Theory of diluted magnetic semiconductors: A minimal model

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Abstract

In this article we review our recent theoretical studies on the carrier induced ferromagnetism of DMS. We propose a minimal model, which is composed of a single tight-binding band of carriers and magnetic impurities, which randomly substitute the host sites. Both of nonmagnetic attractive potentials due to impurities and the exchange interactions between carrier and impurity spins are taken into account. We apply the coherent potential approximation in studying this system. The obtained phase diagrams illustrate the characteristic features of the carrier induced ferromagnetism in DMS. The role of nonmagnetic interaction for the enhancement of the Curie temperature is clarified. The results suggest that the ferromagnetism in Ga1−xMnxAs is caused by a double-exchange-like mechanism mediated by valence band holes. We also report the results of numerical simulations of the model.

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1. Introduction

The so-called magnetic semiconductors have been investigated already for long time. A breakthrough was brought about in 1989 by Munekata et al., who succeeded in doping considerable amount of Mn atoms into InAs by means of the low-temperature molecular beam epitaxy (LTMBE) and realized heavy doping of carriers as well as magnetic impurities [1]. Active investigations of diluted magnetic semiconductors (DMS), i.e. nonmagnetic semiconductors doped with magnetic impurities, followed this discovery and a new field called ‘spintronics’ is now at the focus of strong interest [2]. The clue to realize the spintronic devices may be the creation of a semiconducting material with ferromagnetism at room temperatures. Such a material is, however, still not available.

The most promising candidate for a spintronic material seems to be DMS based on II–VI or III–V compounds. A high Curie temperature (110 K) was obtained in Ga1−xMnxAs with \( x \approx 0.05 \) [3]. It is well established that the ferromagnetism in DMS is carried by localized spins of magnetic impurities and the interactions between them are mediated by carriers incorporated by these impurities. Experimental evidence was given by the fact that the variation of the carrier density by optical excitations [4] or a gate voltage [5] leads to modifications of the ferromagnetism. The ferromagnetism in the DMS is, therefore, called carrier induced ferromagnetism.

At present there is no common understanding on the mechanism for the carrier induced ferromagnetism. The following properties, however, seem to be generally accepted for (Ga,Mn)As: (i) Mn ions substitute randomly for Ga cations [6]. (ii) A Mn ion in GaAs gives rise to an acceptor level at about 0.113 eV above the valence band [7]. (iii) The Mn ion has highly localized \( d \) states with a magnetic moment of \( 5 \mu_B \) (or \( S=5/2 \) ) [7–9]. (iv) According to photo-emission studies [10–12], X-ray absorption spectroscopy [13], and band calculations [14,15], the Mn-induced states near the Fermi level have mainly As \( 4p \) character. (v) The \( p-d \) exchange interaction between the As \( 4p \) hole and the localized Mn \( d \) spin is antiferromagnetic (AF) [14,16,17], and is of about the same magnitude with that in II–VI-based DMS [10,18]. (vi) Antisites and other kinds of defects which may trap holes are common in samples grown by LTMBE [19]. As a result the density of the holes and that of Mn ions are separate sample-dependent quantities to be determined experimentally, though we may expect one hole donated by a Mn atom.
There are already many theoretical studies on the origin of the carrier-induced ferromagnetism [20]. Dietl et al. [21–24] referred to the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction as the origin of the ferromagnetism. Although their theory explains some characteristic magnetic and transport properties of the DMS, the application of the RKKY theory is questionable because of low carrier density in DMS. The RKKY theory is, on the contrary, based on the assumption that the Fermi energy is much larger than the interaction exchange between the localized and the carrier spins. In contrast to the RKKY picture, Akai stressed the assumption that the Fermi energy is much larger than the transport properties of the DMS. The RKKY theory is, on the contrary, based on the RKKY theory. It would be, therefore, useful to examine the property of this model in detail in order to have an insight of the physics in DMS and to obtain suggestions for material designing.

