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# The breakdown of Kohn's theorem in few-electron parabolic quantum dots doped with a single magnetic impurity $\text{Mn}^{2+}$

Nga T. T. Nguyen and F. M. Peeters

Departement Fysica, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium

E-mail: nga.nguyen@ua.ac.be, francois.peeters@ua.ac.be

**Abstract.** The cyclotron resonance (CR) absorption spectrum is calculated for a II-VI parabolic quantum dot (QD) containing few electrons and a single magnetic dopant ( $\text{Mn}^{2+}$ ). We find that Kohn's theorem no longer holds for this system and that the CR spectrum depends on the number of electrons inside the QD. The electron-Mn-ion interaction strength can be tuned for example by the magnetic field and by moving the Mn-ion to different positions inside the QD. We demonstrate that due to the presence of the Mn-ion the relative motion of the electrons couple with their center-of-mass motion through the electron-Mn-ion spin-spin exchange term resulting in an electron-electron interaction dependence of the magneto-optical absorption spectrum. At the ferromagnetic-antiferromagnetic transition we observe significant discontinuities in the CR lines.

## 1. Introduction

Quantum dots (QDs) doped with a single manganese ion ( $\text{Mn}^{2+}$  - spin 5/2) have been fabricated recently [1, 2] in CdTe based semiconductor. The single Mn-ion spin states were probed through multi-peak PL spectroscopy, and signatures of the exciton-Mn-ion spin exchange interaction were observed. Such QD systems are promising for future quantum computing application. For example the Mn-ion magnetic moments can be used to store information facilitating the readout functionalities in a quantum computing system.

Here we investigate a two-dimensional (2D) few-particle parabolic QD model system [3, 4]. We will examine the effect of the electron-electron (e-e) interaction on the magneto-optical absorption spectrum of such a few-electron QD in the presence of a single Mn-ion. Different absorption lines of allowed cyclotron resonance (CR) transitions were predicted as function of an external magnetic field.

We investigate the allowed CR transitions and their corresponding oscillator strength (OS). Our numerical results are for the experimental realized system Cd(Mn)Te where the lateral size is much larger than the height of the QD and consequently the system behaves like a quasi-2D QD. We find crossing and anti-crossing features that depend on the position of the Mn-ion in the QD and on the strength of the confinement potential. We will focus on the allowed transitions and the different CR lines that become possible due to the presence of the Mn-ion. The CR transitions now contain information not only of the electron state but also of the electron-Mn-ion (e-Mn) interaction and the magnetic state of the Mn-ion.

## 2. The model

The Hamiltonian of  $N_e$  interacting electrons ( $\vec{r}_i, \vec{s}_i$ ) confined by a parabolic potential with confinement strength  $\hbar\omega_0$  (tens of meV) embedded in a quasi-2D CdTe host QD doped with a single Mn-ion ( $\vec{R}, \vec{M}$ ) in a perpendicular magnetic field  $\vec{B}$  reads:

$$\hat{H} = \sum_{i=1}^{N_e} \left[ \frac{1}{2m_e^*} \left( -i\hbar\vec{\nabla}_{\vec{r}_i} + e\vec{A}(\vec{r}_i) \right)^2 + \frac{1}{2}m_e^*\omega_0^2\vec{r}_i^2 \right] + \sum_{i<j=1}^{N_e} \frac{e^2}{4\pi\epsilon_0\epsilon|\vec{r}_i - \vec{r}_j|} + \frac{1}{2}\hbar\omega_c (g_e m^* S_z + g_{Mn} m^* M_z) - J_c \sum_{i=1}^{N_e} \vec{s}_i \cdot \vec{M} \delta(\vec{r}_i - \vec{R}). \quad (1)$$

The vector potential  $\vec{A} = B/2(-y, x, 0)$  is taken in the symmetric gauge. The confinement frequency  $\omega_0$  is related to the confinement length by:  $l_0 = \sqrt{\hbar/m_e^*\omega_0}$  with  $m^* = m_e^*/m_0 = 0.106$  the effective electron mass.  $g_e = -1.67$  and  $g_{Mn} = 2.02$  are the Landé g-factor of the host semiconductor and the Mn-ion, respectively. Electron cyclotron frequency is  $\omega_c = eB/m_e^*$ . The strength [5] of the e-Mn spin-spin exchange interaction is typically about  $J_c = 1.5 \text{ eV}\text{\AA}^2$ . We use the set of parameters [1, 6] that is applicable for relatively small Cd(Mn)Te QDs. The dielectric constant  $\epsilon = 10.6$ , the effective Bohr radius  $a_B^* = 52.9 \text{ \AA}$ , and  $l_0$  are of the order of tens of nm. For example, with  $\hbar\omega_0 = 51.32 \text{ meV}$  we have  $l_0 = 26.45 \text{ \AA}$ .

