Zener-like exchange for Mn-doped III-V semiconductors

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Abstract

The proposed microscopic model of ferromagnetism in GaAs:Mn, GaP:Mn is based on the interaction between the transition metal impurities and heavy holes (hh) of host semiconductor. The *kinematic exchange* is derived and the Curie temperature is calculated.

Key words:
Dilute magnetic semiconductors (DMS); Zener exchange; Anderson-Hubbard repulsion

A microscopic model of ferromagnetism with the effective *kinematic* DMS is presented. It takes into account the origin of localized magnetic moments and shallow acceptor levels induced by Mn impurity and derive the effective *kinematic exchange*.

The crystal field resonance (CFR, predominantly d-type) and dangling bond hybrid (DBH, predominantly p-type) arise due to strong hybridization between the atomic t_2 orbitals and p-states of the same symmetry belonging mainly to the heavy hole band [1,2].To describe the indirect exchange, we generalize the single impurity resonance scattering model [3] for the case of two impurities in DMS. The minimal two-impurity Hamiltonian involves t_2-electrons and heavy hole states:

$$H = \sum_{\mathbf{p},\sigma} \varepsilon^h_{\mathbf{p}} c^\dagger_{\mathbf{p}h\sigma} c_{\mathbf{p}h\sigma} + \sum_{\mathbf{p},\sigma;i} \left(V_{\mathbf{p}d} c^\dagger_{\mathbf{p}h\sigma} d_{i\sigma} e^{i\mathbf{p}R_i} + h.c. \right) + \sum_{\sigma,i=1,2} \left(E_d \hat{n}^\sigma_i + \frac{U}{2} \hat{n}^\sigma_i \hat{n}^{\bar{\sigma}}_i \right), \quad (1)$$

with usual notations. It describes the resonant impurity scattering induced by hybridization $V_{\mathbf{p}d}$. The last term contains the localized t_2 electrons with the occupation operator $\hat{n}^\sigma_i = d^\dagger_{i\sigma} d_{i\sigma}$

The solutions of Dyson equations are
$G^\sigma_{dii} = \left[g_{i\sigma}(\varepsilon)^{-1} - V^2 L_{jj}(\varepsilon) \right] / R^\sigma(\varepsilon)$,
$G^\sigma_{dij} = V^2 L^\sigma_{ij}(\varepsilon) / R^\sigma(\varepsilon)$, $(ij = 12; 21)$,
$L_{ij}(\varepsilon) = \sum_{\mathbf{p}} e^{-i\mathbf{p}\cdot(\mathbf{R_i}-\mathbf{R_j})} (\varepsilon - \varepsilon^h_{\mathbf{p}})^{-1}$ is the lattice Green's function for hh and

$$R^\sigma(\varepsilon) = \prod_{i=1,2} \left[g^{-1}_{i\sigma}(\varepsilon) - V^2 L_{ii}(\varepsilon) \right] - V^4 L_{12} L_{21} \quad (2)$$

with $g_{i\sigma}(\varepsilon) = (\varepsilon - E_d - U n^{-\sigma}_i)^{-1}$

The occupied CFR levels correspond to the states (d^5/d^4) of the Mn ions, whereas the empty (d^6/d^5) CFR levels are shifted to the conduction band by the Anderson-Hubbard repulsion U (Fig. 1) responsible for spin-dependent inter-impurity interaction. In GaAs:Mn and GaP:Mn the deep CFR states are completely occupied, and the DBH states in the energy gap are empty [2]). Two competing mechanisms of magnetic interaction arise because the indirect exchange between impurities involves empty states near the top of the valence band and empty (d^6/d^5) CFR levels.

Due to the on-site repulsion, the structure of CFR levels is different for FM and AFM spin orientation.

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For AFM alignment the occupation numbers are $\bar{n}_1^{\uparrow} = \bar{n}_2^{\downarrow} = 1$, $\bar{n}_1^{\downarrow} = \bar{n}_2^{\uparrow} = 0$. The tunneling involves U, and the secular equation $R^{\sigma} = 0$ gives the occupied impurity levels such as E_b^{σ} (see Fig. 1): $E_b^{\uparrow} \approx E_1^{\uparrow} - J_A$, $E_b^{\downarrow} \approx E_2^{\downarrow} - J_A$,. The indirect exchange parameter $J_A = V^4 L^2/U$ is the AFM superexchange. In FM case: $\bar{n}_1^{\uparrow} = \bar{n}_2^{\uparrow} = 1$, $\bar{n}_1^{\downarrow} = \bar{n}_2^{\downarrow} = 0$ and the exchange between impurities is mediated by the empty p states and DBH states; the role of these states for DMS is the same as in the Zener mechanism [4]. The difference is that in Zener's case Mn ions are in different valence states. Since in our case the bonding/antibonding CFR states $E_{(b,a)}^{\uparrow} = E_i^{\uparrow} \pm J_Z$ are occupied, the original Zener mechanism does not work.