2. Minimal model

We assume a lattice model of DMS where the unit cell of the host material is composed of a single site. There is a single orbit for carriers at each site and carriers hop among these sites. Magnetic impurities substitute randomly the host atoms. At each impurity site exists a localized spin. Impurities exert attractive potentials on carriers and localized spins interact with carrier spins. We neglect the Coulomb interactions between carriers as well as direct interactions among localized spins. Then the Hamiltonian for the carriers reads

\[ H = \sum_{m,n,s} t_{mn} a_\dagger_m a_n + \sum_{n,s} u_n a_\dagger_n a_n - \sum_{l(\text{imp.})} \sum_{\mu,\nu} \sigma_{\mu l} a_\dagger_l - S_l, \]

where \( t_{mn} \) is the hopping matrix element between the site \( m \) and \( n \). The localized spin at the site \( l \) is denoted by \( S_l \) and \( \Sigma_{l(\text{imp.})} \) implies the sum over the impurity sites. The nonmagnetic potential \( u_n \) at the site \( n \) is given by

\[ u_n = \sum_{l(\text{imp.})} v(R_n - R_l) \]

where \( v(R) \) is the potential on a carrier at the position \( R \) exerted by an impurity at the origin. For a simplest model we may assume a contact potential \( v(R) = -U_0 \delta_{R,0} \), which is nothing but the difference between the energy levels of an impurity and a host site. We may also simplify the model by assuming the localized spins to be of Ising type, i.e. they have only two possible orientations with \( S^z = \pm 1 \).

In Section 3, we treat this simplest version of the model to overview the characteristic features of the carrier-induced ferromagnetism [35,36], since the essential features of magnetic and electronic properties do not depend on whether the exchange is of Ising- or Heisenberg-type. We assume the exchange constant \( I \) for the Ising-type model to be positive since the result does not depend on the sign of \( I \).

We obtain the averaged density of states (DOS) of carriers using the CPA. Then we calculate the free energy for a set of parameters, i.e. the impurity concentrations \( x \), the carrier density \( n \), magnetization \( m \) and the temperature \( T \). We employ as the DOS of the host material a semicircular one with the half-band width \( \Delta \). We determine the thermal equilibrium for given values of \( x \), \( n \) and \( T \) by minimizing \( F \) in terms of \( m \).
3. Phase diagrams

As the half-bandwidth $\Delta$ scales the energy we measure the strength of the nonmagnetic potential by $\hat{\delta} = -U/\Delta$. Then the normalized effective potential for a carrier at an impurity site is $\hat{\delta} = -I/\Delta$ or $\hat{\delta} + I/\Delta$. If these quantities are less than about $-0.7$ there appear separate impurity bands at the bottom of the DOS. Fig. 1 displays how the DOS changes according to the change in $\hat{\delta}$ for fixed $x$, $m$ and $I/\Delta$. As $\hat{\delta}$ decreases, the impurity band of the carriers with spins parallel with localized ones splits first from the bottom of the host band and then does that of the carriers with antiparallel spins. For the exchange constant not large enough, two separate impurity bands may merge into one. The whole DOS separates into two or three parts according to the values of parameters. We denote the phases with the DOS composed of one, two and three parts by type1, type2 and type3, respectively. The type3 phase is further classified into type3–1 and type3–2 depending on whether the separate impurity bands appear on both sides of the main band or on the same side. The type3–1 phase is realized for large $I/\Delta$ and the type3–2 appears for large $|\hat{\delta}|$. We show the phase diagrams in terms of the DOS in Fig. 2 where $x$ is fixed to be 0.05. The phase diagram for $\hat{\delta} = 0$ was obtained earlier [26]. We can see from these diagrams how the impurity bands split from the main band with change in $I/\Delta$ and $\hat{\delta}$. Please note that the DOS’s for carriers with different spins have different profiles for $\hat{\delta} = 0$, though their phase diagrams are same. Introduction of negative $\hat{\delta}$ causes the difference between phase diagrams of up and down spin carriers which leads to a variety of behaviors in transport properties.