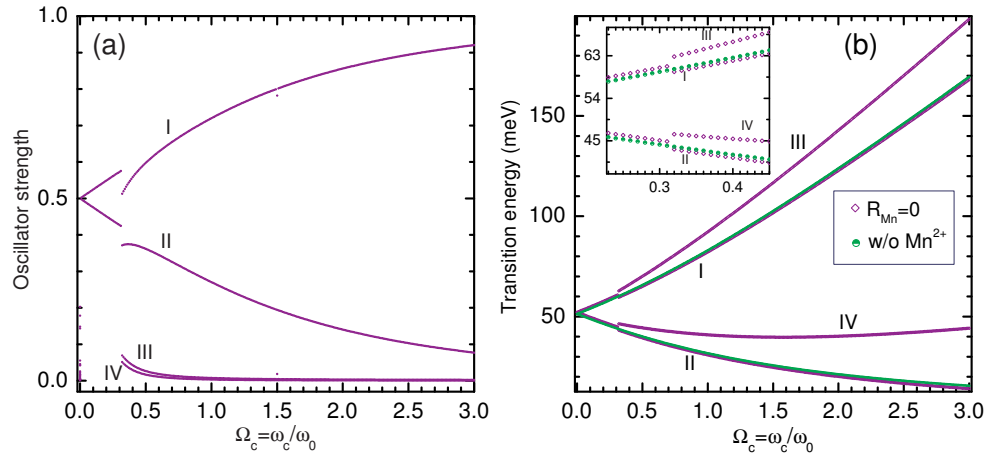
We have adopted configuration interaction method to build up the Hamiltonian [6, 7] matrix and employed exact diagonalization [7] to obtain numerically the many-body eigenstates. Note that the total angular momentum  $L$  and spin  $S_z$  do not commute with  $\hat{H}$  therefore they are no longer good quantum numbers and we have to consider the entire Hilbert space. This rapidly increases the size of the Hamiltonian.

The OS of the intra-band electron transitions (from ground state (GS)  $i$  to excited state  $j$ )  $f_{ij} = 2\Delta E_{ij}/\hbar\omega_H \cdot |A_{ij}|^2/l_H^2$  are calculated using the transition amplitude [8]:  $A_{ij} = \sum_{p=1}^{N_e} \langle \Psi_i(\vec{r}_1, \dots, \vec{r}_{N_e}) | r_p e^{\pm i\theta_p} | \Psi_j(\vec{r}_1, \dots, \vec{r}_{N_e}) \rangle$  with its transition energy  $E_{ij} = E_j - E_i$ . We define  $\omega_H = \omega_0(1 + \Omega_c^2/4)^{1/2}$  where  $\Omega_c = \omega_c/\omega_0$  and  $l_H = [\hbar/(m_e^*\omega_H)]^{1/2}$  defines a new length.  $\Psi_{i(j)}$  is the many-body wave function [7] of state  $i(j)$  which is a linear combination of all possible  $N_e$  quantum state wave function  $\psi_{i(j)}$ , where  $\psi_{i(j)}$  is a product of Slater determinants and spin component of the Mn-ion for configuration  $i(j)$ . The single-electron basis consists of the Fock-Darwin (FD) states in a magnetic field [7]. A sufficiently large number of FD levels are included to guarantee numerical convergence. All allowed transitions with OS exceeding 1% are retained. The following Lorentzian broadened formula:  $\sigma_i(E) = \sum_j \Gamma_{ij}/\pi \cdot f_{ij}/[(E - E_{ij})^2 + \Gamma_{ij}^2]$  is used.  $\Gamma_{ij}$  is the broadening parameter that is taken to be about  $0.01 \div 0.1 \text{ meV}$  in our numerical simulation of the absorption spectrum.

The presence of the Mn-ion leads to different arrangements ferromagnetic (FM) and antiferromagnetic (AFM) of the spins of the electron and the Mn-ion which are tunable by an external magnetic field  $B$ . This is due to the interplay between the Zeeman energies and the exchange interaction, which both depend on  $B$ . The FM phase is found for very small  $B$  when the exchange energy dominates over the Zeeman energies. In the other case the AFM phase is found. The presence of the Mn-ion leads to a mixing of the FD orbitals for the different eigenstates in contrast to the QD without a Mn-ion where those FD orbitals are the quantum eigenstates.

We show in Fig. 1 the OS and CR energies for  $N_e = 1$  electron QD. The main transitions come from transitions to the two  $p$ -orbitals as typically observed in QDs without Mn-doping. But in the presence of a Mn-ion we notice that the OS exhibits a discontinuity at  $\Omega_c = 0.32$  where the FM-AFM transition takes place. I and II, respectively, corresponds to the transitions from the GS with  $(n_r, l, s_z, M_z) = (0, 0, s_z, -5/2)$  to  $(0, \mp 1, s_z, -5/2)$  as the major quantum state. The wave function of the GS changes at the FM-AFM from favoring a configuration where the

electron spin has a large probability to be down to configuration with electron spin up. The other two CR-lines (III and IV) come from spin-spin exchange interaction corresponding to final states that have wave functions containing, respectively,  $(0, -1, -1/2, -3/2)$  and  $(0, 1, -1/2, -3/2)$  as their major FD states.



