+} \gg_{\omega+i\varepsilon}) \right]_{\varepsilon \rightarrow 0}. \end{aligned}$$

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):

$$\begin{aligned} [a_{i\sigma}^{(1)}, H] &= \varepsilon_A a_{i\sigma}^{(1)} + \gamma \sum_{(\Delta)} \left\{ (S + \bar{n}_\sigma + S_{i+\Delta}^z / 2) a_{i+\Delta\sigma}^{(2)} + \right. \\ &\quad \left. + S_{i+\Delta}^\sigma a_{i+\Delta,-\sigma}^{(2)} \right\} - V \xi_{i\sigma}, \\ [a_{i\sigma}^{(2)}, H] &= (\varepsilon_d - \sigma\alpha(S + \bar{n}_\sigma) / 2) a_{i\sigma}^{(2)} + \\ &\quad + \gamma \sum_{(\Delta)} \left\{ [S + \bar{n}_\sigma + (S_i^z + S_{i+\Delta}^z) / 2 + S_i^\sigma S_{i+\Delta}^{-\sigma}] a_{i+\Delta\sigma}^{(2)} + \right. \\ &\quad \left. + (S + \bar{n}_\sigma + S_i^z / 2) a_{i+\Delta\sigma}^{(1)} + \right. \\ &\quad \left. (S_{i+\Delta}^{-\sigma} - S_i^{-\sigma}) a_{i+\Delta,-\sigma}^{(2)} - S_i^{-\sigma} a_{i+\Delta,-\sigma}^{(1)} \right\}. \end{aligned} \quad (16)$$

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

$$\begin{aligned} \omega \ll \hat{A} | \hat{B} \gg_\omega &= \frac{1}{2\pi} \langle [\hat{A}, \hat{B}] \rangle + \ll [\hat{A}, \hat{H}] | \hat{B} \gg_\omega, \\ \omega \ll \hat{A} | \hat{B} \gg_\omega &= \frac{1}{2\pi} \langle [\hat{A}, \hat{B}] \rangle - \ll \hat{A} | [\hat{B}, \hat{H}] \gg_\omega. \end{aligned} \quad (17)$$

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

$$\begin{aligned} (\omega - \varepsilon_A) \ll a_{i\sigma}^{(1)} | a_{i\sigma}^{(1)+} \gg_\omega &= \frac{1}{2\pi} \langle [a_{i\sigma}^{(1)}, a_{i\sigma}^{(1)+}] \rangle + \\ &\quad + \gamma \sum_{(\Delta)} \ll (S + \bar{n}_\sigma + S_{i+\Delta}^z / 2) a_{i+\Delta\sigma}^{(2)} | a_{i\sigma}^{(1)+} \gg_\omega + \\ &\quad + \gamma \sum_{(\Delta)} \ll (S_{i+\Delta}^{-\sigma} a_{i+\Delta,-\sigma}^{(2)} | a_{i\sigma}^{(1)+} \gg_\omega - \ll \xi_{i\sigma}^{(1)} | a_{i\sigma}^{(1)+} \gg_\omega, \\ (\omega + \sigma\alpha(S + \bar{n}_\sigma) / 2) \ll a_{i\sigma}^{(2)} | a_{i\sigma}^{(1)+} \gg_\omega &= \gamma \left\{ \sum_{(\Delta)} \ll (S + \bar{n}_\sigma + \right. \\ &\quad \left. + (S_i^z + S_{i+\Delta}^z) / 2 + S_i^\sigma S_{i+\Delta}^{-\sigma}) a_{i+\Delta\sigma}^{(2)} | a_{i\sigma}^{(1)+} \gg_\omega + \right. \\ &\quad \left. + \sum_{(\Delta)} \ll (S + \bar{n}_\sigma + S_i^z / 2) a_{i+\Delta\sigma}^{(1)} | a_{i\sigma}^{(1)+} \gg_\omega + \right. \\ &\quad \left. + \ll (S_{i+\Delta}^{-\sigma} - S_i^{-\sigma}) a_{i+\Delta,-\sigma}^{(2)} | a_{i\sigma}^{(1)+} \gg_\omega - \right. \\ &\quad \left. - \ll S_i^{-\sigma} a_{i+\Delta,-\sigma}^{(1)} | a_{i\sigma}^{(1)+} \gg_\omega \right\}. \end{aligned} \quad (18)$$

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

$$\begin{aligned} [a_{i\sigma}^{(1)}, H] &= \varepsilon_A a_{i\sigma}^{(1)} + \alpha_{1\sigma}^{(1)} a_{i\sigma}^{(1)} + \alpha_{2\sigma}^{(1)} a_{i\sigma}^{(2)} + Z_{i\sigma}^{(1)}, \\ [a_{i\sigma}^{(2)}, H] &= \varepsilon_d a_{i\sigma}^{(2)} + \alpha_{1\sigma}^{(2)} a_{i\sigma}^{(1)} + \alpha_{2\sigma}^{(2)} a_{i\sigma}^{(2)} + Z_{i\sigma}^{(2)}, \end{aligned} \quad (19)$$

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

$$\left\langle \left\{ a_{i\sigma}^{(1)+}; Z_{i+\Delta\sigma}^{(1,2)} \right\} \right\rangle = 0 \text{ and } \left\langle \left\{ a_{i\sigma}^{(2)+}; Z_{i+\Delta\sigma}^{(1,2)} \right\} \right\rangle = 0. \quad (20)$$

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

$$\begin{aligned} \alpha_{1\sigma}^{(1)} &= 0, \\ \alpha_{2\sigma}^{(1)} &= \alpha_{1\sigma}^{(2)} = \gamma(S + \bar{n}_\sigma + \langle S^z \rangle / 2), \text{ and} \\ \alpha_{2\sigma}^{(2)} &= \gamma(S + \bar{n}_\sigma + \langle S^z \rangle). \end{aligned} \quad (21)$$

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

$$\langle S_{i+\Delta}^z \rangle = \langle S_i^z \rangle = \langle S^z \rangle, \quad \langle S_{i+\Delta}^\sigma \rangle = \langle S_i^\sigma \rangle = \langle S^\sigma \rangle. \quad (22)$$

The equations of motion for each Green's function of the expression (18) with the right-side operator $a_{i\sigma}^{(1)+}$ can be written using the second relation (17). Similar expressions are written for determination of the functions $\langle\langle a_{i\sigma}^{(1)} | a_{i\sigma}^{(2)+} \rangle\rangle$ and $\langle\langle a_{i\sigma}^{(2)} | a_{i\sigma}^{(1)+} \rangle\rangle$.

