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2010 J. Phys.: Conf. Ser. 245 012032

(http://iopscience.iop.org/1742-6596/245/1/012032)

Journal of Physics: Conference Series **245** (2010) 012032 doi:10.1088/1742-6596/245/1/012032

Phase-diagram for the magnetic states of the Mn-ion subsystem in a magnetic quantum dot

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Abstract. The interplay between two types of spin-spin exchange interaction (namely of the electron with the Mn-ions and the Mn-ions with each other) that are governed by the positions of the Mn-ions and the magnetic field is studied in the case of a Mn-ion doped CdTe quantum dot. We investigate the formation of different magnetic phases and the existence of frustrated magnetic states due to the dominant contribution of the Mn-Mn energy.

1. Introduction

Quantum dots (QDs) containing a single, two, three, etc magnetic ions (Mn^{2+}) have been realized and the interaction between the localized magnetic moments and the electron (or hole) in a single dot was investigated through e.g. local probe photoluminescence [1, 2]. In II-VI semiconductor based QDs such as CdTe or CdSe, the dots exhibit ferromagnetism where the number of carriers can be controlled separately from the number of Mn-ions in the QD.

Previously theoretical studies on Cd(Mn)Te QDs containing few Mn-ions include electronic properties of quasi-two-dimensional (2D) few-electron system at zero field [3], ferromagnetism in hard-wall-cubic noninteracting-electron structure [4], intra-band optical absorption spectrum for single-electron nanostructures [5], and magnetism [6, 7] in low-density Mn-ion system. Magnetism of different II-VI materials e.g. Cd(Mn)Se QDs consisting of a very low concentration of Mn-ions was recently realized [8, 9]. When injecting charged particles into these diluted magnetic semiconductor QDs, a long lifetime of excitons was measured which was a consequence of the exchange electron-Mn-ion (e-Mn) interaction. Note that in Cd(Mn)Se the Landé g-factor of electrons and the Mn-ions have opposite sign. This leads to strong magnetic anisotropy which is one of the important requirements of a memory element and was theoretically examined in e.g. Ref. [10] for symmetric QDs.

Here, we study a 2D Cd(Mn)Te single-electron parabolic QD subjected to an external magnetic field $\overrightarrow{B}$ using exact diagonalization. Such system has a relatively complex behavior due to the opposite signs of the g-factors $g_e \cdot g_{Mn} < 0$. Consequently, different local/system magnetic phases can be formed with respect to the spin orientation of the particles in the two exchange interaction extremes. Magnetic polaron states are obtained depending on the Mn-Mn interaction strength and the magnitude of the magnetic field (cyclotron frequency $\omega_c = eB/m_e^*$). Such a QD system can be described by the following Hamiltonian:

$$\hat{H} = \frac{1}{2m_e^*}\left(-i\hbar\overrightarrow{\nabla}_{\overrightarrow{r}} + e\overrightarrow{A}(\overrightarrow{r})\right)^2 + \frac{1}{2}m_e^*\omega_0^2\overrightarrow{r}^2$$

$$+\frac{1}{2}\hbar\omega_c\left[g_e m^* s_z + g_{Mn} m^*(M_{1z}+M_{2z})\right]$$
$$-J_c\overrightarrow{s}\cdot[\overrightarrow{M_1}\delta(\overrightarrow{r}-\overrightarrow{R_1})+\overrightarrow{M_2}\delta(\overrightarrow{r}-\overrightarrow{R_2}]$$
$$+J_{12}^{Mn}(\overrightarrow{R_{12}})\overrightarrow{M_1}\cdot\overrightarrow{M_2}. \quad (1)$$

