INDIRECT EXCHANGE INTERACTION IN Hg1-xMnxTe AND Cd1-xMnxTe ALLOYS

C. Lewiner, J. Gaj, G. Bastard

To cite this version:

C. Lewiner, J. Gaj, G. Bastard. INDIRECT EXCHANGE INTERACTION IN Hg1-xMnxTe AND Cd1-xMnxTe ALLOYS. Journal de Physique Colloques, 1980, 41 (C5), pp.C5-289-C5-292. <10.1051/jphyscol:1980549>. <jpa-00219984>

HAL Id: jpa-00219984
https://hal.archives-ouvertes.fr/jpa-00219984
Submitted on 1 Jan 1980

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
INDIRECT EXCHANGE INTERACTION IN Hg$_{1-x}$Mn$_x$Te AND Cd$_{1-x}$Mn$_x$Te ALLOYS.

C. Lewiner *, J.A. Gaj *, and G. Bastard *

*Groupe de Physique des Solides de l'E.N.S., Laboratoire Associé au C.N.R.S. Université Paris 7, tour 23, 2, Place Jussieu 75251 Paris Cedex 05 - 24 rue Lumond, 75251 Paris Cedex 05, France

† Institute of Experimental Physics, University of Warsaw - Warsaw - Pologne

Abstract.- We investigate in Hg$_{1-x}$Mn$_x$Te and Cd$_{1-x}$Mn$_x$Te alloys, the indirect exchange interaction between two localized moments, which arises from the virtual transitions between the filled valence band and the empty conduction band (Bloembergen and Rowland mechanism). Both cases of zerogap materials (Hg$_{1-x}$Mn$_x$Te alloys of low x) and semiconducting materials (Hg$_{1-x}$Mn$_x$Te alloys of large x and Cd$_{1-x}$Mn$_x$Te alloys) are examined. The Curie Weiss temperature is calculated and compared to the available experimental results.

1. Introduction.- Magnetic susceptibility measurements performed on Hg$_{1-x}$Mn$_x$Te and Cd$_{1-x}$Mn$_x$Te/1-3/ alloys revealed an antiferromagnetic interaction between Mn$^{2+}$ ions : $\chi^{-1}(T)$ behaves like $T + \theta$, $\theta > 0$, at high temperature. Low temperature oscillatory interband magnetoabsorption /4,5/, magneto-transport phenomena /6/ and exciton magnetoreflectivity /7,8/ lead to similar results. These proved impossible to interpret by accounting only for direct exchange between closely spaced moments. In this paper we investigate the Bloembergen and Rowland (B.R) mechanism/9/, in Hg$_{1-x}$Mn$_x$Te and Cd$_{1-x}$Mn$_x$Te alloys and show that it leads to a long range interaction between spins with the right order of magnitude and the right sign. To get this agreement it proves crucial to properly account for the symmetry of the electron Bloch functions; in fact the symmetry imposes the sign of the spin-spin indirect interaction.

2. Background.- In Hg$_{1-x}$Mn$_x$Te/10/ and Cd$_{1-x}$Mn$_x$Te alloys there is not enough free carriers to give a significant indirect intraband effect (RKKY). For these compounds, B.R mechanism is relevant : two localized spins interact via virtual excitation of an electron from the filled valence band to the empty conduction band. Previous calculations used oversimplified description of the electronic band structure; in particular no attention was paid to the symmetry of band edges Bloch functions /9,11/. The band structure of these alloys is reported on figure 1; for more details see ref./14/.

Figure 1: Band structure of Hg$_{1-x}$Mn$_x$Te alloys.

We assume that the mobile electrons interact with the localized electrons of Mn d- levels by an Heisenberg type
hamiltonian:
\[ \mathcal{H} = \sum_{i,j} J(i - \mathbf{R}_i) \mathbf{S}_i \cdot \mathbf{S}_j \]

where \( \mathbf{S}_i \) are the localized spins located at \( \mathbf{R}_i \) and \( \mathbf{S} \) the bare electron spin.

