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OPTICAL CONDUCTIVITY OF (III,Mn)V DILUTED MAGNETIC SEMICONDUCTORS

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The coherent potential approximation (CPA) is used to a minimal model of diluted magnetic semiconductors (DMS), where the carrier feels a nonmagnetic potential at a magnetic impurity site, and its spin interacts with the localized spins of the magnetic impurities through exchange interactions. The CPA equations for one particle Green function are derived and the optical conductivity is investigated in dependence on the system parameters and temperature. For illustration, the case of $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ is considered and compared with experimental data.

Keywords: Optical conductivity; Diluted magnetic semiconductors; Coherent potential approximation

1. Introduction

The discovery of ferromagnetism in $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ and $\text{In}_{1-x}\text{Mn}_x\text{As}$ has recently attracted much interest. With transition temperature in excess of 100 K these systems become one of the most promising materials for spintronic applications¹. At present the ferromagnetism in DMS is not well understood and parameters control of the magnitude of Curie temperature is still open question. To explain ferromagnetism in DMS, various model and approaches have been proposed^{2,3,4,5,6,7,8}. An overview of the theory of ferromagnetic (III,Mn)V semiconductors was recently presented in Ref. 9. The models differ from each other in detail, however, they all agree that the ferromagnetism in DMS is carrier mediated. Currently there is no common understanding on the origin of the carrier induced ferromagnetism. Dietl

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et al.^{2,3} referred to the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction as the origin of the ferromagnetism. Though their theory can give a Curie temperature in agreement with experiment, the RKKY model is questionable because the local coupling between the carrier and the impurity spin is much larger than Fermi energy and cannot be treated perturbatively⁴. In contrast to the RKKY picture, Yagi and Kayanuma⁵ assumed a system where p holes move around interacting with localized spin at impurity sites through the antiferromagnetic exchange interaction as a model for III-V-based DMS. Their model, however, does not contain nonmagnetic (Coulombic) potential arising from magnetic dopant, and therefore does not reproduce the magnetism of (Ga,Mn)As in a reasonable way⁶. Recently, Takahashi and Kubo^{10,11} showed that the nonmagnetic attractive potentials at Mn sites strongly assist the ferromagnetism in (III,Mn)V DMS. Their theory is in good agreement with experimental results for magnetism in (Ga,Mn)As. Based on the minimal model proposed by Takahashi and Kubo, and by using CPA in Ref.12 we have investigated transport properties of DMS system. We note that the impurity band model has been used in many theoretical works on (III,Mn)V DMS, since it is usually believed that such a description can still catch the essential physics^{13,14,15,16}. As well known that the optical spectrum contain important information about the physics of DMS, the purpose of this paper is to calculate the optical conductivity of DMS and to study its dependence on the system parameters and temperature.

2. Model and Theoretical Formulation

We employ the minimal model of $(A_{1-x}Mn_x)B$ -type DMS which includes the exchange interaction and nonmagnetic attractive potential. The Hamiltonian reads

$$H = \sum_{ij\sigma} t_{ij} c_{i\sigma}^+ c_{j\sigma} + \sum_i u_i, \quad (2.1)$$

where t_{ij} is the hopping matrix element between the site i and j , u_i depends on the ions species occupying the i site:

$$u_i = \begin{cases} E_A \sum_{\sigma} c_{i\sigma}^+ c_{i\sigma}, & i \in A \\ E_M \sum_{\sigma} c_{i\sigma}^+ c_{i\sigma} + \Delta \sum_{\sigma} (\sigma S_i) c_{i\sigma}^+ c_{i\sigma}, & i \in Mn. \end{cases} \quad (2.2)$$

Here $c_{i\sigma}^+$ ($c_{j\sigma}$) is the creation (annihilation) operator for a carrier at site i with spin σ . The localized spins are approximated as Ising spins and $S_i (= \pm 1)$ denotes the direction of localized spin at site i , $\Delta = JS/2$ is the effective coupling constant, E_A (E_M) represents a nonmagnetic local potential at an A (Mn) site. The difference of the nonmagnetic potential on the impurity atom (Mn) from that on the host atom (A), $E_M - E_A$, acts as an attractive potential in III-V-based DMS.