Fig. 3 shows the DOS in arbitrary unit for $x = 0.05$, $m = 0.0$ and $I/\Delta = 0.6$. The local DOS at an impurity site shows the probability for a carrier with a definite energy to stay at impurity sites. Since the effective exchange interaction between the carrier and the localized spins are proportional to the local DOS, this quantity plays an important role in the magnetism. Fig. 3(a) shows the case where $\hat{\delta} = 0.0$ and the impurity band is formed but still not separated from the main band. It is clearly seen from these figures that the impurity band at the bottom of the DOS is mostly composed of the carrier states with spin parallel with the localized ones. It implies that the low energy carriers are strongly coupled to localized spins even if the impurity bands are not well separated. Fig. 3(b) shows the case where $\hat{\delta} = -0.3$ and the impurity band at the bottom of DOS is well separated from the main one. In this case the carriers in the impurity band is almost completely parallel to the localized spins. We will show this fact again in Section 4 as to the model with Heisenberg-type exchange interactions. These results imply that the carriers are strongly coupled to localized spins and the coupling cannot be regarded as a small perturbation as is assumed in the RKKY theory.

Next we show the magnetic ground state phase diagram for $x = 0.05$ in Fig. 4. You can see from this figure that the perfectly ferromagnetic ground state is always realized for small $n$ and finite $I/\Delta$ and negative $\hat{\delta}$. With increase in $n$, the magnetization starts to decrease at a critical value $n_{c1}$ (solid line in Fig. 4) and the partially ferromagnetic state is realized. The polarization continuously decreases with $n$ to vanish at another critical value $n_{c2}$ (dashed line in Fig. 4) where the ground state becomes paramagnetic. The critical densities $n_{c1}$ and $n_{c2}$ show different dependence on $I/\Delta$ according to the magnitude of $\hat{\delta}$. In the case where there is no nonmagnetic attractive potential ($\hat{\delta} = 0$), $n_{c1}$ and $n_{c2}$ first increase and each has a maximum with the increase in $I/\Delta$. The characteristic feature of this case is that $n_{c2}$ can be much larger than both $n_{c1}$ and $x$ for small $I/\Delta$. It rapidly decreases with increase in $I/\Delta$ and almost agrees with $n_{c1}$ for $I/\Delta \geq 0.3$. For $I/\Delta \geq 0.7$, $n_{c1}$ and $n_{c2}$ stay nearly constant and are almost equal to $x$. These features were reported earlier by Yagi et al. [26]. It should be noted that the value $I/\Delta \approx 0.7$ agrees with that on the phase boundary where impurity bands split from the main one. Finite attractive nonmagnetic potential ($\hat{\delta} < 0$) causes the reduction of the partially ferromagnetic phase. The maximum of $n_{c2}$ is suppressed and $n_{c2}$ stays almost always $\approx x$. Though for some parameter regions $n_{c1}$ and $n_{c2}$ are very close to each other, the transitions at $n = n_{c1}$ and $n_{c2}$ are always continuous [38].

The obtained magnetization shows usual temperature-dependence. We show $T_c$ as a function of $n$ in Fig. 5 for $I/\Delta = 1.0$ and 0.5 and various values of $\hat{\delta}$. The maximum of $T_c$ occurs at $n \leq x/2$. For $\hat{\delta} = 0$, the $n$-dependence of $T_c$ changes

Fig. 1. The DOS for various values of $\hat{\delta}$ while the other parameters are fixed as $x = 0.05$, $I/\Delta = 0.2$ and $m = 0.5$. Figures show the cases where (a) $\hat{\delta} = -0.4$, (b) $-0.7$, (c) $-0.8$ and (d) $-1.0$. 
according to whether \( I/D \geq 0.7 \) or not. For small \( I/D \), \( T_c \) gradually decreases with increase in \( n \) after the maximum value and vanishes at \( n_{c2} \), which is much larger than \( x \). On the other hand, \( T_c \) decreases quite rapidly and vanishes at \( n_{c2} \) for large \( I/D \).

According to above difference we may classify the system into two categories, i.e. the weak-coupling and the strong-coupling systems. When we introduce negative \( \delta \), the weak-coupling region is suppressed and the system starts to show the strong-coupling behavior already for small \( I/D \). Therefore, we understand that the main effect of a negative \( \delta \) on the ferromagnetism is to enhance the effect of exchange interaction. At the bottom of the DOS, \( I/D - \delta \) may be interpreted as the strength of an effective exchange interaction since the DOS at the bottom has almost same profile if \( I/D - \delta \) is same. The boundary of the weak-coupling and the strong-coupling is roughly given by the condition \( I/D - \delta = 0.7 \). We must note, however, that the effects of \( I/D \) and \( -\delta \) are not identical. We compare \( T_c \) of two cases with same \( I/D - \delta \) but with different \( I/D \) in Fig. 6. Fig. 6 shows that the increase in \( I/D \) favors ferromagnetism more than the decrease in \( \delta \) does. This tendency is more pronounced for weaker interaction. We may still regard \( I/D - \delta \) as the quantity regulating the properties of low energy carriers.