The e-Mn and Mn-Mn exchange interactions are, respectively, the fourth and fifth term in Eq. (1). Their strength as a function of the relative position between two Mn-ions can be estimated from Fig. 1. The electrons interact with the Mn-ions by the contact spin-exchange interaction whose form can be expressed in term of second-quantization $J_{ij}(\overrightarrow{R}) = J_c\varphi_i^*(\overrightarrow{R})\varphi_j(\overrightarrow{R})$ with strength [11] $J_c = 1.5\,\mathrm{eV}\mathring{A}^2$. $\{\varphi_i\}$ are the Fock-Darwin single-electron states. The two Mn-ions interact with each other through the anti-ferromagnetic (AFM) spin exchange interaction [12, 13] whose strength $J_{12}^{Mn}(\overrightarrow{R_{12}}) = J_{12}^0\exp\{-\lambda(|\overrightarrow{R_{12}}|/a_0-1)\}$ decreases exponentially with their separation $|\overrightarrow{R_{12}}| = |\overrightarrow{R_1}-\overrightarrow{R_2}|$. $J_0^{12} = 0.5$ meV and $\lambda = 5.1$ are chosen according to experiment work [13] where the two Mn-ions are assumed to interact most strongly when they are nearest neighbors in the Mn-lattice with lattice spacing $a_0 = 5.4\mathring{A}$. Parameters applicable to Cd(Mn)Te QDs are used: the electron effective mass $m^* = m_e^*/m_0 = 0.106$, dielectric constant $\epsilon = 10.6$, effective Bohr radius $a_B^* = 52.9\ \mathring{A}$ and $l_0 = \sqrt{\hbar/m_e^*\omega_0} \sim$ tens of nanometers, g_e=-1.67, and $g_{Mn} = 2.02$.

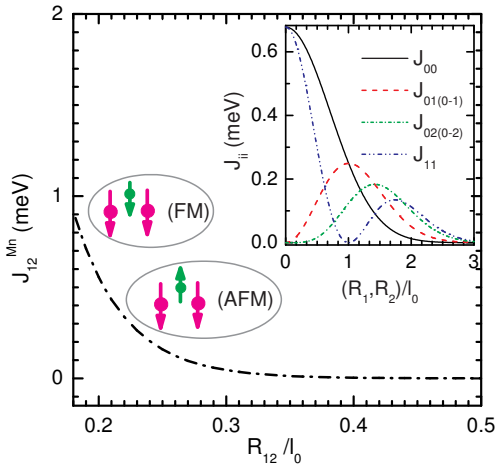

Figure 1. Electron-Mn (the inset) and Mn-Mn (big arrows) exchange interaction as a function of the separation between the Mn-ions. The strength of the e-Mn exchange interaction is evaluated as the diagonal elements in the exchange matrix for the *s*-, *p*-, and *d*-shell. The lower left insets show schematic plots of the FM and AFM phases in case of a single electron (small arrow). Subscripts of J in the inset refer to (n_r, l) as the radial and azimuthal quantum numbers.

We define ferromagnetic (FM) and AFM phases in accordance with the spin couplings of the two subsystems (of the electrons and the Mn-ions) with each other. In fact, at high magnetic fields the electrons and the Mn-ions have anti-parallel spins, which can be considered as the AFM phase. For small magnetic fields the FM phase is found mostly, at least in the case of $N_e = 1$ electron. The Mn-ions in their subsystem also exhibit different orderings (*AFM* and *FM*) in accordance with their spin orientations. We distinguish these local states with the FM and AFM phases of the system by writing them in *italic*.

2. Phase-diagram

The FM and AFM phase diagram for $N_e = 1$ electron [14] and $N_{Mn} = 1$ is summarized in Fig. 2(a) as a function of the Mn-ion position relative to the center of the QD and magnetic field. This result shows that the single-electron case samples the dominant FM region around the center of the dot. By moving the Mn-ion out of the center, the e-Mn interaction decreases and a slightly larger than zero field is sufficient to transit the system to the AFM phase.

Now we introduce a second Mn-ion. We found that the Mn-ion now becomes less sensitive to the presence of the field as compared to the one Mn-ion situation with the stable minimum value $M_z = -5/2$ [14]. Here, the Mn-ion(s) transit to spin $-5/2$ after the intermediate phases where M_z of the Mn-ions can be $-1/2$ or $-3/2$. The e-Mn and Mn-Mn exchange interaction compete most strongly in the very-small-field limit (see Fig. 1). Note that the e-Mn interaction strength is larger with increasing magnetic field. It is worth noting that the Mn-Mn exchange energy is only comparable with the e-Mn energy when they are positioned close to each other, say $R_{12} < 0.4l_0$. Plus, the Mn-ions can repel/attract the electrons differently if they are located asymmetrically with respect to the center of the QD. In case they are located symmetrically and for small Mn-Mn separation their spin exchange strength is enhanced and the Mn-ions stay in the AFM state. On the other hand when they equally attract the electron and the system they stay in the FM phase. Such a state is named *frustration*. To understand the physics that takes place with changing the magnetic field and the Mn-ion positions (symmetry and asymmetry) it is important to have information on the Mn-ion position dependence of the local AFM and FM states. Such information is made visible in Fig. 2(b). The phase diagram has a step-like form because the Mn-Mn interaction strength depends on the $M_{(1,2)z}$ which changes by steps of unity when changing their relative separation or their individual positions. In case the Mn-ions are very close to each other, say $R_{12} < 0.28l_0$, the subsystem stays in the AFM phase regardless they are symmetrically or asymmetrically positioned.

