Far Infrared absorption of non center of mass modes and optical sum rule in a few electron quantum dot with Rashba spin-orbit coupling

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Introduction.

Semiconducting Quantum Dots (QD) with few confined electrons are possible candidates for applications in future quantum electronics\textsuperscript{1}. The separation of the electron levels in such artificial atoms, of size of hundred of nanometers, is of the order of few meV, so that optical spectroscopy requires Far Infrared Radiation (FIR). Indeed, FIR absorption is a common tool in large scale QD arrays\textsuperscript{2} (e.g. in In QDs\textsuperscript{3} or field-effect confined GaAs QDs\textsuperscript{4}) ever since their first fabrication. However, in parabolically confined dots, it is well established that the FIR spectrum is rather poor of information, because the dipole approximation holds to a high degree of accuracy and light couples only to the electron center of mass (CM) modes (so called Kohn’s modes $\omega_{\pm}$). The latter, are free-oscillator like and are decoupled from the internal dynamics of the correlated electrons (Kohn’s theorem\textsuperscript{5}). Hence, the location of the absorption peaks does not depend on the number of electrons $N$ confined in the dot. Non parabolic corrections to the confinement potential have been invoked to defeat Kohn’s theorem\textsuperscript{2}, what would provide also information about $e-e$ correlations by using FIR. Indeed, weak plasma modes have been spotted just below the upper Kohn frequency $\omega_{+}$\textsuperscript{4,6}. Recently, Raman scattering is improving as a tool to probe correlation effects\textsuperscript{6}, and to prepare spin states in QDs\textsuperscript{7}.

Much interest is being focused on the Rashba Spin Orbit (RSO) interaction\textsuperscript{8}, which arises in QD structures due to the two-dimensional (2D) confinement, since it can be tuned by gate voltages parallel to the $x-y$ structure\textsuperscript{8}. RSO interaction offers a precious tool for the manipulation of the dot spin states and is quite relevant for the proposed application of QDs as spin qubits\textsuperscript{9,10}. In this context, the study of the effects of the various spin-orbit (SO) couplings (e.g. including Dresselhaus, etc.) is quite crucial, because, in conjunction with the electron-phonon interaction, it is one of the causes of spin relaxation and dephasing, which limits the coherent evolution of the spin\textsuperscript{11,12}. Besides, SO affects conductivity directly, by turning weak localization corrections into antilocalization ones, as probed in large QDs\textsuperscript{12}.

In the presence of SO coupling, the CM dynamics of the electrons and that of their relative coordinates cannot be separated\textsuperscript{13}. Hence a simple FIR experiment on a QD with SO coupling can probe any excitation mode and correlation effects compatible with optical selection rules. By exciting a few electron QD in the presence of RSO coupling and of an external orthogonal magnetic field $B$ with circularly polarized light, it is possible to identify the collective spin excitations, as we discussed previously\textsuperscript{13,14}. The intensities of the non–CM peaks increase with SO coupling at the expenses of the CM ones. We find that the absorption intensities satisfy the optical sum rule, encountered in single atoms as well as in solids\textsuperscript{15}. In particular, the total intensity is proportional to the number of electrons $N$ confined in the dot. In the case of a circularly polarized light, the sum rule is independent of the strength of the RSO coupling, even in a constant magnetic field. This property of the sum rule, that we proof analytically and check numerically, could help in identifying the relative weight of the RSO coupling, with respect to other sources of intrinsic SO interactions\textsuperscript{17}.

Center of mass excitations in Quantum Dot. The electrons are confined in the $(x,y)$ plane by a parabolic potential of characteristic frequency $\omega_{\perp}$, in the presence of an uniform orthogonal magnetic field $\mathbf{B} = -B\hat{z}$ . The total Hamiltonian for electrons of charge $-e$, interacting via the Coulomb potential, in the effective mass ($m_{e}^*$) approximation, in the absence of SO coupling, is:

$$H = \sum_{i=1}^{N} \left[ \frac{1}{2m_{e}^*} \left( \frac{\hbar}{e} A_{i} \right)^{2} + \frac{1}{2} m_{e}^* \omega_{\perp}^{2} \hat{r}_{i}^{2} \right] + \sum_{i,j=1}^{N} \frac{U}{|\hat{r}_{i} - \hat{r}_{j}|},$$

(1)

with $A_{i} = B/2(y_{i} - x_{i}, 0)$. The strength of the Coulomb interaction $U$ is dictated by the screening in the dot and
is a parameter in our calculation. In the presence of an orthogonal magnetic field \( B \) (cyclotron frequency \( \omega_c = eB/m^*_c \)), the characteristic length due to the lateral geometrical confinement \( l = \sqrt{\hbar/m^*_c \omega_c} \) depends on the frequency \( \omega_c = \sqrt{\omega_0^2 + \omega_i^2}/4 \).