\( J(i) \) is the exchange integral supposed to be contact-like. Due to spin-orbit coupling the second order energy shift may be rewritten as the sum of an isotropic and pseudodipolar spin-pin Hamiltonian. In what follows we have neglected all anisotropic effects and calculated the \( I_{ij}^{ZZ} \) exchange integral (\( \mathbf{S}_i // \mathbf{R}_i \)):
\[ \Delta e(2) = \sum_{i,j} \alpha^\beta \alpha^\beta \mathbf{S}_i \cdot \mathbf{S}_j \]

\[ I_{ij}^\alpha \beta = \frac{1}{R^2} \sum_{\nu \nu'} \frac{f(\nu \nu')}{(1 - F(\nu \nu'))} \exp(i \mathbf{k} \mathbf{R}_i) \mathbf{S}_i \cdot \mathbf{S}_j \]

\[ I_{ij} = \frac{\mathbf{S}_i \cdot \mathbf{S}_j}{R^2} \]

where \( \mathbf{S}_i \) are the periodic part of the Bloch states (\( \nu \) labels the bands and \( \mathbf{S}_i \) their Kramers degeneracy). Note the crucial part played by the symmetry of the bands edges in the evaluation of the matrix element. One usually assumes it to be constant which is only valid for parabolic spherical s-type bands. For p symmetry levels their matrix elements depend on \( k_x/k \) and \( k_y/k \).

3. Analytic calculations (\( \Delta \alpha \)).

3.1 Parabolic zero-gap semiconductors (\( H_{1-x}M_n_n_x \) alloys \( x < 1 \)). - The absence of forbidden gap leads to a power law decline for \( I_{ij} \) /10/:
\[ I_{ij} = \frac{\beta^2 m_n f(s)}{16 \pi^2 \hbar^2 R^4} \]

where \( \beta = \langle \mathbf{S}_i \mathbf{J}(\mathbf{r}) \mathbf{S}_j \rangle \) is the exchange integral in the p bands, \( m_n \) the effective mass of the heavy hole valence band and
\[ s = \left( \frac{m_n}{m_e} \right)^{1/2}. \]

\( f(s) \) has been evaluated for two cases: actual symmetry induced band (\( f_{s1} \)) and accidental band degeneracy (\( f_{a} \)).

Fig. 2: Dependence of the effective exchange integral for parabolic ZG materials in the cases of accidental band degeneracy (\( f_a \)) and symmetry induced degeneracy (\( f_{s1} \)).

Note that \( f_a \) and \( f_{s1} \) vanish in the limit of infinite \( s \) (\( m_n \) finite, \( \epsilon_\sigma = m_e \)). In this limit however, it is impossible to use a parabolic dispersion relation for the conduction band which would be linear in \( k \).

3.2 Extreme non parabolic limit (\( \epsilon_\sigma = 0 \)).

There are two types of virtual interband transitions:
The former is analogous to case a) and involves only the matrix elements of \( \mathbf{J}(\mathbf{r}) \) between p symmetry states since \( \langle \mathbf{S}_i \mathbf{J}(\mathbf{r}) \mathbf{S}_j \rangle = 0 \) /15/. The latter is induced by s and p mixing and involves two matrix elements:
\[ \beta = \langle \mathbf{S}_i \mathbf{J}(\mathbf{r}) \mathbf{S}_j \rangle \] and \( \langle \mathbf{S}_i \mathbf{J}(\mathbf{r}) \mathbf{S}_j \rangle = \alpha. \]

Then /15/:
\[ I_{ij} = I_{ij}^a \]

\[ I_{ij}^h h \alpha c = \frac{m_n \beta^2}{96 \pi \hbar^2 R^4} \psi(\delta) \]

with \( \delta = \frac{R}{\lambda} \) and \( \lambda = \frac{\sqrt{3 \pi m_n}}{2 \sqrt{2} m_n} \left[ \langle \mathbf{S}_i \mathbf{v} \rangle^2 \right] \)

