Origin of carrier-induced ferromagnetism of (Ga,Mn)As

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Abstract

Taking into account both random impurity distribution and thermal fluctuations of localized spins, we have performed a model calculation for the carrier (hole) state in $Ga_{1-x}Mn_xAs$ by using the coherent potential approximation (CPA). The result reveals that a p-hole in the band tail of $Ga_{1-x}Mn_xAs$ is not like a free carrier but rather is virtually bound to impurity sites. The carrier spin strongly couples to the localized d spins on Mn ions. The hopping of the carriers among Mn sites causes the ferromagnetic ordering of the localized spins through the double-exchange mechanism. The present result is consistent with the picture recently obtained by the studies of infrared optical conductivity and photoemission spectroscopy.

Key words: magnetic semiconductor; exchange interaction; double-exchange mechanism; $Gd_{1-x}Mn_xAs$

Although a considerable amount of experimental results has already been accumulated [1], the origin of the ferromagnetism in III-V-based diluted magnetic semiconductors (DMS's) has still not been clarified theoretically. In this work, we investigate the effect of magnetization on carrier states in DMS's to clarify the mechanism of the ferromagnetism. The present model is described by

$$H = \sum_{m,n,\mu} \varepsilon_{mn} a^\dagger_{m\mu} a_{n\mu} + \sum_m U_m, \qquad (1)$$

where $a^\dagger_{m\mu}$ ($a_{m\mu}$) creates (annihilates) a carrier with spin μ at the m-th site. Here, U_m denotes either $E_A \sum_\mu a^\dagger_{m\mu} a_{m\mu}$ or $E_M \sum_\mu a^\dagger_{m\mu} a_{m\mu} - I \sum_{\mu\nu} a^\dagger_{m\mu} \boldsymbol{\sigma}_{\mu\nu} \cdot \mathbf{S}_m a_{m\nu}$, depending on whether the site m is occupied by Ga or Mn. E_A (E_M) denotes the spin-independent potential of a Ga (Mn) ion; $-I\boldsymbol{\sigma} \cdot \mathbf{S}_m$ represents the exchange interaction between the carrier and the localized spin $\mathbf{S}_m$ of Mn at site m. We apply the dynamical coherent potential approximation (dynamical CPA) [2] to the above model, assuming a semicircular model density of states (DOS) with half-bandwidth Δ for the host valence (p-hole) band. We set $E_A \equiv 0$, and adopted the parameters $\Delta = 2$eV, $IS/\Delta = -0.4$ and $E_M/\Delta = -0.3$ for $Ga_{1-x}Mn_xAs$.

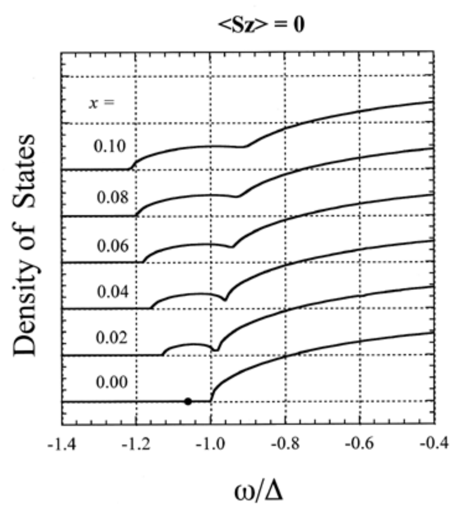

Fig. 1. Carrier (hole) DOS with $\langle S_z \rangle_{av} = 0$ for various values of Mn mole fraction x. The impurity level is represented by a dot on the line of $x = 0.00$.