Denote by N_+ and N_- the number of localized up-spin and the down-spin sites,

respectively, then the average magnetization of localized spin is given by $M = (N_+ - N_-)/N_s$, where $N_s = xN$. Here N is the number of lattice sites and x is the mole fraction of Mn atom. For the average magnetization M , each site is occupied by an A atom (denoted as 0 site) with probability $p_0 = 1 - x$, by a Mn atom with up-spin (denoted as + site) with probability $p_+ = x(1 + M)/2$, by a Mn atom with down-spin (denoted as - site) with probability $p_- = x(1 - M)/2$. According to CPA, the local Green function at α -site ($\alpha = +, -, 0$) for carriers with σ -spin $G_\sigma^\alpha(\varepsilon)$ is determined by

$$G_\sigma^\alpha(\varepsilon) = G_\sigma(\varepsilon) + G_\sigma(\varepsilon)T_\sigma^\alpha(\varepsilon)G_\sigma(\varepsilon), \quad (2.3)$$

where $T_\sigma^\alpha(\varepsilon)$ is the single site T -matrix for carriers with σ -spin at α -site, $G_\sigma(\varepsilon)$ is the Green function for the effective medium which is given by

$$G_\sigma(\varepsilon) = \int \frac{\rho_0(z)dz}{\varepsilon - z - \sum_\sigma(\varepsilon)} \quad (2.4)$$

Here $\rho_0(z)$ denotes the unperturbed density of states (DOS), $\sum_\sigma(z)$ denotes the coherent potential which is determined self-consistently.

The CPA demands that the scattering matrix vanishes on average over all possible configuration of the random potential $\langle T_\sigma^\alpha(\varepsilon) \rangle = 0$. This is equivalent to

$$G_\sigma(\varepsilon) = \left\langle (G_\sigma^{-1}(\varepsilon) + \sum_\sigma(\varepsilon) - u_\sigma^\alpha)^{-1} \right\rangle, \quad (2.5)$$

where $u_\sigma^\alpha - \sum_\sigma(\varepsilon)$ being the scattering potential for carriers with σ -spin at α -site, and u_σ^α is equal to E_A , $E_M + \Delta\sigma$, $E_M - \Delta\sigma$ for $\alpha = 0, +, -$, respectively. By using the semi-elliptical DOS $\rho_0(z) = \frac{2}{\pi W^2} \sqrt{W^2 - z^2}$, where W is the half-width of the band, Green function (2.4) takes the form

$$G_\sigma(\varepsilon) = \frac{2}{W^2} [\varepsilon - \sum_\sigma(\varepsilon) - \sqrt{(\varepsilon - \sum_\sigma(\varepsilon))^2 - W^2}]. \quad (2.6)$$

Eliminating $\sum_\sigma(\varepsilon)$ from Eq. (2.6) we get

$$\sum_\sigma(\varepsilon) = \varepsilon - \frac{W^2}{4} G_\sigma(\varepsilon) - \frac{1}{G_\sigma(\varepsilon)}. \quad (2.7)$$

Substituting u_σ^α and $\sum_\sigma(\varepsilon)$ into Eq. (2.5) we obtain

$$G_\sigma(\varepsilon) = \frac{1-x}{\varepsilon - wG_\sigma(\varepsilon) - E_A} + \frac{x(1+M)/2}{\varepsilon - wG_\sigma(\varepsilon) - E_M - \Delta\sigma} + \frac{x(1-M)/2}{\varepsilon - wG_\sigma(\varepsilon) - E_M + \Delta\sigma}, \quad (2.8)$$

where $w = W^2/4$ and $\sigma = \pm 1$.