\( m_e \) is the bare electron mass.
\( \psi(\delta) \) presented in figure 3, shows a sign reversal for \( \delta \gtrsim 0.4 \) corresponding to \( R \approx 0.44 \) Å which is much less than the nearest neighbour distance (4.53 Å). We may thus conclude that the electron heavy hole contribution is in all realistic cases antiferromagnetic with \( R^{-5} \) dependence at large \( R \):

\[
I_{ij} \propto \frac{1}{R^5} c = -\frac{m_v}{64\pi^2 \hbar^2} \frac{\lambda}{R} \left( \alpha^2 - \frac{10}{3} \beta^3 + \frac{43}{9} \beta^6 \right)
\]

for the experimental values of \( \alpha \) and \( \beta \) the electron light hole contribution is ferromagnetic and behaves like \( R^{-5} \); however the total effect remains antiferromagnetic for all distances.

\[
\varphi(\delta) \text{ versus } \delta
\]

4. General calculation.- For non parabolic Z.G. alloys (Hg\(_{1-x}\)-Mn\(_x\)Te \( 15<\alpha<7\)% or for opengap semiconductors (Hg\(_{1-x}\)-Mn\(_x\)Te \( x > 7\)% or Cd\(_{1-x}\)-Mn\(_x\)Te of all \( x \)) it is crucial to use the correct dispersion relation since \( s \) and \( p \) band mixing are then responsible for part of the effect (Z.G) or for the whole effect (S.G.) . For finite spin-orbit coupling the latter is no longer analytic and numerical calculations were performed using a very simplified band model (the Kane four band approximation /16/) and limiting \( k \) and \( k' \) to a spherical Brillouin zone. This sharp cut off leads to an oscillatory behaviour of \( I_{ij} \) with the distance exactly as a sharp Fermi level is needed to get the RKKY oscillations. These oscillations are spurious and will be smeared out by several factors among them the use of a non spherical Brillouin zone /17/ and of a finite spatial range of \( J(z) \). As long as a summation of \( I_{ij} \) over many neighbours is performed these oscillatory effects will compensate; however if only one or two neighbours are involved it will be necessary to smoothen the dependence of \( I_{ij}(R) \) on \( R \).

Superimposed on this behaviour eq(3) shows that as long as \( R<<\l_a \) the extreme non parabolic limit results may be used and a power law \( I_{ij} \propto R^{-2} \) with \( 4<n<5 \) prevails. For large \( R \) an exponential decay /9/ will be recovered.

5. Results and conclusion.- In order to compare our theory with susceptibility measurements /1-2/ (high temperature) it is necessary to calculate the Curie-Weiss temperature /18/:

\[
k_B T_0 = \frac{35}{12} \sum_{R_0j>a} I_{ij} \delta_{ij} \quad \text{for } a \text{ and } b \text{ the experimental values of } \alpha \text{ and } \beta.
\]

In low temperature experiments /5,8/ the first and second neighbouring pairs are frozen and the long range interaction involved is \( T_0 \) given by /5/:

\[
k_B T_0 = \frac{35}{12} (1-x)^{18} \sum_{R_0j>a} I_{ij} \delta_{ij}
\]

(a is the lattice parameter).

As pointed out the oscillatory behaviour of \( I_{ij} \) prevents us of obtaining any reliable values of \( T_0 \). For Cd\(_{1-x}\)-Mn\(_x\)Te we get \( \theta = 2.2^\circ \) for \( x = 1\% \) and the results for HgMnTe are displayed in table I and show a qualitative agreement with experimental measurements.

Table 1.- Curie Weiss temperature \( \theta \) as a function of \( x \) in Hg\(_{1-x}\)-Mn\(_x\)Te alloys. The numerical values of \( \alpha \) and \( \beta \) are from ref. /14/ and \( m_v = 0.6 m_o \).

In conclusion, the B.R. mechanism used together with a Kane band structure provides an interpretation of the antiferromagnetic long range interaction observed in Hg\(_{1-x}\)-Mn\(_x\)Te and Cd\(_{1-x}\)-Mn\(_x\)Te alloys. However for opengaps the wave vectors near the Brillouin zone edge contribute significantly showing clearly the limitations of the Kane model. Moreover one should take properly into account anisotropic effects.
References


/15/ Lewiner, C., and Bastard, G., (to be published in Jour. Phys. C)


/18/ Kittel, C., Introduction to Solid State Physics, (J. Wiley Editor).