In the strong-coupling system there appear impurity bands at the bottom of DOS, in which the local DOS at the impurity sites is strongly confined. The spins of carriers in the impurity bands are strongly coupled to the localized spins. Then the increase of the magnetization enhances hopping probabilities of carriers and induces the broadening of the impurity band, which leads to the decrease in the total kinetic energy.

![Fig. 2. The phase diagram in terms of the DOS for \( x = 0.05 \). In the phase type1 and type 2 the DOS is composed of one and two components, respectively. In the type3–1 phase two separate impurity bands appear on both sides of main band and in the type3–2 phase they appear on the same side.](image)

![Fig. 3. The total and the local DOS for \( x = 0.05, m = 0, I/D = 0.6 \): (a) \( \delta = 0.0 \) and (b) \( \delta = -0.3 \). The full (broken) lines in the figures on the second row depict the local DOS at the impurity sites with upward (downward) localized spins. Notice that the scales of the DOS are different for different rows.](image)
and stabilizes the ferromagnetism. This is the mechanism causing the ferromagnetism in the strong-coupling systems. The decrease in the kinetic energy is maximal if the impurity band is half-filled and no decrease occurs when it is fully-filled. This explains why $T_c$ is maximal at $n = x/2$ and vanishes at $n = x$. This mechanism is similar to the DE mechanism in (La,Sr)MnO$_3$ [39,40]. We may, therefore, call this mechanism ‘DE-like’ mechanism.

Now that we have two categories of carrier induced ferromagnetism, which is more appropriate to describe (Ga,Mn)As or (In,Mn)As? We discuss this problem in the following section.

4. (Ga,Mn)As and (In,Mn)As

We applied the CPA to the model with Heisenberg-type exchange interactions in order to describe typical III–V based DMS, (Ga,Mn)As and (In,Mn)As [30,31]. The magnitude of the localized spins are taken to be $S$. For (Ga,Mn)As, we employed the parameter $IS/\Delta = -0.4$ ($I$ was chosen to be negative according to the experimental results), $\delta = -0.3$ and $\Delta = 2$ eV [14,15]. The present parameters are chosen to be consistent with an acceptor level at 0.113 eV in the dilute limit $(x \to 0)$ [7].

The DOS is shown as a function of the carrier energy $\lambda$ in Fig. 7 for $m = 0$ (a) and $m = 1$ (b) for various $x$. An impurity band forms around the acceptor level with the increase in $x$. When $m = 0$ the impurity band merges into the host valence band at $x \geq 0.035$, while when $m = 1$ the down-spin DOS is composed of a single band at $x \geq 0.017$. The result roughly agrees with the experimental observation of impurity-band-like states [12,43]. We restrict ourselves to the case $x = 0.05$ where a high $T_c$ was reported. The low energy band tail shown in Fig. 8(a) is strongly affected by the change in $m$. The analysis

![Fig. 4. The ground state magnetic phase diagram for $x = 0.05$ and various values of $\delta$.](image)

![Fig. 5. The Curie temperature as a function of the carrier density for $x = 0.05$: (a) $I/\Delta = 1.0$, (b) $I/\Delta = 0.5$.](image)
Fig. 6. Comparison of the Curie temperatures in the two cases with a same value of $I/\Delta - \delta$: (a) $I/\Delta - \delta = 0.6$, (b) $I/\Delta - \delta = 0.9$. Both are for $x = 0.05$.

Fig. 7. The low energy part of the DOS of Ga$_{1-x}$Mn$_x$As for various $x$: (a) $m = 0$, (b) $m = 1$. The DOS for down and up spin carriers are depicted by full and dashed lines as functions of the energy $\lambda$ of the carrier, respectively. The impurity level for an isolated impurity is indicated by a dot.

