

Proceedings of the XX International School of Semiconducting Compounds, Jaszowiec 1991

PECULARITIES OF p - d INTERACTION IN SEMIMAGNETIC SEMICONDUCTORS WITH Cr^{2+1} *

J. BLINOWSKI

Institute of Theoretical Physics, Warsaw University
Hoża 69, 00-681 Warszawa, Poland

AND P. KACMAN

Institute of Physics, Polish Academy of Sciences
Al. Lotników 32/46, 02-668 Warszawa, Poland

In cubic DMS crystals with Cr^{2+} content the non-Heisenberg part of the p - d interaction together with the strong, static Jahn-Teller effect may lead to a zero-magnetic field splitting and significant modifications of the spin splittings for the valence band. The effect reaches a maximum when all Jahn-Teller distortions are oriented along one of the [100]-type crystallographic directions.

PACS numbers: 75.50.Pp, 75.30.-m, 71.70.-d

In zinc-blende type DMS the tetrahedral crystal field splits the ground state of the free ion Cr^{2+} into the excited orbital doublet E and the ground orbital triplet T_2 (as long as the weak T_2 - E mixing due to the spin-orbit interaction is neglected). For each of the 5T_2 states one of the one-electron orbitals t_{2g} is empty. In such a case as it was demonstrated in [1] the usual Heisenberg-like Hamiltonian $\hat{H}_H = -BS \cdot J$, which describes the spin-dependent part of the p - d interaction, has to be completed by additional non-Heisenberg terms. If we denote by S the total spin operator of the impurity ion ($S = 2$), by \mathcal{L} the fictitious orbital angular momentum for the T_2 triplet ($\mathcal{L} = 1$) and by J the fictitious total angular momentum ($J = 3/2$) for the Γ_8 valence-band electron (for which the Luttinger basis was used), the non-Heisenberg part of the p - d interaction can be expressed in the form:

$$\hat{H}_{\text{NH}} = (B + 3C)\hat{A} + (B + 2C) \left\{ (1/2)[\hat{A}, \mathcal{L} \cdot S + S \cdot J]_+ + S \cdot J \right\}; \quad (1)$$

*This work was partially supported by the grant G-MEN-128/90.

where

$$\hat{A} = (\mathcal{L} \cdot \mathbf{J})^2 - (1/2)\mathcal{L} \cdot \mathbf{J} - (5/2). \quad (2)$$

The formulae for the negative "exchange constants" B and C can be found in [1]. This operator has to be multiplied by a phase factor $\exp[i(\mathbf{k} - \mathbf{k}')\mathbf{R}_I]$ originating from the envelope parts of the Luttinger functions, where \mathbf{R}_I is the position of the Cr^{2+} ion.

According to the Jahn-Teller theorem, the orbital degeneracy makes the ground state of Cr^{2+} unstable against an asymmetric displacement of the neighboring ions. The Cr^{2+} impurities in $\text{A}^{\text{II}}\text{B}^{\text{VI}}$ compounds are known to undergo a strong, static Jahn-Teller effect, in which the local distortion reduces the symmetry around each ion to D_{2d} ; the ground state becomes an orbital singlet 5B_2 separated from the upper states by the Jahn-Teller energy $3E_{\text{JT}}$ roughly constant for all $\text{A}^{\text{II}}\text{B}^{\text{VI}}$ compounds ($\approx 400\text{--}600 \text{ cm}^{-1}$) [2]. Such a static distortion is possible along each of the cubic axes.

For the distortion in z -direction along the [001] crystallographic axis the orbital ground state has the form:

$$|\zeta\rangle = |\mathcal{M} = 0\rangle, \quad (3)$$

where $|\mathcal{M} = 0\rangle$ is the state with the projection of the fictitious angular momentum \mathcal{L} on the [001] direction equal to zero. The ground states for the remaining two distortions, along [100] and [010] axes, are conventionally denoted by $|\xi\rangle$ and $|\eta\rangle$, respectively.

In DMS crystals the mobile band electrons interact simultaneously with all magnetic ions. Within the mean field approximation this interaction is diagonal in \mathbf{k} and can be obtained by calculating the thermodynamic average of $\hat{H}_H + \hat{H}_{\text{NH}}$ for each Cr^{2+} ion and summing over all ions in the unit volume of the crystal. For $kT < 3E_{\text{JT}}$ the thermodynamic average involves only the orbital ground singlets $|\xi\rangle$, $|\eta\rangle$ or $|\zeta\rangle$. The final p - d interaction depends strongly on the relative number of ions with the Jahn-Teller distortion along the three cubic axes.

It is well-known that one can change these numbers by, e.g. an application of uniaxial stress [2]. In the limit case, with all the Jahn-Teller distortions and the external magnetic field along the [001] axis, the part of the mean field effective mass Hamiltonian representing the p - d interaction is diagonal in the Luttinger $m_{\mathbf{J}}$, \mathbf{k} representation. The eigenvalues of this part, which determine the band splittings at $\mathbf{k} = 0$ are:

$$\begin{aligned} E_{\pm 3/2} &= -(B + 3C)xN_0 \mp (3/2)BM, \\ E_{\pm 1/2} &= +(B + 3C)xN_0 \mp (1/2)(B + 4C)M, \end{aligned} \quad (4)$$

where M represents the total magnetization of xN_0 Cr^{2+} ions per unit volume. One can see from Eqs. (4) that two important effects of p - d hybridization might be expected in this case. First, there is a zero-field splitting proportional to the concentration of Cr^{2+} ions. Second, the dependence of the valence band Zeeman splittings on the magnetization differs considerably from the form $B_{\text{Mn}}M J_Z$ established for DMS with Mn^{2+} content.

In the opposite limit, when none of the three possible axes of the Jahn-Teller distortion is privileged, the effective mass p - d Hamiltonian for the magnetic field along the [001] direction is again diagonal but with quite different eigenvalues:

$$E_{\pm 3/2} = \mp(B - C)M \mp (1/3)(B + 2C)\Delta M,$$

$$E_{\pm 1/2} = \mp(1/3)(B - C)M \mp (5/9)(B + 2C)\Delta M, \quad (5)$$

where ΔM is the difference between contributions to the magnetization M from ions with the distortion axes parallel ([001]) and perpendicular ([100] or [010]) to the magnetic field. In this case, there is no zero-field splitting due to p - d hybridization. Still, the expected pattern of the Zeeman splittings and its temperature and magnetic field dependencies are not standard, since in general $\Delta M \neq 0$. It seems that among all zinc-blende type DMS based on II-VI compounds one can put $\Delta M \cong 0$ only for CdTe crystals, where the spin-orbit interaction for Cr^{2+} ions is really very small.

References

- [1] J. Blinowski, P. Kacman, in *Proc. XX ICPS, Thessaloniki, 1990*, Eds. E.M. Anastassakis, J.D. Joannopoulos, World Scientific, Singapore 1990, Vol. 3, p. 1827.
- [2] J.T. Vallin, G.D. Watkins, *Phys. Rev. B* **9**, 2051 (1974).