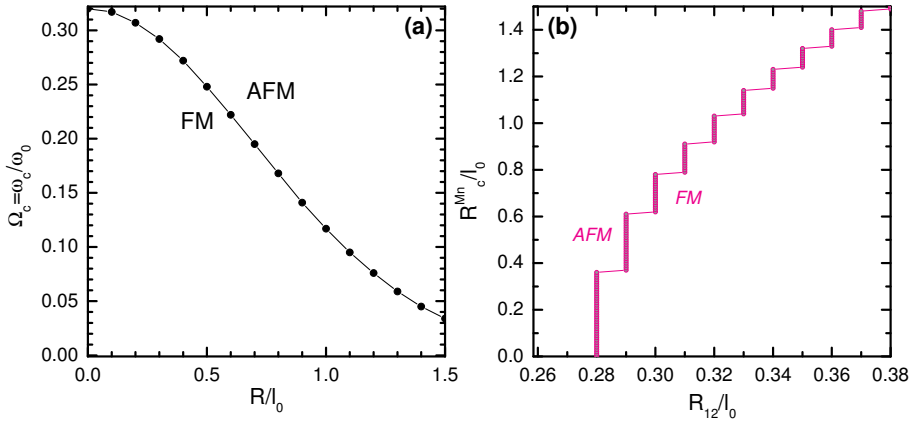

Figure 2. Magnetic phase diagram of a single-electron QD doped with one (a) and two (b) Mn-ions for zero field as function of the Mn-ion positions. $\overrightarrow{R_c^{Mn}} = (\overrightarrow{R_1} + \overrightarrow{R_2})/2$ is the Mn-ion center of mass coordinate.

Magnetic polaron state occurs when a single electron FM or AFM couples with a collection of FM-coupled Mn-ions. The FM polaron is found when the Mn-ion separation is engineered such that their magnetic coupling is FM and the e-Mn interaction is found FM. Therefore, such FM polaron can be obtained in the small-field limit. Because in the high-polarized situation,

the electron will couple AFM with the Mn-ions and the system forms an AFM polaron.

We also calculate the ground-state (GS) magnetization $< M >_{GS} = -\partial < E_{GS} > /\partial B$ and the thermodynamic magnetization $< M(T) > = -\partial < E(T) > /\partial B$ for $T = 5.8$ K and show the results in Fig. 3 for a typical symmetric positioning of the Mn-ions $\overrightarrow{R_{1,2}} = (\pm 0.15 l_0, 0)$ as a function of magnetic field. The magnetic-field dependence of the magnetic polaron states (circles containing electron and two Mn-ions) is observed in different manners with and without T. The step appears each time the spins of either the electron or the Mn-ions transit to a smaller/larger intermediate state. In this case the magnetic polaron state starts at very small field, $\Omega_c = \omega_c/\omega_0 \approx 0$, the system exhibits a unique step that is the FM-AFM transition.

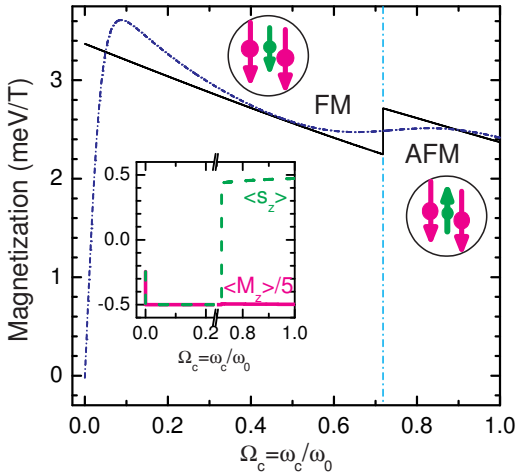

Figure 3. Magnetization as a function of magnetic field calculated for the GS energy (black solid) and $T = 5.8$ K (blue dash-dotted) in case $\overrightarrow{R_{1,2}} = (\pm 0.15 l_0, 0)$. Cyan dash-dotted separates the FM and AFM regions. Inset is the average of s_z and M_z for reference. Small and big arrows refer to the electron and Mn-ions, respectively.

Acknowledgments

This work was supported by FWO-Vl (Flemish Science Foundation) and the Belgian Science Policy (IAP).

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