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

$$\begin{aligned} &\begin{pmatrix} \omega - \varepsilon_A - \alpha_{1\sigma}^{(1)} & -\alpha_{2\sigma}^{(1)} \\ -\alpha_{1\sigma}^{(2)} & \omega - \varepsilon_d^\sigma - \alpha_{2\sigma}^{(2)} \end{pmatrix} \hat{G}_\sigma = \begin{pmatrix} 1/2\pi & 0 \\ 0 & 1/2\pi \end{pmatrix} + \\ &+ \begin{pmatrix} \langle\langle Z_{i\sigma}^{(1)} | Z_{i\sigma}^{(1)+} \rangle\rangle & \langle\langle Z_{i\sigma}^{(1)} | Z_{i\sigma}^{(2)+} \rangle\rangle \\ \langle\langle Z_{i\sigma}^{(2)} | Z_{i\sigma}^{(1)+} \rangle\rangle & \langle\langle Z_{i\sigma}^{(2)} | Z_{i\sigma}^{(2)+} \rangle\rangle \end{pmatrix} \times \\ &\times \begin{pmatrix} \omega - \varepsilon_A - \alpha_{1\sigma}^{(1)} & -\alpha_{2\sigma}^{(1)} \\ -\alpha_{1\sigma}^{(2)} & \omega - \varepsilon_d^\sigma - \alpha_{2\sigma}^{(2)} \end{pmatrix}^{-1}. \end{aligned} \quad (23)$$

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

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

$$\text{where } \hat{G}_{0\sigma} = \begin{pmatrix} \frac{1/2\pi}{\omega - \varepsilon_A - \alpha_{1\sigma}^{(1)} - \frac{\alpha_{2\sigma}^{(1)}\alpha_{1\sigma}^{(2)}}{\omega - \varepsilon_d^\sigma - \alpha_{2\sigma}^{(2)}}} & \frac{\alpha_{2\sigma}^{(1)}}{(\omega - \varepsilon_A - \alpha_{1\sigma}^{(1)})(\omega - \varepsilon_d^\sigma - \alpha_{2\sigma}^{(2)}) - \alpha_{2\sigma}^{(1)}\alpha_{1\sigma}^{(2)}} \\ \frac{\alpha_{1\sigma}^{(2)}}{(\omega - \varepsilon_A - \alpha_{1\sigma}^{(1)})(\omega - \varepsilon_d^\sigma - \alpha_{2\sigma}^{(2)}) - \alpha_{2\sigma}^{(1)}\alpha_{1\sigma}^{(2)}} & \frac{1/2\pi}{\omega - \varepsilon_d^\sigma - \alpha_{2\sigma}^{(2)} - \frac{\alpha_{2\sigma}^{(1)}\alpha_{1\sigma}^{(2)}}{\omega - \varepsilon_A - \alpha_{1\sigma}^{(1)}}} \end{pmatrix},$$

$$\hat{P}_\sigma = (2\pi)^2 \begin{pmatrix} \langle\langle Z_{i\sigma}^{(1)} | Z_{i\sigma}^{(1)+} \rangle\rangle & \langle\langle Z_{i\sigma}^{(1)} | Z_{i\sigma}^{(2)+} \rangle\rangle \\ \langle\langle Z_{i\sigma}^{(2)} | Z_{i\sigma}^{(1)+} \rangle\rangle & \langle\langle Z_{i\sigma}^{(2)} | Z_{i\sigma}^{(2)+} \rangle\rangle \end{pmatrix}, \text{ and } \hat{G}_\sigma = \begin{pmatrix} \langle\langle a_{i\sigma}^{(1)} | a_{i\sigma}^{(1)+} \rangle\rangle & \langle\langle a_{i\sigma}^{(1)} | a_{i\sigma}^{(2)+} \rangle\rangle \\ \langle\langle a_{i\sigma}^{(2)} | a_{i\sigma}^{(1)+} \rangle\rangle & \langle\langle a_{i\sigma}^{(2)} | a_{i\sigma}^{(2)+} \rangle\rangle \end{pmatrix}.$$

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

$$\hat{G}_\sigma = \hat{G}_{0\sigma} + \hat{G}_{0\sigma} \hat{M}_\sigma \hat{G}_\sigma, \quad (25)$$

where

$$\hat{M}_\sigma = {}^{irr}\hat{P}_\sigma + {}^{irr}\hat{P}_\sigma \hat{G}_{0\sigma} {}^{irr}\hat{P}_\sigma + \dots \quad (26)$$

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

$$\begin{aligned} {}^{irr}\langle\langle Z_{i\sigma}^{(1)} | Z_{i\sigma}^{(1)+} \rangle\rangle &= -\gamma^2 \tilde{S} \{ (\tilde{S} + \langle S^z \rangle + \langle S^\sigma \rangle + \\ &+ \frac{1}{2\tilde{S}} (\frac{\langle S^{z2} \rangle}{2} + \langle S^z S^\sigma \rangle)) A_{\sigma,\omega}^{22} - \langle S^{-\sigma} \rangle + \end{aligned} \quad (27)$$

$$+ \frac{1}{2} (\langle S^{-\sigma} S^z \rangle + 2 \langle S^{-\sigma} S^\sigma \rangle) \Theta_{\sigma,\sigma}^{22} \} - J_\sigma(\omega) / 2\pi,$$

where

$$A_{\mu,\nu}^{jk} = \langle\langle a_{i\mu}^{(j)} | a_{i\mu}^{(k)+} \rangle\rangle_\nu, \quad \tilde{S} = S + \bar{n}_\sigma, \text{ and}$$