Fig. 8. The low energy part of (a) the DOS and (b) the spin-coupling strength $Q(\omega)$ of Ga$_{1-x}$Mn$_x$As for $x = 0.05$ and various values of $m$. The DOS for down and up spin carriers are depicted by full and dashed lines, respectively, in (a). The arrow indicates the Fermi level for $n = x (= 0.05)$. The impurity level is shown by a dot.
of the local DOS reveals that the change in the band tail is mainly due to the change in the local DOS at Mn sites. The result indicates that a carrier at the band tail stays mainly due to the change in the local DOS at Mn sites. The spin-coupling strength $Q(\lambda)$ defined by

$$Q(\lambda) \equiv -\frac{\langle \delta(\lambda - H) \sum_{\mu \nu} a_{\nu}^\dagger a_{\mu} \sigma_{\mu \nu} S_i \rangle / S}{\langle \delta(\lambda - H) \rangle}$$

at an impurity site $i$, is almost unity in the band tail irrespective to the value of $m$ (see Fig. 8(b)). It implies that the spin of a carrier in the band tail is oriented always antiparallel to the localized spin when the carrier is at a Mn site. The result implies that the system is in the strong-coupling region though a separate impurity band does not occur in (Ga,Mn)As for $x \gtrsim 0.03$. For given $m$, we obtained the total energy $E(m)$ assuming that the carriers are degenerate. This approximation may be justified for $T \lesssim T_c$, for $n \gtrsim 0.1x$ when the Fermi energy is larger than $k_B T_c$. As is shown in Fig. 9(a) the energy decrease due to magnetization is maximal for $n = x/2$ and vanishes at $n = x$. We estimated the Curie temperature approximately by using $E(m)$ instead of using the free energy (for details see the original paper [31]). This estimation of $T_c$ was shown to roughly agree with that obtained by the dynamical mean field theory [32]. Fig. 9(b) displays $T_c$ as a function of $n$.

Fig. 10 shows the maximal $T_c$ as a function of $x$, with the experimental ones [6]. Theoretical results for $T_c$ show reasonable agreement with experimental results. The maximum of $T_c$ increases with $x$ nearly proportionally to $\sqrt{x}$. The carrier concentration at which $T_c$ is maximal slightly decreases with increase in $x$ and equals to $\sim (0.4-0.3)x$ for $0.01 < x < 0.08$.

From above results we conclude that (Ga,Mn)As belongs to the strong-coupling systems and its ferromagnetism is caused by the DE-like mechanism of $p$-hole carriers. Note that the strong effective interaction between the carrier and the localized spins are realized by the aid of the nonmagnetic attractive potentials.

Another III–V-based DMS which exhibits the carrier induced ferromagnetism is (In,Mn)As. A recent spectroscopic study confirmed that the hole character is not Mn 3$d$ but As 4$p$ [18]. In (In,Mn)As, however, there are several features different from (Ga,Mn)As: (i) the highest $T_c$ of In$_{1-x}$Mn$_x$As thick films ever reported is 10 K (for $x \sim 0.01$) and is much lower than that of (Ga,Mn)As [8], though $T_c \approx 35$ K was achieved in In$_{1-x}$Mn$_x$As/(Ga,Mn)Sb heterostructures [41]. (ii) A Drude-like behavior in the optical absorption indicates that the holes in (In,Mn)As behave like free carriers [42]. (iii) The split-off state is not observed in (In,Mn)As [12,18,43]. Some of above differences can be explained within the framework of the present theory. The acceptor level in (In,Mn)As is reported to be about 0.03 eV [44], which is very shallow in comparison with that in (Ga,Mn)As (0.113 eV). Since, the exchange energy in (In,Mn)As is reported to be somewhat smaller than that in (Ga,Mn)As [18], we may choose the parameters as $J/\Delta = -0.3$ for (In,Mn)As. We assume as $\Delta = 2$ eV as for (Ga,Mn)As. Then we determined $\delta = -0.3$ so as to reproduce the acceptor level. Fig. 11 shows the result for $x = 0.05$. The result shows that the magnetic impurity band is almost united

![Fig. 9](image1.png)

![Fig. 10](image2.png)
with the host band because of the shallowness of the impurity level. This result explains why it is difficult to observe the split-off states in (In,Mn)As. Since, the Fermi level soon reaches the bottom of the host band, the holes are only weakly bound to Mn sites. Thus, the many holes move all over the crystal and behave like free carriers. The present theory, however, predicts rather high $T_c \sim 80$ K for $x=0.05$.