The Eq. (2.8) is easily transformed into a quartic equation for $G_\sigma(\varepsilon)$ and it is solved analytically. The total DOS $\rho_\sigma(\varepsilon)$ is then obtained by

$$\rho_\sigma(\varepsilon) = -\frac{1}{\pi} \text{Im} G_\sigma(\varepsilon). \quad (2.9)$$

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The free energy F per site is given by

$$F = n\mu - k_B T \int_{-\infty}^{\infty} [\rho_{\uparrow}(\varepsilon) + \rho_{\downarrow}(\varepsilon)] \ln[1 + e^{\frac{\mu - \varepsilon}{k_B T}}] d\varepsilon - \frac{TS}{N}, \quad (2.10)$$

where n is the density of the carriers, which is considered as an independent input parameter, μ is the chemical potential for the carriers, S is the entropy due to the localized spins given by

$$S = k_B \ln \frac{N_s!}{N_+! N_-!}. \quad (2.11)$$

By minimizing F with respect to μ and M we obtain the following equations

$$n = \int_{-\infty}^{\infty} [\rho_{\uparrow}(\varepsilon) + \rho_{\downarrow}(\varepsilon)] f(\varepsilon) d\varepsilon, \quad (2.12)$$

$$M = \tanh \left\{ \frac{1}{x} \int_{-\infty}^{\infty} \left[\frac{\partial \rho_{\uparrow}}{\partial M} + \frac{\partial \rho_{\downarrow}}{\partial M} \right] \ln[1 + e^{\frac{\mu - \varepsilon}{k_B T}}] d\varepsilon \right\}, \quad (2.13)$$

where $f(\varepsilon) = \left(1 + e^{\frac{\varepsilon - \mu}{k_B T}}\right)^{-1}$ is the Fermi distribution function. Eqs. (2.8)–(2.9) and (2.12)–(2.13) form a set of self-consistent equations for μ and M for a given set of parameter values x, n, Δ, E_A, E_M and T . If these equations have nontrivial solution $M \neq 0$, the system has a magnetic order. The Curie temperature T_C is determined by differentiating the both sides of Eq. (2.13) with respect to M at $M = 0$. Note that in contrast to ^{11,16} where the local moment magnetization M is left as an input parameter, this value is determined self-consistently in our calculations.

To derive the optical conductivity of a disordered one-particle system in CPA, we follow the procedure described in Ref. 17, which gives

$$\sigma(\omega) = \sigma_0 \int \frac{f(\varepsilon - \omega) - f(\varepsilon)}{\omega} Y(\varepsilon, \omega) d\varepsilon, \quad (2.14)$$

with σ_0 being the Mott minimal metallic conductivity, and

$$Y(\varepsilon, \omega) = \frac{4\pi W}{3} \sum_{\sigma} \int_{-W}^W \left(1 - \frac{z^2}{W^2}\right)^{3/2} A_{\sigma}(\varepsilon, z) A_{\sigma}(\varepsilon - \omega, z) dz, \quad (2.15)$$

$$A_{\sigma}(\varepsilon, z) = -\frac{1}{\pi} \text{Im} \frac{1}{\varepsilon - z - \sum_{\sigma}(\varepsilon)}. \quad (2.16)$$

The static conductivity is found from Eqs. (2.14)–(2.15) in the limit $\omega \rightarrow 0$.