$$\begin{aligned} \Theta_{\xi,\xi}^{jk} &= \frac{1}{\tilde{S}} \left\{ e^{-\xi\beta h} A_{\xi,\omega+\xi h}^{jk} - \right. \\ &\left. (e^{-\xi\beta h} - 1) \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega + \xi h - \omega'} \left[-2 \text{Im} A_{\xi,\omega'+i\varepsilon}^{jk} \right]_{\varepsilon \rightarrow 0} \right\}, \end{aligned} \quad (28)$$

$$\begin{aligned} {}^{irr}\langle\langle Z_{i\sigma}^{(2)} | Z_{i\sigma}^{(1)+} \rangle\rangle &= {}^{irr}\langle\langle Z_{i\sigma}^{(1)} | Z_{i\sigma}^{(2)+} \rangle\rangle = -\gamma^2 \tilde{S} \{ (\tilde{S} + \\ &+ \langle S^z \rangle + \langle S^\sigma \rangle \langle S^{-\sigma} \rangle + \frac{1}{2\tilde{S}} (\langle S^\sigma \rangle \langle S^z S^{-\sigma} \rangle + \frac{1}{2} \langle S^{z2} \rangle)) \times \end{aligned}$$

$$\begin{aligned} &A_{\sigma,\omega}^{22} + (\tilde{S} + \langle S^z \rangle + \frac{1}{4\tilde{S}} \langle S^z \rangle^2) A_{\sigma,\omega}^{12} - \langle S^\sigma S^{-\sigma} \rangle - \\ &- \langle S^{-\sigma} \rangle \langle S^\sigma \rangle \Theta_{-\sigma,-\sigma}^{22} + \langle S^\sigma \rangle \langle S^{-\sigma} \rangle \Theta_{-\sigma,-\sigma}^{12} \} \end{aligned}$$

and

$$\begin{aligned}
& \text{irr} \ll Z_{i\sigma}^{(2)} | Z_{i\sigma}^{(2)+} \gg \text{irr} = -\gamma^2 \tilde{S} \{ (\tilde{S} + 2 \langle S^z \rangle + \langle S^\sigma \rangle \langle S^{-\sigma} \rangle + \\
& + \langle S^\sigma S^{-\sigma} \rangle + \frac{1}{\tilde{S}} (\langle S^{z2} \rangle + \langle S^z \rangle^2) / 2 + \langle S^z S^\sigma \rangle \langle S^{-\sigma} \rangle + \\
& \langle S^\sigma \rangle \langle S^z S^{-\sigma} \rangle + \langle S^{-\sigma} S^\sigma \rangle \langle S^\sigma S^{-\sigma} \rangle) A_{\sigma,\omega}^{22} + (\tilde{S} + \frac{3}{2} \langle S^z \rangle + \\
& + \langle S^{-\sigma} \rangle \langle S^\sigma \rangle + \frac{1}{2\tilde{S}} (\langle S^{z2} \rangle + \langle S^z \rangle^2) / 2 + \\
& \langle S^z S^\sigma \rangle \langle S^{-\sigma} \rangle) A_{\sigma,\omega}^{21} + (\tilde{S} + \frac{3}{2} \langle S^z \rangle + \langle S^{-\sigma} \rangle \langle S^\sigma \rangle + \\
& + \frac{1}{2\tilde{S}} (\langle S^{z2} \rangle + \langle S^z \rangle^2) / 2 + \langle S^z S^{-\sigma} \rangle \langle S^\sigma \rangle) \times \\
& \times A_{\sigma,\omega}^{12} + (\tilde{S} + \langle S^z \rangle + \frac{1}{4\tilde{S}} \langle S^{z2} \rangle) A_{\sigma,\omega}^{11} - 2 \langle S^\sigma S^{-\sigma} \rangle \times \\
& \times \Theta_{-\sigma,-\sigma}^{22} + (\langle S^\sigma \rangle \langle S^{-\sigma} \rangle - \langle S^\sigma S^{-\sigma} \rangle) \times \\
& \times (\Theta_{-\sigma,-\sigma}^{21} + \Theta_{-\sigma,-\sigma}^{12}) + (\langle S^\sigma \rangle \langle S^{-\sigma} \rangle + \langle S^\sigma S^{-\sigma} \rangle) \Theta_{-\sigma,-\sigma}^{11} \}.
\end{aligned} \quad (29)$$

Such general expressions of the irreducible parts are hardly suitable for the analytical treatment, but allow the perfect numerical analysis.

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

$$\langle S^z \rangle, \langle S^\sigma \rangle, \langle S^{z2} \rangle, \langle S^+ S^- \rangle, \langle S^+ S^z \rangle, \langle S^- S^z \rangle. \quad (30)$$

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 $\ll S_i^+ | S_i^- \gg_\omega$ and $\ll S_i^z | S_i^z \gg_\omega$ 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_i^z and S_i^σ :

$$\begin{aligned}
[S_i^z, \hat{H}] = & \gamma \left\{ \sum_{\Delta} [S_i^+ S_{i+\Delta}^- a_{i\uparrow}^{(2)+} a_{i+\Delta\uparrow}^{(2)} - S_{i-\Delta}^+ S_i^- a_{i-\Delta\uparrow}^{(2)+} a_{i\uparrow}^{(2)} + \right. \\
& + S_{i-\Delta}^- S_i^+ a_{i-\Delta\downarrow}^{(2)+} a_{i\downarrow}^{(2)} - S_i^- S_{i+\Delta}^+ a_{i\downarrow}^{(2)+} a_{i+\Delta\downarrow}^{(2)}] + \\
& + \sum_{\Delta} [S_i^+ (a_{i-\Delta\downarrow}^{(2)+} a_{i\downarrow}^{(2)} - a_{i\downarrow}^{(2)+} a_{i+\Delta\uparrow}^{(2)} + a_{i-\Delta\downarrow}^{(1)+} a_{i\uparrow}^{(2)} - a_{i\downarrow}^{(2)+} a_{i+\Delta\uparrow}^{(1)}) - \\
& \left. - S_i^- (a_{i-\Delta\uparrow}^{(2)+} a_{i\downarrow}^{(2)} - a_{i\uparrow}^{(2)+} a_{i+\Delta\downarrow}^{(2)} + a_{i-\Delta\uparrow}^{(1)+} a_{i\downarrow}^{(2)} - a_{i\uparrow}^{(2)+} a_{i+\Delta\downarrow}^{(1)}) \right\},
\end{aligned} \quad (31)$$