The ratio \( v = U/\omega_i \) gives an estimate of how strong the correlations are. By tuning \( U \) and \( \omega_i \), one can range from a Fermi liquid behavior \( (v \sim 1) \), up to very strongly correlated regimes \( (v \sim 5-7) \), in which crystallized phases appear, the so called Wigner molecule \[18\]. We will focus on intermediate regimes \( v \sim 2 - 4 \) in what follows, in which correlations are too strong to be dealt with by using an Hartree Fock approach, but not enough to allow for breaking of azimuthal symmetry and for creation of a Wigner molecule \[19\]. We use exact numerical diagonalization as done previously \[20\].

The Hamiltonian of Eq. (1) separates as: \( H = H_{CM} + H_r \), with \( [H_{CM}, H_r] = 0 \). Here \( H_{CM} \) is the Hamiltonian for the CM coordinates \( \vec{R} = \sum_i \vec{r}_i, \vec{P} = \sum_i \vec{p}_i \), with total mass \( M^* = Nm^*_c \) and \( H_r \) involves only the relative coordinates \( \vec{p}_{ij} = \vec{p}_i - \vec{p}_j, \vec{r}_{ij} = \vec{r}_i - \vec{r}_j \).

Let us first consider the case of \( N = 2 \) electrons for sake of illustration. The quantum numbers labeling the two particle states are particularly simple. Indeed, the spin wavefunction factorizes, as well as the two-dimensional harmonic oscillator wavefunction of the CM. Finally, just a single particle orbital wavefunction for the relative coordinate is present. The CM wavefunction is always symmetric w.r.t. to the exchange of the two particles. Hence, the requirement of overall antisymmetry for the total wavefunction, fixes reciprocally the symmetries of the relative motion and of the spin wavefunctions. The ground state (GS), at zero magnetic field, is a singlet of energy \( E_0 = 4.097\omega_o \), for \( \omega_o = 5meV, U = 13meV \). The CM excitations are always equally spaced at each \( B \). Indeed, we find, at \( B = 0 \), the first two CM excitations at energies \( E_1 = 5.099\omega_o \) and \( E_2 = 6.100\omega_o \), with a relative error \( \sim 2/1000 \) r.w. to the correct result.

For more than two electrons the analytical factorization of spin and orbital wavefunction is possible only when the dot is fully spin polarized. This implies that, in the general case, the CM modes can be identified only by comparing the energies of the states numerically. In Fig. (a) we have plotted a few low lying energy levels for \( N = 3 \) vs \( \omega_c \), in the absence of SO coupling. Good quantum numbers are the total orbital angular momentum \( M \) orthogonal to the dot disk, the total spin \( S \) and the projection of the spin along \( \hat{z} \), \( S_z \). We have singled out the GS (bold black line) and the first two CM modes \( E_1, E_2 \) (red and green line respectively) with the same \( S = S_z = 0 \) as the GS, but with \( M \) increasing by one. They are equally spaced at each \( B \) (within numerical errors), as shown in the inset, where the energy differences \( E_1 - E_{GS} \) (red circles), \( E_2 - E_1 \) (green triangles) and the expected difference \( \omega_c \) (black line) are reported in units of \( \omega_o \).

The RSO coupling, included in Fig. (b), adds to the non interacting Hamiltonian of eq. (1) the potential:

\[
V_{RSO} = \frac{\alpha}{\hbar} \hat{z} \times \sum_i \left( \vec{p}_i + \frac{e}{c} \vec{A}_i \right) \cdot \vec{\sigma}_i.
\]  

