

Comparison between the coherent potential approximation and the mean field approximation

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Abstract

We have calculated the Curie temperature T_C of diluted magnetic semiconductors (DMS) by applying three approximations for a simple model; the coherent potential approximation (CPA), the virtual crystal approximation (VCA), and the mean-field approximation (MFA). Comparison of the results reveals that both the VCA and the MFA overestimate the T_C for appropriate carrier density n , suggesting that the high T_C 's predicted on the basis of the VCA are artificial.

Key Word: diluted magnetic semiconductor (DMS), $\text{Ga}_{1-x}\text{Mn}_x\text{As}$, coherent potential approximation (CPA), mean field approximation (MFA), virtual crystal approximation (VCA)

1 Introduction

In spite of a great deal of recent experimental and theoretical activity, there is not yet a consensus on the fundamental mechanism leading to the ferromagnetism of $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ [1]. The mean-field Zener model (the phenomenological model) predicts the possibility of high Curie temperature for some materials [2]. The applicable range of the approximation, however, has not yet been clarified. To shed light on this problem, we calculate the Curie temperature T_C of diluted magnetic semiconductors (DMS) by applying three approximations for a simple model; the coherent potential approximation (CPA), the virtual crystal approximation (VCA), and the mean-field approximation (MFA).

2 Model and Methods

In the present model [3–6], $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ is regarded as a semiconducting alloy in which a mole fraction x of Ga ions (symbol: A) in GaAs are replaced at random by Mn ions (symbol: M). A single carrier (a p hole) moving in $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ is subject to the local

potential E_A or $E_M - I\sigma \cdot \mathbf{S}_n$ depending on whether it is on a Ga site or a Mn site. Here, E_A and E_M denote the spin independent potential on the Ga ion and Mn ion, respectively; $-I\sigma \cdot \mathbf{S}_n$ represents the p - d exchange interaction between the carrier (p hole) and the localized spin \mathbf{S}_n (d spin) of Mn located on the n site. Hereafter we set $E_A = 0$. Assuming that the carriers are degenerate, we calculate the total energy by

$$E(\langle S_z \rangle) = \int_{-\infty}^{\varepsilon_F} \omega [D_{\uparrow}(\omega) + D_{\downarrow}(\omega)] d\omega, \quad (1)$$

where $D_{\uparrow}(\omega)$ [$D_{\downarrow}(\omega)$] is the spin-polarized carrier density of states (DOS) with \uparrow (\downarrow) spin. The Curie temperature T_C is calculated employing the energy gain between the paramagnetic ($\langle S_z \rangle = 0$) and completely ferromagnetic ($\langle S_z \rangle = S$) states as

$$k_B T_C = \frac{2}{3x} [E(0) - E(S)]. \quad (2)$$

This approximation has been proven to give a reasonable estimation of T_C [7].

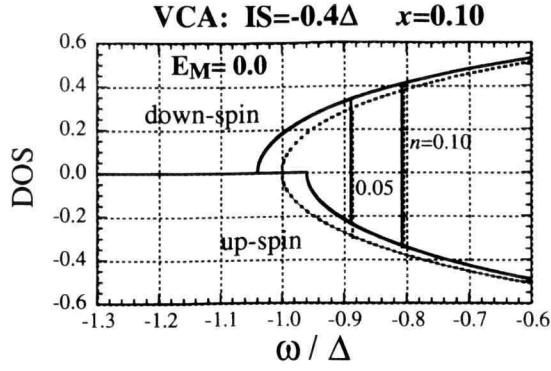


Figure 1: Result for the DOS calculated using the VCA; $IS = -0.4\Delta$, $E_M = 0.0$ and with $x = 0.10$. $D_{\uparrow}(\omega)\Delta$ and $-D_{\downarrow}(\omega)\Delta$ are depicted as functions of energy ω/Δ . Solid lines are for completely ferromagnetic states, and dotted lines are for paramagnetic states. Fermi levels of ferromagnetic (paramagnetic) states for $n = 0.05$ and $n = 0.10$ are shown by the vertical solid (dotted) lines.