$$\begin{aligned}
[S_i^\sigma, H] = & \sigma h S_i^\sigma - \sigma \gamma \left\{ \sum_{\Delta, \sigma'} \frac{S_i^\sigma}{2} (a_{i\sigma'}^{(2)+} a_{i+\Delta\sigma'}^{(2)} + a_{i-\Delta\sigma'}^{(2)+} a_{i\sigma'}^{(2)} + \right. \\
& + a_{i\sigma'}^{(2)+} a_{i+\Delta\sigma'}^{(1)} + a_{i-\Delta\sigma'}^{(1)+} a_{i\sigma'}^{(2)}) + \sum_{\Delta} [2 S_{i-\Delta}^\sigma S_i^z a_{i-\Delta\sigma}^{(2)+} a_{i\sigma}^{(2)} - \\
& - S_i^z S_{i-\Delta}^\sigma a_{i-\sigma}^{(2)+} a_{i+\Delta, -\sigma}^{(2)} + 2 S_i^z (a_{i-\Delta\uparrow}^{(2)+} a_{i\downarrow}^{(2)} - \\
& \left. - a_{i\uparrow}^{(2)+} a_{i+\Delta\downarrow}^{(2)} + a_{i-\Delta\uparrow}^{(1)+} a_{i\downarrow}^{(2)} - a_{i\uparrow}^{(2)+} a_{i+\Delta\downarrow}^{(1)}) \right\}.
\end{aligned} \quad (32)$$

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,

$$\begin{aligned}
[S_i^+, H] = & h S_i^+ + \beta_1^{(1)} S_i^+ + \beta_2^{(1)} S_i^z + \hat{Y}_i^{(1)} \text{ and} \\
[S_i^z, H] = & \beta_1^{(2)} S_i^+ + \beta_2^{(2)} S_i^z + \hat{Y}_i^{(2)}.
\end{aligned} \quad (33)$$

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

$$\langle [S_i^-; \hat{Y}_i^{(1,2)}] \rangle = 0 \text{ and } \langle [S_i^z; \hat{Y}_i^{(1,2)}] \rangle = 0, \quad (34)$$

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

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

$$\begin{aligned}
\omega \ll \hat{A} | \hat{B} \gg_\omega = & \frac{1}{2\pi} \langle [\hat{A}, \hat{B}] \rangle + \ll [\hat{A}, \hat{H}] | \hat{B} \gg_\omega, \\
\omega \ll \hat{A} | \hat{B} \gg_\omega = & \frac{1}{2\pi} \langle [\hat{A}, \hat{B}] \rangle - \ll \hat{A} | [\hat{B}, \hat{H}] \gg_\omega,
\end{aligned} \quad (35)$$

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

$$\begin{aligned}
(\omega - h) \ll S_i^+ | S_i^- \gg_\omega = & 2 \langle S_i^z \rangle + \ll Y_i^{(1)} | S_i^- \gg_\omega, \\
\omega \ll S_i^z | S_i^- \gg_\omega = & \langle S_i^- \rangle + \ll Y_i^{(2)} | S_i^- \gg_\omega.
\end{aligned} \quad (36)$$

Constructing the equations for searching the Green functions $\ll S_i^+ | S_i^z \gg_\omega$ and $\ll S_i^z | S_i^z \gg_\omega$, and performing the procedure (35) with these functions, one gets the matrix equation

$$\begin{aligned}
& \begin{pmatrix} \omega - h & 0 \\ 0 & \omega \end{pmatrix} \begin{pmatrix} \ll S_i^+ | S_i^- \gg_\omega & \ll S_i^+ | S_i^z \gg_\omega \\ \ll S_i^z | S_i^- \gg_\omega & \ll S_i^z | S_i^z \gg_\omega \end{pmatrix} = \\
& = \frac{1}{2\pi} \begin{pmatrix} 2 \langle S_i^z \rangle & - \langle S_i^+ \rangle \\ \langle S_i^- \rangle & 0 \end{pmatrix} + \\
& + \begin{pmatrix} \text{irr} \ll Y_i^{(1)} | Y_i^{(1)+} \gg_\omega & \text{irr} \ll Y_i^{(1)} | Y_i^{(2)+} \gg_\omega \\ \text{irr} \ll Y_i^{(2)} | Y_i^{(1)+} \gg_\omega & \text{irr} \ll Y_i^{(2)} | Y_i^{(2)+} \gg_\omega \end{pmatrix} \times \\
& \times \begin{pmatrix} \omega - h & 0 \\ 0 & \omega \end{pmatrix}^{-1},
\end{aligned} \quad (37)$$

where the notions are introduced as follows

$$\begin{aligned}
\hat{S} &= \begin{pmatrix} \langle\langle S_i^+ | S_i^- \rangle\rangle_\omega & \langle\langle S_i^+ | S_i^z \rangle\rangle_\omega \\ \langle\langle S_i^z | S_i^- \rangle\rangle_\omega & \langle\langle S_i^z | S_i^z \rangle\rangle_\omega \end{pmatrix}, \\
\hat{Y} &= \begin{pmatrix} irr \langle\langle Y_i^{(1)} | Y_i^{(1)+} \rangle\rangle_{irr \omega} & irr \langle\langle Y_i^{(1)} | Y_i^{(2)+} \rangle\rangle_{irr \omega} \\ irr \langle\langle Y_i^{(2)} | Y_i^{(1)+} \rangle\rangle_{irr \omega} & irr \langle\langle Y_i^{(2)} | Y_i^{(2)+} \rangle\rangle_{irr \omega} \end{pmatrix} \\
S_0 &= \begin{pmatrix} \frac{1}{\omega-h} & 0 \\ 0 & \frac{1}{\omega} \end{pmatrix} \begin{pmatrix} \langle S_i^z \rangle / \pi & -\langle S_i^+ \rangle / 2\pi \\ \langle S_i^- \rangle / 2\pi & 0 \end{pmatrix} = \\
&= \frac{1}{2\pi} \begin{pmatrix} \frac{2\langle S_i^z \rangle}{\omega-h} & -\frac{\langle S_i^+ \rangle}{\omega-h} \\ \frac{\langle S_i^- \rangle}{\omega} & 0 \end{pmatrix}, \\
\hat{A}_1 &= \begin{pmatrix} \langle S_i^z \rangle / \pi & -\langle S_i^+ \rangle / 2\pi \\ \langle S_i^- \rangle / 2\pi & 0 \end{pmatrix}, \\
\hat{A}_2 &= \frac{2\pi}{(\omega-h)\omega \langle S_i^- \rangle \langle S_i^+ \rangle} \times \\
&\times \begin{pmatrix} 0 & \omega^2 \langle S_i^+ \rangle \\ (\omega-h)^2 \langle S_i^- \rangle & 2(\omega-h)\omega \langle S_i^z \rangle \end{pmatrix}.
\end{aligned} \tag{38}$$