Then the band contribution due to two-impurity scattering is.

$$E_{ex} = -\frac{V^4}{4\pi} \cdot (\vec{\sigma}_1 \cdot \vec{\sigma}_2 + 3) \left\{ \int_{\varepsilon_F}^{0} d\varepsilon \frac{\Gamma_{12}(\varepsilon) P_{12}(\varepsilon)}{[\varepsilon - E_d - V^2 P_{11}(\varepsilon)]^2 + \frac{V^4}{4}\Gamma_{11}^2} + 3x \cdot \frac{P_{12}(\varepsilon_i) P'_{12}(\varepsilon_i)}{[1 - V^2 P'_{11}(\varepsilon_i)]^2} \right\}, \quad (3)$$

($\vec{\sigma}_{1,2}$ are the vectors of Pauli matrices). The terms in curly brackets correspond to the contribution of mobile and localized holes. Here $P_{11}(\varepsilon)$ is the Hilbert transform of the hh density of states ρ, $\Gamma_{11}(\varepsilon) \approx \pi\rho(\varepsilon)$, $\Gamma_{12}(\varepsilon) \approx \pi\rho(\varepsilon) \sin kR_{12}/kR_{12}$ and

$$P_{12}(\varepsilon) = \int d\omega \frac{\sin kR_{12}}{kR_{12}} \frac{\rho_{hb}(\omega)}{\varepsilon - \omega}. \quad (4)$$

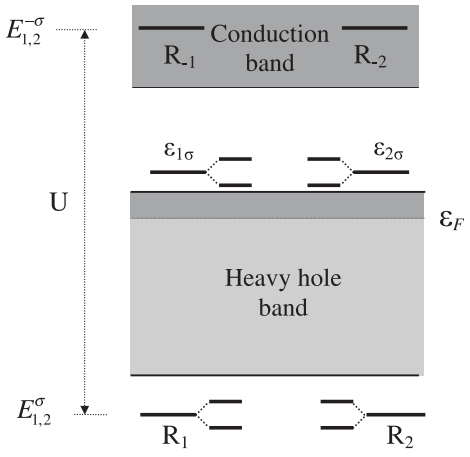

Fig. 1. The scheme of energy levels in GaAs:Mn and GaP:Mn: $R_{1,2}$ stand for CFR levels. The DBH levels $\varepsilon_{1\sigma,2\sigma}$ (acceptor levels) are splitted from the heavy hole band and pushed in the energy gap due to the interaction with the CFR levels.

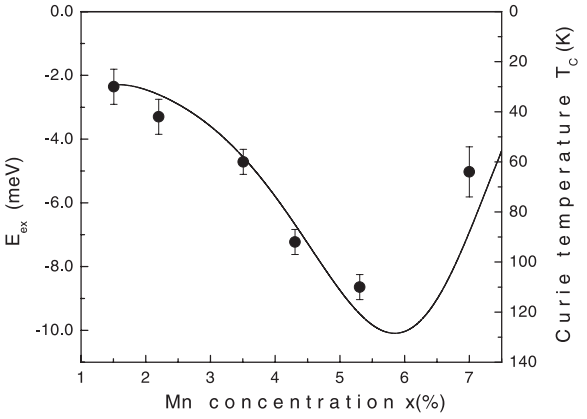

Fig. 2. The dependence of the kinematic exchange (left axis) and T_C (right axis) on Mn concentration. Experimental results (filled circles) are taken from Ref. [5]. The hh bandwidth is 2.9eV (after Ref. [7]); the d-level E_d=-1.5 eV and the hybridization parameter $V = 1.27eV$ are calculated.

The Fermi level dependence $\varepsilon_F(x)$ is calculated using the hole density data [5] (with error bars). The hybridization parameter $V = 1.27$eV is obtained for the acceptor level $\varepsilon_i = 85$ meV ($\varepsilon_i^{\rm exp} = 110$ meV [1]) and the CFR level $E_i = -3.0$eV ($E_i^{\rm exp} = -3.4$eV [6]). By means of Eq. (3) for GaAs:Mn the Curie temperature $T_C(x) = E_{ex}(x)/k_B$, has been computed. The contribution of the localized holes is negligible at small x, and for $x > 5\%$ the formation of impurity band was not taken into account. The results are presented in Fig. 2. Our results are in good agreement both with experimental data, and theoretical predictions.

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