5. Numerical results

In the present section, we report on a numerical study of the minimal model (1). For this purpose we employed the model on the square lattice with the hopping matrix element $t$ only between nearest neighbor sites. We assume the Ising-type exchange interactions with the strength $I$ and the nonmagnetic attractive potential of contact-type with the strength $U$. In order to compare the results with those in previous sections we employ the half-bandwidth $\Delta = 4t$ as a unit of the energy and express the strength of the attractive potential in terms of $\delta = - U/\Delta$.

The numerical simulation was done in the following way. First, we fix a randomly chosen spatial configuration of impurities. Then we perform numerical diagonalization of the Hamiltonian $H$ for each states of localized spins at the impurity sites. The physical quantities are averaged by using the exact grand partition function taking into account of all states of localized spins. We average furthermore the physical quantities over randomly chosen real-space impurity configurations. The desired carrier density is given by the adjustment of the chemical potential $\mu$. In this work we employed a $10 \times 10$ lattice with periodic boundary conditions and the impurity and carrier concentrations are fixed as $x=0.05$ and $n=0.025$, respectively.

Since, we are dealing with a finite size system we cannot expect a long-range order. Therefore, we measure the magnetization by $M$ defined by

$$M = \sqrt{\langle \left( \frac{1}{N_i} \sum_i S_i \right)^2 \rangle}$$

where $\langle \rangle$ indicates the thermal average and $N_i$ is the number of the magnetic impurities. In Fig. 12 the $I$-dependence of $M$ is shown for $\delta=0$, $-0.375$ and $-0.648$. The value of $M$ for $I=0$ is $1/\sqrt{N_i}$ irrespective to $\delta$ though it should vanish in the thermodynamic limit. In the absence of the attractive potential, $M$ starts to decrease when the exchange $I$ is introduced and then it turns to increase at $I=0.5$. The fact that $M$ is smaller than $M_{I=0}$ implies that the effective interactions between the localized spins may be antiferromagnetic rather than ferromagnetic for weak $I/\Delta$. The magnetization $M$ becomes larger than $M_{I=0}$ at $I/\Delta = 0.7$ and takes a maximal value at $I/\Delta = 1.2$. Then it decreases quite slowly with the increase in $I/\Delta$. We may consider that effective ferromagnetic interactions are working between localized spins for $I/\Delta \geq 0.7$. The optimum value of the exchange coupling at which $M$ takes a maximum is denoted by $I_{\text{opt}}$. When we introduce a negative $\delta$ the graph of $M$ vs. $I/\Delta$ in Fig. 12 is shifted leftwards with a slight change of its profile. This result is a numerical evidence for the fact that

$$\text{Fig. 11. (a) The DOS of In}_{0.95}\text{Mn}_{0.05}\text{As for various values of } m. \text{ (b) The Curie temperature } T_c \text{ as a function of } n.$$
the attractive potential enhances exchange coupling between the carrier and the localized spins as we argued in previous sections. Similar results were also obtained in the simulations of a three-dimensional system [37].

Though the shifts of the curves in Fig. 12 are not quite equal to the values of \( \delta \), we may roughly consider that \( I - U \) is playing the role of an effective exchange coupling. We may estimated the optimal effective exchange coupling as \( I_{\text{op}}/\Delta - \delta \approx 1.2 \).

In Fig. 13(a) we show the DOS for \( I/\Delta = 0.5 \) and \( \delta = 0 \), where the effective AF couplings between localized spins is working. There is no impurity band split from the host band in this case. On the contrary, in Fig. 13(b)–(d) which correspond to the cases where the effective ferromagnetic coupling is operative, we observe a impurity band separated from the host one. The width of the impurity band in Fig. 13(c) is larger than those in Fig. 13(b) and (d). In the latter cases we may expect that the DE-like mechanism for ferromagnetism is operative. However, more detailed study is necessary to examine this expectation.

