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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 $\vec{B}$ using exact diagonalization. Such system has a relatively complex behavior due to the opposite signs of the g-factors $g_e \cdot g_{\text{Mn}} < 0$. 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:

$$\hat{H} = \frac{1}{2m_e^*} \left(-i\hbar \nabla \cdot \vec{A}(\vec{r}) + eA(\vec{r})\right)^2 + \frac{1}{2}m_e^*\omega_0^2\vec{r}^2$$
\( + \frac{1}{2} \hbar \omega_c [g_e m^* s_z + g_{Mn} m^* (M_{1z} + M_{2z})] \)
\[ - J_c \vec{s} \cdot [M_1 \delta(\vec{r} - \vec{R}_1) + M_2 \delta(\vec{r} - \vec{R}_2)] \]
\[ + J_{12}^{Mn} (\vec{R}_{12}) \cdot M_1 \cdot M_2. \]

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 terms of second-quantization

\[ J_{ij}(\vec{R}) = J_c \varphi_i^*(\vec{R}) \varphi_j(\vec{R}) \]

with strength \( J_c = 1.5 \text{ eVÅ}^2 \). \( \{\varphi_i\} \) are the Fock-Darwin single-electron states. The two Mn-ions interact with each other through the anti-ferromagnetic (AFM) spin exchange interaction whose strength \( J_{12}^{Mn}(\vec{R}_{12}) = J_0^{12} \exp\{-\lambda(|\vec{R}_{12}|/a_0 - 1)\} \)

decreases exponentially with their separation \( |\vec{R}_{12}| = |\vec{R}_1 - \vec{R}_2| \).
\( J_0^{12} = 0.5 \text{ meV} \) 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 \( a_0 = 5.4 \text{Å} \). 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 \( a_B^e = 52.9 \text{ Å} \) and \( l_0 = \sqrt{\hbar/m^*_e \omega_0} \sim \text{tens of nanometers} \), \( g_e = -1.67 \), 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 \( R_{12} < 0.4 l_0 \). 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 \( R_{12} < 0.28 l_0 \), the subsystem stays in the AFM phase regardless they are symmetrically or asymmetrically positioned.

![Figure 2](image_url)

**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. \( R_{Mn}^c = (\vec{R}_{1} + \vec{R}_{2})/2 \) 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 \( T = 5.8 \text{ K} \) and show the results in Fig. 3 for a typical symmetric positioning of the Mn-ions \( \vec{R}_{1,2} = (\pm 0.15l_0, 0) \) 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 \( T = 5.8 \text{ K} \) (blue dash-dotted) in case \( \vec{R}_{1,2} = (\pm 0.15l_0, 0) \). 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.

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