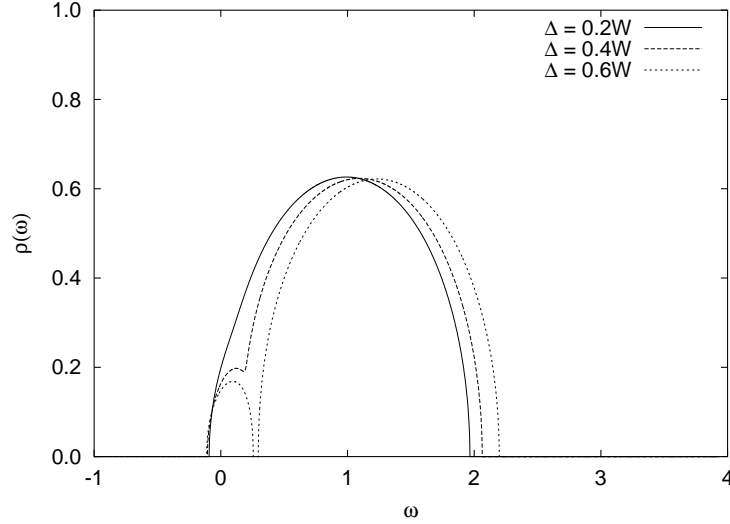


Fig. 1. The calculated majority spin DOS for various coupling constants for $x = 0.05$, $T = 0$ and $E_M = -0.3W$.

3. Numerical Results and Discussion

Through this work we take E_A as the origin ($= 0$) and W as the unit of energy. We assume the effective coupling constant Δ to be positive since the result does not depend on the sign of Δ . From Eq. (2.8), it is easily seen that for fixed x and M the DOS is determined by combined coupling $E_M \pm \Delta$, and not solely by the exchange coupling Δ . In Fig. 1, examples of the calculated majority spin DOS are shown for parameter values $x = 0.05$ (we focus on the doping of $x = 0.05$ associated with the highest T_c in $\text{Ga}_{1-x}\text{Mn}_x\text{As}$), $T = 0$, $E_M = -0.3W$ and three values of Δ . If the combined coupling is not strong ($|E_M - \Delta| = 0.5W$) the impurity band is not formed, at the intermediate combined coupling ($|E_M - \Delta| = 0.7W$) the impurity band is formed but not well separated from the main band; however, when the combined coupling is relatively large ($|E_M - \Delta| = 0.9W$), we find a separated impurity band below the main band. As well known that the carrier density is much smaller than the impurity concentration due to the heavy compensation, therefore the chemical potential μ is located in the lower impurity band or the lower band edge. Thus the key physics issue is, obviously, whether the combined potential $E_M \pm \Delta$ is weak or strong, and all physics properties are determined in the lower energy band edge.

Fig. 2 displays the change of the conductivity with the change coupling Δ for fixed values of x, E_M, n and temperature T . This optical conductivity has two main features: i) a zero-frequency or Drude peak corresponding to motion within the impurity band or the lower energy band, and ii) a finite-frequency broad peak

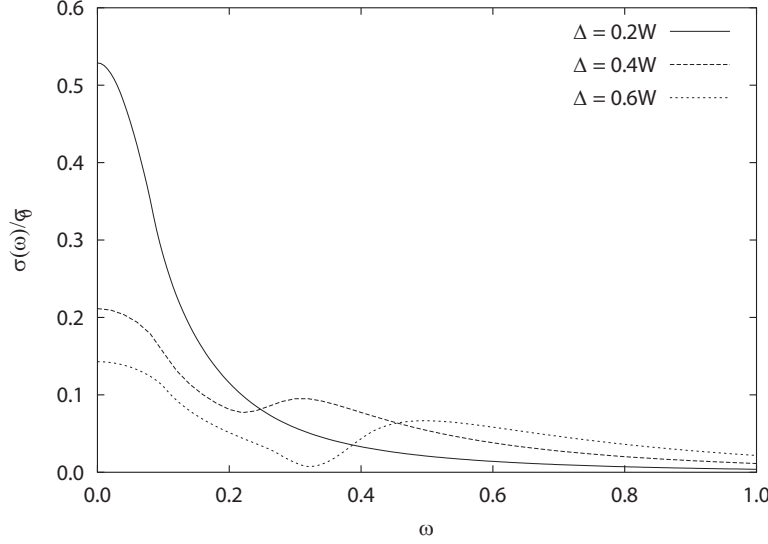


Fig. 2. Coupling dependence of the conductivity for $x = 0.05$, $n = 0.01$, $T = 0$ and $E_M = -0.3W$.