**Figure 1.** OS (a) and CR energies (b) of single-electron QD in case the Mn-ion is located at  $R = 0$  as a function of magnetic field. The results without Mn-ion are added in the inset for reference.

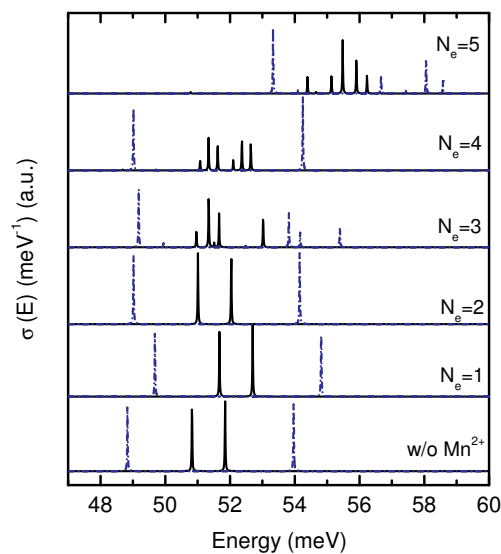
Many-body effects in the FIR spectroscopy are examined in Fig. 2 where the CR energies for different  $N_e$  QDs are shown when the Mn-ion is located at  $R = 0$  for two different  $\Omega_c = 0.02$  ( $\approx 0.15$  T) and 0.1. The number of allowed electron transitions depends on  $N_e$ . We refer to Ref. [9] for a detailed study on how the e-e interaction weakens the e-Mn exchange interaction and how it affects the FIR spectrum.

The  $N_e$ -dependence of the CR spectrum is due to a breaking of Kohn's theorem. The reason is that the center-of-mass motion couples with the relative motions and also with the Mn-ion through the e-Mn spin exchange. Note that the relative motions contain information about the e-e interaction. This fact leads to the existence of various IR absorption spectra for different  $N_e$  in which many transitions have different energies.

For  $N_e = 3$ , the number of major CR lines is four in the FM phase. The contribution  $(0, 1, -1/2, -3/2)$ , which becomes dominant in the excited-state wave function, is ascribed to the presence of the double (circularly) right-polarized modes (of the spin-down  $s$ -electron and spin-up  $p_{(n_r, l)=(0,1)}^+$ -electron) as the first (sorted ascending in energy) two large-OS peaks and double left-polarized modes (the other two large-OS peaks) for  $\Omega_c = 0.02$ , and triple left-polarized modes for  $\Omega_c = 0.1$  (the three largest-energy peaks). The very-low-OS (4% of the total OS) black solid peak is the left-polarized mode combining the  $\sigma^+$ (s) of the spin-down  $s$ -electron and the  $p^+$ -electron where the configuration  $(0, 1, -1/2, -3/2)$  strongly dominates the final state.

We note that for  $N_e = 2, 4, \dots$  electrons the FM phase is the GS up to lower B-fields as compare to the case  $N_e = 1, 3, 5, \dots$  electrons (see Ref. [7]). This fact leads to the appearance of only two major peaks for  $N_e = 2$  and 4 electrons when  $\Omega_c = 0.1$  which are the major transitions ( $S_z = 0$ ) to the  $p$ -orbitals without exchanging spins. However, for  $N_e=4$  the total spin can be such that we have triplet state for  $\Omega_c = 0.02$  which results in a larger number of CR-lines in

this case. Apparently, Fermi-Dirac statistics plays an essential role because the filling effect, as seen in the case  $N_e = 4$  for the intermediate states  $S_z = \pm 1$  and 0, influences directly the spin exchange interaction. The FIR absorption energies for  $N_e = 5$  are different from those of  $N_e = 3$  due to  $p$ - $p$  (orbital) e-e interaction effect. For  $\Omega_c = 0.02$  a left-polarized mode can be at a smaller energy as compared to a right-polarized mode where the left-polarized combined modes of the spin-down  $s$ -, spin-up  $p^+$ -, and spin-up  $p_{(n_r, l)=(0, -1)}^-$ -electron and of the two spin-up  $p$ -electrons are, respectively, the first and the fourth peak (sorted in energy). The existence of the very-low-OS peaks ( $\approx 2 \div 5\%$  of the total OS) in all cases of  $N_e$  are evidence of the influence of the e-Mn interactions when the small component to the GS, e.g.  $(0, 0, -1/2, -3/2)$  for  $N_e = 1$  electron QD, becomes the dominant one in the excited states.



**Figure 2.** CR energies of a  $N_e$ -electron QD in case the Mn-ion is located at  $R=0$  for two different fields  $\Omega_c = 0.02$  (black solid) and  $0.1$  (blue dash-dotted). Absorption energies in case without the Mn-ion are added for reference.

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