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

$$\hat{S} = \hat{S}_0 + \hat{S}_0 \hat{A}_1^{-1} \hat{Y} \hat{A}_2 \hat{S}_0. \tag{39}$$

Transform the equation (39) into the Dyson equation

$$\hat{S} = \hat{S}_0 + \hat{S}_0 \hat{D} \hat{S}, \tag{40}$$

with the mass operator in the form

$$\hat{D} = \hat{A}_1^{-1} irr \hat{Y} irr \hat{A}_2 + \hat{A}_1^{-1} irr \hat{Y} irr \hat{A}_2 \hat{S}_0 \hat{A}_1^{-1} irr \hat{Y} irr \hat{A}_2 + \dots \tag{41}$$

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:

$$\begin{aligned}
irr \langle\langle Y_i^{(1)} | Y_i^{(1)+} \rangle\rangle_{irr \omega} &= \gamma^2 \{ n_{\uparrow\uparrow}^{22} \left[\frac{1}{2} S_\omega^{+-} + \langle S^+ \rangle S_\omega^{z-} + \langle S^- \rangle \Lambda_h^{z+}(\omega) \right] + \left(n_{\uparrow\uparrow}^{21} \Lambda_{-(\varepsilon_d^\uparrow - \varepsilon_A)}^{+-}(\omega) + n_{\uparrow\uparrow}^{12} \Lambda_{\varepsilon_d^\uparrow - \varepsilon_A}^{+-}(\omega) \right) + \\
&+ n_{\downarrow\downarrow}^{12} \Lambda_{\varepsilon_d^\downarrow - \varepsilon_A}^{+-}(\omega) + n_{\downarrow\downarrow}^{21} \Lambda_{-(\varepsilon_d^\downarrow - \varepsilon_A)}^{+-}(\omega) \} / 4 + \\
&+ 4n_{\uparrow\uparrow}^{22} \{ \Xi_\omega^{zz} + \langle S^- \rangle \langle S^+ \rangle \Lambda_h^{zz}(\omega) + \langle S^z \rangle^2 S_\omega^{+-} \} + \\
&+ n_{\downarrow\downarrow}^{22} \{ 4\Xi_\omega^{zz} + 4\langle S^- \rangle \langle S^+ \rangle \Lambda_h^{zz}(\omega) + S_\omega^{+-} / 2 - \\
&- \langle S^- \rangle \Lambda_h^{z+}(\omega) + 4\langle S^z \rangle^2 S_\omega^{+-} \} - n_{\downarrow\downarrow}^{22} \langle S^+ \rangle S_\omega^{z-} + \\
&+ 4n_{\downarrow\downarrow}^{22} \{ \Lambda_{\varepsilon_d^\downarrow - \varepsilon_d^\uparrow}^{zz}(\omega) + \Lambda_{-(\varepsilon_d^\downarrow - \varepsilon_d^\uparrow)}^{zz}(\omega) \} + \\
&+ 4[n_{\uparrow\downarrow}^{12} \Lambda_{\varepsilon_d^\downarrow - \varepsilon_A}^{zz}(\omega) + n_{\uparrow\downarrow}^{21} \Lambda_{-(\varepsilon_d^\uparrow - \varepsilon_A)}^{zz}(\omega)],
\end{aligned} \tag{42}$$

where

$$\begin{aligned}
\Lambda_\zeta^{jk}(\omega) &= e^{-\beta\zeta} S_{\omega+\zeta}^{jk} + \\
&+ (e^{-\beta\zeta} - 1) \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega + \zeta - \omega'} \left[-2 \text{Im} S_{\omega'+i\varepsilon}^{jk} \right]_{\varepsilon \rightarrow 0}, \\
\Xi_\omega^{jk} &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega - \omega'} (e^{\beta\omega'} - 1) \times \\
&\times \int_{-\infty}^{\infty} \frac{d\omega''}{2\pi} \left[-2 \text{Im} S_{\omega''-i\varepsilon_1}^{+-} \right]_{\varepsilon_1 \rightarrow 0} \left[-2 \text{Im} S_{\omega'-\omega''-i\varepsilon_2}^{jk} \right]_{\varepsilon_2 \rightarrow 0},
\end{aligned}$$

$$n_{ij}^{kl} = (1 - n_i^k) n_j^l \text{ and } S_\tau^{lm} = \langle\langle S_i^l | S_i^m \rangle\rangle_\tau.$$