corresponding to transitions from the impurity band to the main band. It is seen that interband transitions are not much relevant at the weak combined coupling ($|E_M - \Delta| = 0.5W$), but they appear with more weight at the intermediate combined coupling ($|E_M - \Delta| = 0.7W$). At the combined coupling strong enough ($|E_M - \Delta| = 0.9W$), when the impurity band is formed and separated from the main band, the finite-frequency peak is weaker in strength than for the intermediate case due to carrier localization. In Fig. 3 we present the evolution of the conductivity with temperature. Here we use the parameters $\Delta = 0.4W$, $E_M = -0.3W$. These parameters for $W = 2$ eV are considered to be appropriate to $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ ^{11,18}. It is observed that as T is increased, the static conductivity changes slightly, whereas the width of zero-frequency peak decreases and the finite-frequency peak moves down in energy and increases in intensity. Our CPA results are in reasonable agreement with ones obtained using the dynamical mean field theory (DMFT)¹³. However, in Ref. 13 a detailed comparison between the calculated results and the optical phenomena observed in real DMS has not yet been performed. As was noted in Ref. 13 the temperature dependence of the conductivity may be readily understood from the density of states curves and the spin disorder scattering. Our optical spectrum for $T = T_c$ and $n = 0.01$ show a peak at $\omega^* = 0.24W = 0.48$ eV. This value is higher than value 0.22 eV experimentally observed in the optical conductivity of $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ for $x = 0.052$ ^{6,19}. With growing n the discrepancy between calculated and experimental values reduces, for example, for $n = 0.04$ we found $\omega^* = 0.36$ eV. This discrepancy may be caused by the neglecting of band structure of (Ga,Mn)As in the model as well as nonlocal effects in CPA calculations.

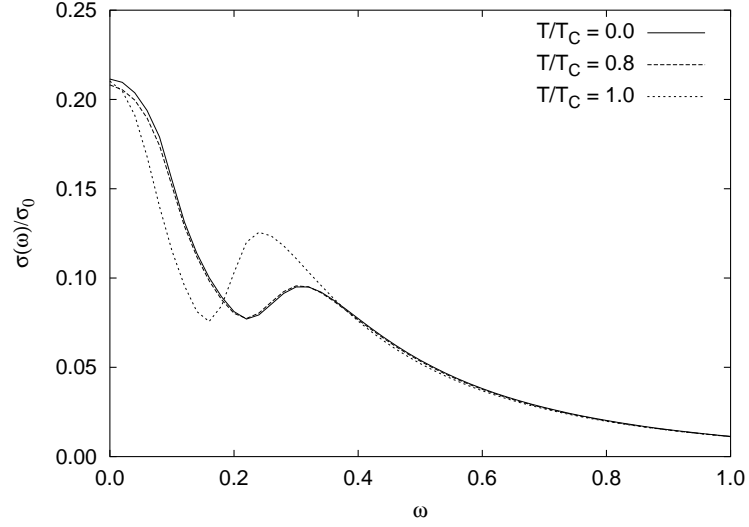


Fig. 3. Temperature dependence of the conductivity for $x = 0.05$, $n = 0.01$, $\Delta = 0.4W$ and $E_M = -0.3W$.

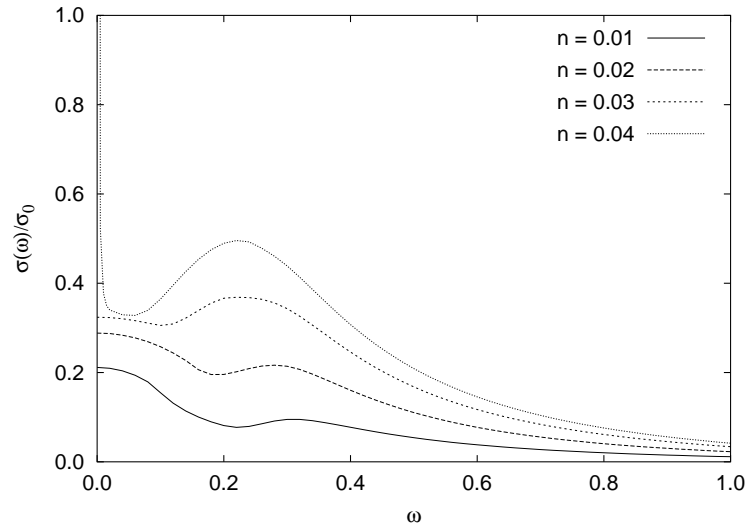


Fig. 4. Density dependence of the conductivity for $x = 0.05$, $T = 0$, $\Delta = 0.4W$ and $E_M = -0.3W$.