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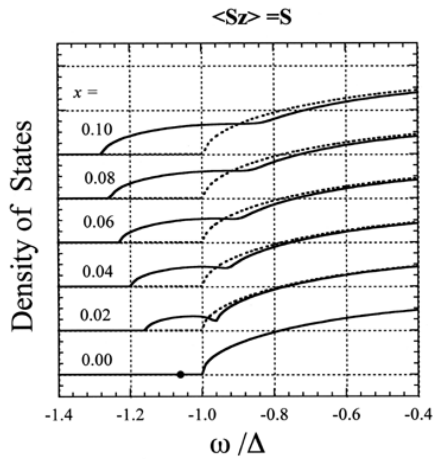

Fig. 2. DOS with $\langle S_z\rangle_{\rm av} = S$ for various values of x. The solid and dotted lines represent $D_\downarrow(\omega)$ and $D_\uparrow(\omega)$, respectively.

Figure 1 shows the variation in the carrier DOS with Mn mole fraction x in a paramagnetic region. An impurity (acceptor) level appears at the energy of $E_{\rm a} = -1.057\Delta$, which is consistent with an acceptor energy of 0.113eV [3]. With increase in x, an impurity band forms. For $x > 0.02$, the impurity band merges into the host band. The results consistently explain the experimental observation of impurity-band-like states [4] and the insulator-metal transition at $x \sim 0.03$ [5]. In Fig. 2, the DOS with a saturating magnetization is shown for various values of x. As a consequence of exchange interaction, the tail of the down-spin band stretches toward the lower-energy side, whereas the tail of the up-spin band merges well into the host band.

The DOS of $x = 0.05$ depicted in Fig. 3(a) shows that the band tail that originates from the magnetic impurity state extends around the impurity level with increasing magnetism. Hence the ferromagnetic state has lower energy than the paramagnetic one when n is small. The gain of kinetic energy causes the ferromagnetism under a certain temperature. This implies that the double-exchange mechanism for ferromagnetism is operative. We also present the relative local DOS at Mn sites defined by $R(\omega) = (D^{\rm M}_\uparrow(\omega) + D^{\rm M}_\downarrow(\omega))/(D_\uparrow(\omega) + D_\downarrow(\omega))$ in Fig.3(b), which shows that $R(\omega)$ is almost independent of $\langle S_z\rangle_{\rm av}$. The result for $R(\omega)$ shows that majority of carriers in the band tail remain at Mn sites ($R(\omega) \sim 0.6$) in spite of small x; this is consistent with the nearly bound-hole picture suggested by the results of experiments [6,7]. A simple calculation shows that the carrier spin couples strongly with the localized d spins. The Curie temperature $T_{\rm c}$ estimated from the magnetization dependence of DOS is in good agreement with the value of 110K observed in $Ga_{1-x}Mn_xAs$ for $x = 0.053$ and $n \simeq 0.3x$ [1]. The detail will be published elsewhere.

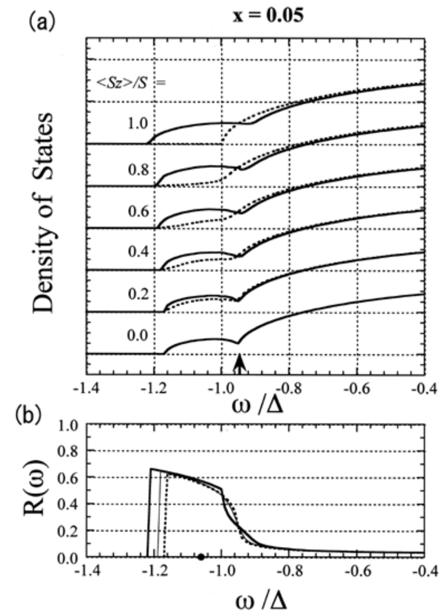

Fig. 3. (a) DOS with x=0.05 for various values of magnetization. The arrow indicates the Fermi level for $n = x$ (= 0.05). (b) The ratio $R(\omega)$ of the local DOS at Mn site to the total DOS for $\langle S_z\rangle_{\rm av}/S$ = 1.0 (thick full line), 0.5 (thin full line), and 0.0 (dotted line).

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