$$\begin{aligned}
irr \langle\langle Y_i^{(1)} | Y_i^{(2)+} \rangle\rangle_{irr \omega} &= \gamma^2 \left\{ -n_{\uparrow\uparrow}^{22} \langle S^+ \rangle S_\omega^{+-} / 2 + \right. \\
&+ n_{\uparrow\uparrow}^{22} \{ 2\Xi_\omega^{z+} + \langle S^+ \rangle \langle S^- \rangle \Lambda_h^{z+}(\omega) + \langle S^z \rangle S_\omega^{+-} \} - \\
&- \frac{n_{\downarrow\downarrow}^{22}}{2} \langle S^+ \rangle S_\omega^{+-} - n_{\downarrow\downarrow}^{22} \{ 2\Xi_\omega^{z+} + 2\langle S^- \rangle \langle S^+ \rangle \Lambda_h^{z+}(\omega) + \\
&+ 2\langle S^+ \rangle \langle S^z \rangle \Lambda_{-h}^{z+}(\omega) \} + 2n_{\uparrow\downarrow}^{22} \left(\Lambda_{\varepsilon_d^\downarrow - \varepsilon_d^\uparrow}^{z+}(\omega) + \Lambda_{-(\varepsilon_d^\downarrow - \varepsilon_d^\uparrow)}^{z+}(\omega) \right) + \\
&+ 2 \left(n_{\uparrow\downarrow}^{12} \Lambda_{\varepsilon_d^\downarrow - \varepsilon_A}^{z+}(\omega) + n_{\uparrow\downarrow}^{21} \Lambda_{-(\varepsilon_d^\uparrow - \varepsilon_A)}^{z+}(\omega) \right) \left. \right\},
\end{aligned} \tag{43}$$

$$\begin{aligned}
irr \langle\langle Y_i^{(2)} | Y_i^{(2)+} \rangle\rangle_{irr \omega} &= \gamma^2 \{ (n^{(2)} - (n_{\uparrow}^{(2)2} + n_{\downarrow}^{(2)2})) \times \\
&\times \{ 2\Xi_\omega^{++} + \langle S^- \rangle \langle S^+ \rangle \Lambda_h^{++}(\omega) + \Lambda_{-h}^{++}(\omega) \} + \\
&- n_{\uparrow\downarrow}^{22} \left\{ \Lambda_{\varepsilon_d^\downarrow - \varepsilon_d^\uparrow}^{+-}(\omega) + \Lambda_{\varepsilon_d^\uparrow - \varepsilon_d^\downarrow}^{+-}(\omega) + \tilde{\Lambda}_{\varepsilon_d^\downarrow - \varepsilon_d^\uparrow}^{+-}(\omega) + \right. \\
&+ \tilde{\Lambda}_{\varepsilon_d^\uparrow - \varepsilon_d^\downarrow}^{+-}(\omega) \left. \right\} - n_{\downarrow\uparrow}^{12} \Lambda_{\varepsilon_A - \varepsilon_d^\uparrow}^{+-}(\omega) \\
&- n_{\downarrow\uparrow}^{21} \Lambda_{\varepsilon_A - \varepsilon_d^\downarrow}^{+-}(\omega) - n_{\uparrow\downarrow}^{12} \tilde{\Lambda}_{\varepsilon_A - \varepsilon_d^\uparrow}^{+-}(\omega) - n_{\uparrow\downarrow}^{21} \tilde{\Lambda}_{\varepsilon_A - \varepsilon_d^\downarrow}^{+-}(\omega) \left. \right\},
\end{aligned} \tag{44}$$

with

$$\begin{aligned}
\tilde{\Lambda}_\zeta^{jk}(\omega) &= e^{-\beta\zeta} S_{-\omega-\zeta}^{jk} + \\
&+ (e^{-\beta\zeta} - 1) \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega + \zeta - \omega'} \left[-2 \text{Im} S_{-\omega'-i\varepsilon}^{jk} \right]_{\varepsilon \rightarrow 0}.
\end{aligned}$$

5. Conclusions

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^σ have been neglected when the Vonsovskii Hamiltonian was written in the spin-polaron approximation (8, 9). In the case of

DMS, these components occur of importance, which can be seen from the equations for the electron propagators. Writing the Vonsovskii Hamiltonian in the spin-polaron approximation we assumed that S value is a large number ($S > 1/2$). It is seen from the self-energy electron parts (27–29) that the genuine parameter of the model is the t^2/S parameter corresponding to the Hubbard model and to the $t - J$ model [23] with the t^2/S parameter. There exists the peculiarity of the electron Green functions $\hat{G}_{0\sigma}$ in the approximation of the atomic limit (24) for DMS in comparison with the atomic limit for the magnetic semiconductors [38]. In DMS, the zero order Green function contains the carrier transfer. It has been pointed out that the more complicated averages of the spin operators have to be calculated for correct finding the electron spectra in magnetic semiconductors [28]. This statement is true for the case of DMS, too. As far as all the experimental studies of the temperature dependence of magnetization are performed in magnetic field [11–18], the Hamiltonian (1) includes the term of interaction between the localized magnetic moments and external magnetic field. The equations for the self-energy parts of the electron (27–29) and the spin (42–44) Green functions reveal entangled picture of the magnetic field participation rather than simple Zeeman splitting. The substantial requirements of our scheme are the homogeneity of the magnetic properties (22) and the single-node character of electron and spin Green functions. Under violation of the first requirement one can expect the phase layering [19, 23, 36], while breaking the second requirement leads to a more complicated problem [32] that has not been solved yet for the strongly correlated systems.

Appendix. Calculation of the irreducible electron and spin parts by means of two-time decoupling of the Green functions

In order to find the irreducible parts of the scattering matrix \hat{P}_σ , the two-time decoupling of the Green functions is exploited. For example, let us consider the following term of the matrix:

$$\sum_{\Delta', \Delta''}^{irr} \ll (1 + \frac{1}{2S} S_{i+\Delta'}^z) a_{i+\Delta'\uparrow}^{(2)} | (1 + \frac{1}{2S} S_{i+\Delta''}^z) a_{i+\Delta''\uparrow}^{(2)+} \gg^{irr} \equiv A_1^{irr}. \quad (A.1)$$

Since this term is diagonal at the lattice node, one can use the spectral theorem for the Fermi-operators [38,41,42]:

$$A_1^{irr} = \sum_{\Delta'}^{irr} \ll (1 + \frac{1}{2S} S_{i+\Delta'}^z) a_{i+\Delta'\uparrow}^{(2)} | (1 + \frac{1}{2S} S_{i+\Delta'}^z) a_{i+\Delta'\uparrow}^{(2)+} \gg^{irr} = \sum_{\Delta'} \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega - \omega'} (e^{\beta\omega'} + 1) \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{-i\omega't} \times \left\langle \left(1 + \frac{1}{2S} S_{i+\Delta'}^z\right)_i a_{i+\Delta'\uparrow}^{(2)+}(t) \left(1 + \frac{1}{2S} S_{i+\Delta'}^z\right) a_{i+\Delta'\uparrow}^{(2)} \right\rangle. \quad (A.2)$$