It is interesting that the numerical results indicate the decrease of effective ferromagnetic coupling for large \( I - U \). This behavior was not found in the CPA treatment of the model (see Figs. 13 and 14 of Ref. [31]). A possible explanation is that carriers are localized too strongly due to the strong attractions and cannot mediate the ferromagnetic interactions effectively. However, the decrease in \( M \) is small as can be seen in Fig. 12 and there is no clear difference between the width of the impurity band in Fig. 13(b) which corresponds to \( I = I_{\text{op}} \) and that in (d) corresponding to \( I > I_{\text{op}} \).

6. Summary and discussion

We constructed a minimal model for carriers in the DMS, which takes into account of both nonmagnetic attractive potentials due to impurity centers and the exchange interactions between carrier spins and localized spins. According to the analysis based on the CPA, we clarified the conditions for the carrier induced ferromagnetism to occur. It turned out that the system shows different characteristic behaviors according to the strength of the effective interaction determined by the exchange coupling and the nonmagnetic potential.

In the weak-coupling systems there is no pronounced impurity band. The local DOS at the impurity sites spreads to the whole energy range of the DOS. Therefore, the carriers with rather high energy can interact with localized spins. This leads to the ferromagnetism in a wide range of carrier density. On the other hand the effective interaction is weak and, therefore, the Curie temperature is low. A mean field type treatment based on the RKKY theory might be relevant in this region.

On the other hand in the strong-coupling systems there appear impurity bands at the bottom of DOS. The local DOS at the impurity sites is strongly confined in the impurity band and the carriers only in the impurity band strongly interact with localized spins. As a result the ferromagnetism occurs only for \( n < x \). The ferromagnetic mechanism is similar to that of the DE interaction.

Preliminary results of our numerical study in two-dimensions are consistent with the above picture.

We applied our theory to (Ga,Mn)As and (In, Mn)As employing parameters consistent with the optical data and obtained reasonable agreement with experimental results for magnetism. It turned out that (Ga,Mn)As belongs to the strong-coupling systems though the impurity band is not well separated from the host one. (In,Mn)As may be regarded to be marginal between the strong-coupling and the weak-coupling. The difference between these two materials comes

Fig. 13. Density of states for a fixed impurity configuration in the system with (a) \( I/\Delta = 0.5, \delta = 0 \), (b) \( I/\Delta = 0.5, \delta = -0.648 \), (c) \( I/\Delta = 1, \delta = 0 \), and (d) \( I/\Delta = 1, \delta = -0.648 \).
mainly from the difference in the strength of the nonmagnetic potential.

We also obtained the electrical conductivity in the framework of the CPA [34–36]. The results of the static and optical conductivities show various behaviors according to the parameters. Preliminary results were already reported in Refs. [34,35] and details will be reported elsewhere.

Sakai performed numerical simulations of the model with nearest neighbor hopping on the $6 \times 6 \times 6$ simple cubic lattice [37]. They found that the most favorable condition for the ferromagnetism for $x=0.6$ and $n=0.3$ is realized when the attractive potentials are rather weak and there is no impurity band at the bottom of the DOS. Their results showed that the optimal condition is $I - U \sim 2.5$, i.e., $\sim 0.3 \times$ the half-bandwidth. The result is in contrast with our result in two dimensions where $|I - \delta| = 1.15$ is the optimal condition. On the other hand the acceptor level is experimentally observed and rather strong ferromagnetism is realized in (Ga,Mn)As.

These facts may imply that the minimal model with contact attractive potentials is not quite appropriate for explaining the magnetic and optical properties in (Ga,Mn)As in a consistent way. If it is the case we need to improve the model.

A possible way of improving the model is to take into account of the long-ranged character of the attractive potential. In real systems the potential due to a charged impurity should be a screened Coulomb potential. Bound states due to an impurity may be too strongly localized if we employ a contact potential and as a result the hopping probabilities to other impurity sites may not have enough sizes to bring about carrier induced ferromagnetism. In the case of long-ranged attractive potentials, the bound states may be more loosely localized and may lead to a broad impurity band. If it is the case, the CPA calculation for a model with contact potentials might play a role of an effective theory for the exact treatment of a more realistic model with long-ranged potentials, since the CPA tends to overestimate the width of the impurity band. We are practicing at present a numerical study of a model with long-ranged nonmagnetic potentials. The results will be reported elsewhere. In addition to the improvements of the model, more detailed numerical studies of the model, for its simplest version as well, are necessary to understand the physics of the DMS.

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