In addition, the carrier concentration is not known experimentally with precision. The density dependence of the optical conductivity of $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ for $x = 0.05$ and $T = 0$ K is shown in Fig. 4, and it is as follows: as the density increases the con-

ductivity increases and the finite-frequency peak moves down in energy. The shift of finite-frequency peak to the left is caused by the decrease in separation between the chemical potential and the edge of the main band (as n is increased), since increasing the carrier density by a small amount was found to simply shift the chemical potential to the right. Fig. 5 displays the sensitivity of the conductivity to nonmagnetic potential. Here we use the parameters: $x = 0.05$, $\Delta = 0.4W$, $n = 0.01$, $T = 0$ K and four values of E_M . The behavior of the conductivity is similar to ones shown from Fig. 2, where we fixed E_M and changed Δ . The similarity is due to fact that the case of $\Delta = 0.4W$, $E_M = -0.1W$ ($\Delta = 0.4W$, $E_M = -0.5W$) in Fig. 5 and that of $\Delta = 0.2W$, $E_M = -0.3W$ ($\Delta = 0.6W$, $E_M = -0.3W$) in Fig. 2 have the same low energy part of DOS, which is determined by the combined coupling energy $E_M - \Delta$.

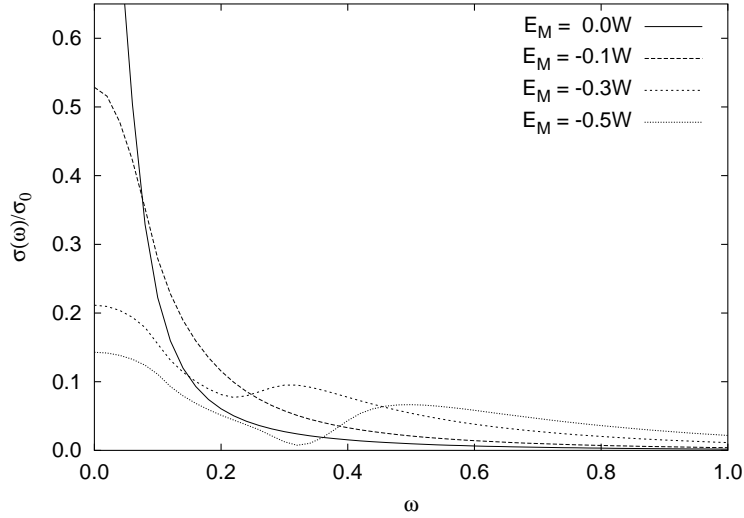


Fig. 5. Nonmagnetic potential dependence of the conductivity for $x = 0.05$, $n = 0.01$, $T = 0$ and $\Delta = 0.4W$.

To summarize, in this paper we have applied CPA to calculate the optical conductivity in diluted magnetic semiconductors $A_{1-x}Mn_xB$. We derived CPA equations for one particle Green function and the optical conductivity in the minimal model, where carrier feels a nonmagnetic potential at a magnetic impurity site, and its spin interacts with the localized spins through exchange interaction. We have shown that the optical conductivity strongly depends on the temperature and the system parameters, i. e., exchange coupling, carrier density, nonmagnetic potential. Our results are in good agreement with ones obtained by DMFT, and in qualita-

tively agreement with experiments for (Ga,Mn)As. The minimal model provides useful insights for interpreting experiments, however, in order to explain optical properties in (Ga,Mn)As and other (III,Mn)V DMS in a consistent way further improvements of the model are required.

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