The Bogolyubov-Tyablikov decoupling of the operators gives

$$\left\langle \left(1 + \frac{1}{2S} S_{i+\Delta'}^z\right)_i a_{i+\Delta'\uparrow}^{(2)+}(t) \left(1 + \frac{1}{2S} S_{i+\Delta'}^z\right) a_{i+\Delta'\uparrow}^{(2)} \right\rangle \approx \left\langle \left(1 + \frac{1}{2S} S_{i+\Delta'}^z\right)_i \left(1 + \frac{1}{2S} S_{i+\Delta'}^z\right) \right\rangle \left\langle a_{i+\Delta'\uparrow}^{(2)+}(t) a_{i+\Delta'\uparrow}^{(2)} \right\rangle. \quad (A.3)$$

While the localized magnetic moments do not interact immediately, it appears that

$$S_{i+\Delta'}^z(t) = e^{-itH_0} S_{i+\Delta'}^z e^{itH_0} = S_{i+\Delta'}^z. \quad (A.4)$$

Then one gets

$$A_1^{irr} = \sum_{\Delta'} \left\langle \left(1 + \frac{1}{2S} S_{i+\Delta'}^z\right)^2 \right\rangle \ll a_{i+\Delta'\uparrow}^{(2)} | a_{i+\Delta'\uparrow}^{(2)+} \gg_{\omega}. \quad (A.5)$$

It is assumed that the system after the configuration averaging becomes homogeneous one. Using this assumption A_1^{irr} expression can be written as

$$A_1^{irr} = \left(1 + \frac{1}{S} \langle S^z \rangle + \frac{1}{4S} \langle S^z{}^2 \rangle\right) \ll a_{i\uparrow}^{(2)} | a_{i\uparrow}^{(2)+} \gg_{\omega}. \quad (A.6)$$

For the irreducible Green functions like $^{irr} \ll (1 + \frac{1}{2S} S_{i+\Delta'}^z) a_{i+\Delta'\uparrow}^{(2)} | S_{i+\Delta''}^- a_{i+\Delta''\uparrow}^{(2)+} \gg^{irr}$ due to relations

$$S_{i+\Delta}^-(t) = e^{-itH_0} S_{i+\Delta}^- e^{itH_0} = e^{-iht} S_{i+\Delta}^-, \quad (A.7)$$

the more complicated result can be derived,

$$\sum_{\Delta', \Delta''}^{irr} \ll (1 + \frac{1}{2S} S_{i+\Delta'}^z) a_{i+\Delta'\uparrow}^{(2)} | S_{i+\Delta''}^- a_{i+\Delta''\uparrow}^{(2)+} \gg^{irr} = \left(\langle S^- \rangle + \frac{1}{2S} \langle S^z \rangle \right) \times \left\{ e^{-\beta h} \ll a_{i\uparrow}^{(2)} | a_{i\uparrow}^{(2)+} \gg_{\omega+h} - (e^{-\beta h} - 1) \times \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega + h - \omega'} \left[-2 \text{Im} \ll a_{i\uparrow}^{(2)} | a_{i\uparrow}^{(2)+} \gg_{\omega+i\varepsilon} \right]_{\varepsilon \rightarrow 0} \right\}$$

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 \hat{P}_σ (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 Bose operators, the irreducible Green function is written as:

$$S_1^{irr} \equiv \sum_{\Delta', \Delta''}^{irr} \ll \frac{S_i^+}{2} (a_{i\uparrow}^{(2)+} a_{i+\Delta'\uparrow}^{(1)} + a_{i-\Delta'\uparrow}^{(1)+} a_{i\uparrow}^{(2)}) | \frac{S_i^-}{2} (a_{i\uparrow}^{(2)} a_{i+\Delta''\uparrow}^{(1)+} + a_{i-\Delta''\uparrow}^{(1)} a_{i\uparrow}^{(2)+}) \gg_{\omega}^{irr} = \sum_{\Delta', \Delta''} \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega - \omega'} (e^{\beta\omega'} - 1) \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{-i\omega't} \left\langle \frac{S_i^-(t)}{2} (a_{i\uparrow}^{(2)} a_{i+\Delta''\uparrow}^{(1)+} + a_{i-\Delta''\uparrow}^{(1)} a_{i\uparrow}^{(2)+}) \right\rangle \left(\frac{S_i^+(t)}{2} (a_{i\uparrow}^{(2)+} a_{i+\Delta'\uparrow}^{(1)} + a_{i-\Delta'\uparrow}^{(1)+} a_{i\uparrow}^{(2)}) \right). \quad (A.9)$$

Then, performing the Bogolyubov-Tyablikov decoupling, one receives:

$$\left\langle \frac{S_i^-(t)}{2} \left(a_{i\uparrow}^{(2)} a_{i+\Delta\uparrow}^{(1)+} + a_{i-\Delta\uparrow}^{(1)} a_{i\uparrow}^{(2)+} \right) \right\rangle \frac{S_i^+}{2} \left(a_{i\uparrow}^{(2)+} a_{i+\Delta\uparrow}^{(1)} + a_{i-\Delta\uparrow}^{(1)+} a_{i\uparrow}^{(2)} \right) \rangle = \left\langle \left(a_{i\uparrow}^{(2)} a_{i+\Delta\uparrow}^{(1)+} + a_{i-\Delta\uparrow}^{(1)} a_{i\uparrow}^{(2)+} \right) \right\rangle (t) \times \left\langle \left(a_{i\uparrow}^{(2)+} a_{i+\Delta\uparrow}^{(1)} + a_{i-\Delta\uparrow}^{(1)+} a_{i\uparrow}^{(2)} \right) \right\rangle, \quad (\text{A.10})$$