3 Results and Discussion

First we show the results for the DOS calculated using VCA with $IS = -0.4\Delta$ and $E_M = 0$ for $x = 0.10$. In the VCA, the paramagnetic DOS accords with the model band, and the magnetization ($\langle S_z \rangle = S$) yields the spin-dependent shift $\pm xIS$ uniformly in the entire energy range. The Fermi level ε_F is nominally changed due to the magnetization when $n > 0.05$. If the carrier density n is sufficiently large, the energy gain is estimated using the DOS at the undisturbed Fermi level ε_F^0 , so that we obtain the mean-field approximation (MFA) result as

$$k_B T_C^{\text{MFA}} = \frac{2}{3} x (IS)^2 \rho(\varepsilon_F^0). \quad (3)$$

In Fig. 2, we depict the results for T_C obtained using the VCA, T_C^{VCA} , as a function of n for various values of x , together with T_C^{MFA} . Note that T_C^{MFA} depends only on the DOS at the Fermi level while T_C^{VCA} depends on the whole energy range of DOS that the carriers occupy. Comparing both results, T_C^{MFA} and T_C^{VCA} are in good agreement for small values of $|xIS|$ except in the case of a very small n .

Next, we compare the results with $E_M = 0$ obtained using the CPA with that using the VCA/MFA.

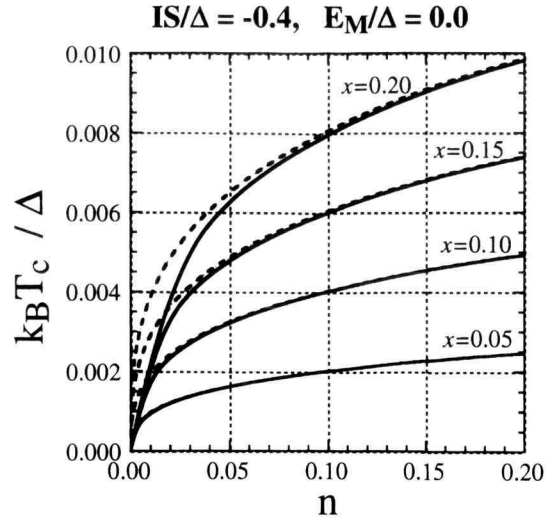


Figure 2: Result for T_C ; broken lines are for MFA using Eq. (3), solid lines are for VCA. $x = 0.05, 0.10, 0.15, 0.20$ (bottom to top).

The DOS shown in Fig. 3(a) reveals that the paramagnetic DOS is already broadened due to the disorder caused by the incorporation of magnetic ions. With the development of magnetization, the tail of the down-spin band stretches to the low-energy side, while that of the up-spin band shrinks. The change due to the development of magnetization, however, occurs only in the narrow energy range of the band-tail ($-1.1\Delta < \omega < -0.8\Delta$), where the coupling between carrier spin and localized spins is strong, as has been previously shown by us [4]. Thus, the increase in n does not accompany the energy gain due to the development of magnetization when n is as high as $n > x$. In consequence, T_C^{CPA} as a function of n has a peak at $n \sim x/2$, as shown in Fig. 4. Comparing the results for T_C with $E_M = 0$ as shown in Figs. 2 and 4, T_C^{VCA} is markedly higher than T_C^{CPA} when n exceeds a quarter of x for $x > 0.1$. The present result indicates that the prediction of high T_C on the basis of the MFA [2] needs to be re-examined. Note that $k_B/\Delta = 0.002$ corresponds to $T_C = 46\text{K}$ when we take the bandwidth $2\Delta = 4\text{eV}$. Thus, neither of the results obtained with $E_M = 0$ can explain the T_C as high as 110 observed in $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ with $x \sim 0.05$ [1].