$$\frac{1}{4} \langle S_i^-(t) S_i^+ \rangle = \frac{1}{4} \delta_{\Delta, \Delta''} \left\langle \left(a_{i+\Delta\uparrow}^{(1)+} a_{i+\Delta\uparrow}^{(1)} \right) \left\langle a_{i\uparrow}^{(2)} a_{i\uparrow}^{(2)+} \right\rangle e^{i(\varepsilon_d^{\uparrow} - \varepsilon_A)t} + \left\langle a_{i-\Delta\uparrow}^{(1)} a_{i-\Delta\uparrow}^{(1)+} \right\rangle \left\langle a_{i\uparrow}^{(2)+} a_{i\uparrow}^{(2)} \right\rangle e^{-i(\varepsilon_d^{\uparrow} - \varepsilon_A)t} \right\rangle \left\langle S_i^-(t) S_i^+ \right\rangle,$$

where the following relation is utilized:

$$a_{i\uparrow}^{(2)}(t) = e^{-itH_0} a_{i\uparrow}^{(2)} e^{itH_0} = e^{i\varepsilon_d^{\uparrow} t} a_{i\uparrow}^{(2)}, \quad (\text{A.11})$$

$$a_{i+\Delta\uparrow}^{(1)+}(t) = e^{-itH_0} a_{i+\Delta\uparrow}^{(1)+} e^{itH_0} = e^{-i\varepsilon_A t} a_{i+\Delta\uparrow}^{(1)+}.$$

Finally, the irreducible spin part S_1^{irr} takes the following form:

$$S_1^{irr} = \frac{(1-n_{\uparrow}^{(2)})n_{\uparrow}^{(1)}}{4} \left\{ e^{\beta(\varepsilon_d^{\uparrow} - \varepsilon_A)} \langle\langle S_i^+ | S_i^- \rangle\rangle_{\omega - (\varepsilon_d^{\uparrow} - \varepsilon_A)} + \frac{(e^{\beta(\varepsilon_d^{\uparrow} - \varepsilon_A)} - 1)}{2\pi} \times \int_{-\infty}^{\infty} \frac{d\omega'}{\omega - (\varepsilon_d^{\uparrow} - \varepsilon_A) - \omega'} \left[-2\text{Im} \langle\langle S_i^+ | S_i^- \rangle\rangle_{\omega' + i\varepsilon} \right]_{\varepsilon \rightarrow 0} \right\} + \frac{(1-n_{\uparrow}^{(1)})n_{\uparrow}^{(2)}}{4} \left\{ e^{-\beta(\varepsilon_d^{\uparrow} - \varepsilon_A)} \langle\langle S_i^+ | S_i^- \rangle\rangle_{\omega + (\varepsilon_d^{\uparrow} - \varepsilon_A)} + \frac{e^{-\beta(\varepsilon_d^{\uparrow} - \varepsilon_A)} - 1}{2\pi} \times \int_{-\infty}^{\infty} \frac{d\omega'}{\omega + (\varepsilon_d^{\uparrow} - \varepsilon_A) - \omega'} \left[-2\text{Im} \langle\langle S_i^+ | S_i^- \rangle\rangle_{\omega' + i\varepsilon} \right]_{\varepsilon \rightarrow 0} \right\}.$$

Similarly for the part $S_2^{irr} \equiv \sum_{\Delta, \Delta''}^{irr} \langle\langle S_{i-\Delta}^+ S_i^z a_{i-\Delta\uparrow}^{(2)+} a_{i\uparrow}^{(2)} \rangle\rangle_{\omega}$ one has

$$S_2^{irr} = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega - \omega'} (e^{\beta\omega'} - 1) \times \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{-i\omega t} \sum_{\Delta, \Delta''} \left\langle \left(S_{i-\Delta}^- S_i^z \right)_t \left(S_{i-\Delta}^+ S_i^z \right) \right\rangle \times \left\langle \left(a_{i-\Delta\uparrow}^{(2)} a_{i\uparrow}^{(2)+} \right)_t \left(a_{i-\Delta\uparrow}^{(2)+} a_{i\uparrow}^{(2)} \right) \right\rangle =$$

$$n_{\uparrow}^{(2)} (1 - n_{\uparrow}^{(2)}) \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega - \omega'} (e^{\beta\omega'} - 1) \times \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{-i\omega t} \left\{ \langle S_{i-\Delta}^- (t) S_{i-\Delta}^+ \rangle \langle S_i^z (t) S_i^z \rangle + \langle S_{i-\Delta}^- (t) \rangle \langle S_{i-\Delta}^+ \rangle \times \langle S_i^z (t) S_i^z \rangle = \langle S_{i-\Delta}^- (t) S_{i-\Delta}^+ \rangle \langle S_i^z (t) \rangle \langle S_i^z \rangle \right\} = n_{\uparrow}^{(2)} (1 - n_{\uparrow}^{(2)}) \times \left\{ \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega - \omega'} (e^{\beta\omega'} - 1) \times \int_{-\infty}^{\infty} \frac{d\omega''}{2\pi} \left[-2\text{Im} \langle\langle S_i^+ | S_i^- \rangle\rangle_{\omega'' - i\varepsilon_1} \right]_{\varepsilon_1 \rightarrow 0} \times \left[-2\text{Im} \langle\langle S_i^z | S_i^z \rangle\rangle_{\omega' - \omega'' - i\varepsilon_2} \right]_{\varepsilon_2 \rightarrow 0} + \langle S^- \rangle \langle S^+ \rangle \times \left\{ e^{-\beta h} \langle\langle S_i^z | S_i^z \rangle\rangle_{\omega+h} + (e^{-\beta h} - 1) \times \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega + h - \omega'} \left[-2\text{Im} \langle\langle S_i^z | S_i^z \rangle\rangle_{\omega' + i\varepsilon} \right]_{\varepsilon \rightarrow 0} \right\} + \langle S^z \rangle \langle S^z \rangle \langle\langle S_i^+ | S_i^- \rangle\rangle_{\omega} \right\}.$$

By analogy, all other terms entering the irreducible electron and spin Green functions can be calculated, if the condition of independence of the averages on the site number is preserved. Thus, combining the calculated terms, the equations (27–29) and (42–44) are derived.

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