In the VCA and/or MFA, the finite nonmagnetic

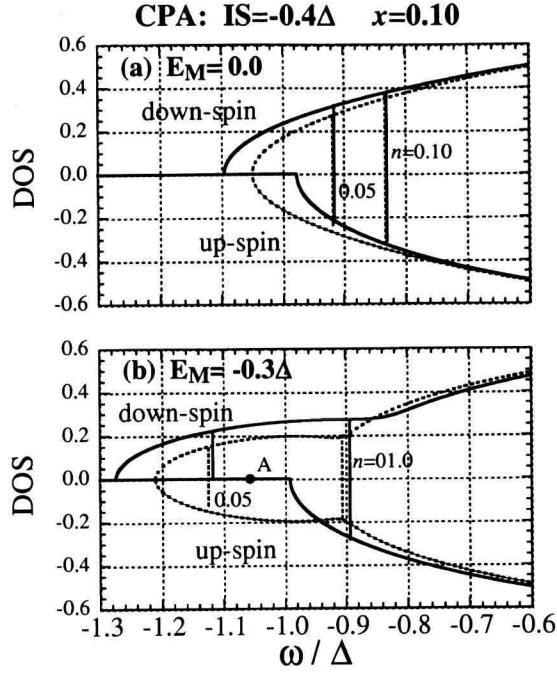


Figure 3: Result of the DOS calculated using the CPA; (a) $E_M = 0$, and (b) $E_M = -0.3\Delta$. Solid lines are for completely ferromagnetic states, and dotted lines are for paramagnetic states. Fermi levels of ferromagnetic (paramagnetic) states for $n = 0.05$ and $n = 0.10$ are shown by the vertical solid (dotted) lines. The dot on the abscissa of (b) indicates an impurity level A of $x \rightarrow 0$ limit.

potential (E_M) does not affect the calculation because the substitutional disorder is completely neglected in these approximations. In the CPA, on the contrary, the disorder is considered together with the multiple scattering effect, as has been previously discussed by us [3, 4]. In Fig 3(b), we show the result for DOS with $IS = -0.4\Delta$ and $E_M = -0.3\Delta$. Note that these parameters reproduce an acceptor energy of 0.11eV when $x \rightarrow 0$. The negative E_M forms the bandtail originated from the impurity band, and the spin polarization in the bandtail induces the ferromagnetism of high T_C though $IS = -0.4\Delta$ as shown in Fig. 4.

4 Conclusion

To summarize, the present study reveals the limitation of the MFA/VCA application for the carrier states and ferromagnetism in DMS, indicating the im-

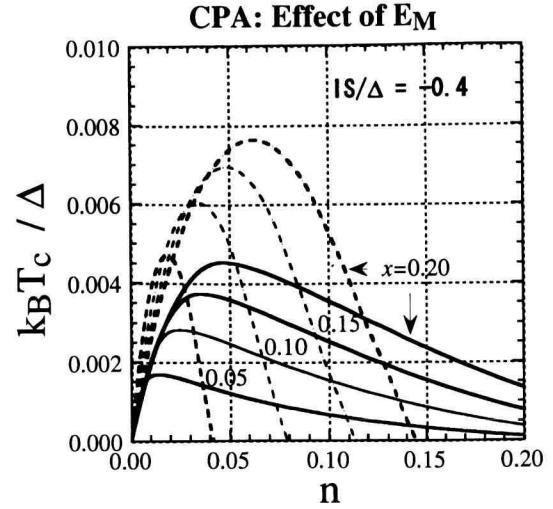


Figure 4: Result of the CPA for T_C ; solid lines for $E_M = 0.0$, broken lines for $E_M = -0.3\Delta$. $x = 0.05, 0.10, 0.15, 0.20$ (bottom to top).

portance of the attractive nonmagnetic potential that cannot be taken into account within the MFA/VCA frame.

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