Here \( \vec{\sigma} \) are the Pauli matrices and \( \alpha \) is proportional to the effective (crystal plus applied) electric field in the \( \hat{z} \) direction. In a biased dot, the actual size of this perturbation would depend also on the screening of the source drain bias voltage \( V_{sd} \) applied to the contacts. For a reference dot with \( \omega_d = 5meV \) and \( U = 13meV \), we choose \( \alpha \) in the range \( 0 \leq 25meV nm \). In the presence of the term of eq. (2) in the Hamiltonian, the orbital angular moment-
FIG. 2: (Color online) N=2 (left) and N=3 (right). Bottom panels: the excitation modes energies \( \omega_\alpha \equiv E_\lambda - E_{GS} \) vs. \( \omega_c \), in units of \( \omega_o \), for \( \alpha = 0 \) (d) and 25 meV nm (e). The intensities of their FIR absorption peaks are represented by a greyscale plot underlying the heavy lines. At \( \alpha = 0 \) a single peak appears, corresponding to the CM excitation mode. By increasing the RSO, other excitation branches appear, whose weight increases with magnetic field. The broadening is artificial and equal for all the peaks \( [2] \). Middle panels: the intensities of the excitation modes are plotted with colors corresponding to the curves in (d),(e), in arbitrary units. The top plots show the sum rule vs \( \omega_c \) in units of \( \omega_o \). The plotted sum is independent of the RSO interaction. Numerical discrepancy occurs in the neighborhood of a level crossing ( \( \omega_c \sim 4 \text{ meV} \) ), due to the truncation of the Hilbert space.

tum \( M \) and the spin \( S_z \) cease to be separately conserved, while the total angular momentum along \( z \), \( J_z = M + S_z \), is. The total spin \( S \) of the CM levels in Fig. (1b) keeps being the same as that of the GS. Nevertheless, \( S \) of the GS increases with \( \omega_o \) due to crossings.

**FIR absorption, Kohn modes, and optical sum rule.**

The FIR interaction in the dipole approximation can be written as

\[
H_{FIR} = A_0(\omega) \hat{e} \cdot \vec{P} e^{i\omega t} + h.c. \tag{3}
\]

where \( A_0(\omega) \) is the envelope function of the FIR wavepacket in the \( \omega \)-space, which we suppose to be almost monochromatic and \( \hat{e} \) is the polarization vector of the light. The Kohn modes are excited at frequency \( \omega_\pm = \omega_o \pm \omega_c/2 \). It is apparent from eq. (2) that the CM and the relative coordinates no longer decouple, in the presence of the RSO term. As a consequence, more excitations appear in the FIR spectrum and we now discuss the relative intensities of the peaks we find.

We choose circularly polarized light in the \( x, y \) plane, in order to excite modes in subspaces with \( \Delta J_z = \pm 1 \). If we take right hand polarization \( \epsilon_R = \hat{x} + i\hat{y} \), the radiation transfers one unit of angular momentum to the dot, \( H_{FIR} \propto \rho^+_c + h.c. \) where:

\[
\rho^+_c = \sum_{n \sigma} \frac{m}{|m|} \left( c^\dagger_{n-1m+1\sigma} c_{n\sigma} + c^\dagger_{n+1m+1\sigma} c_{n\sigma} \right) \tag{4}
\]

The operators \( c_{n\sigma} \) correspond to the single particle Darwin-Fock orbitals \( \phi_{n\sigma} \). These are the eigenfunctions of the 2D harmonic oscillator with frequency \( \omega_o \) and energy: \( \epsilon_{n,m} = (n + 1)\hbar\omega_o - \frac{m}{2}\hbar\omega_c \). Here \( m \) is the angular momentum in the \( z \) direction ( \( m \in (-n, -n + 2, ..., n - 2, n) \) with \( n \in (0, 1, 2, 3, ... ) \) ) and \( \sigma \) is the spin projection along the \( z \) axis. The prime in eq. (4) restricts the sum in such a way that the labels containing \( n \) and \( m \) are compatible with the given rules. \( \rho^+_c \) is the operator creating an excitation which increases \( M = \sum_i^n m_i \) by one. The energy location of the FIR absorption peaks for two (left panels) and three electrons (right panels) is shown in Fig. 2 vs. \( \omega_c \) for \( \alpha = 0 \) (d), and \( \alpha = 25 \text{ meV nm} \) (e) and their intensity,

\[
I_\lambda = |\langle J^{GS}_z + 1, \lambda | H_{FIR} | J^{GS}_z \rangle |^2, \tag{5}
\]

appears as a grey scale plot in arbitrary units. The broadening of the lineshapes is artificial and equal for all the
peaks. The excitation energies $\omega_0 \equiv E_\lambda - E_{GS}$, for $\Delta J_z = 1$, are also plotted in units of $\omega_0$ vs. the magnetic field $\propto \omega_z$ as colored curves in Fig.(2a,d,e). $\lambda$ is a generic label [21]. In the absence of RSO, only the lower Kohn mode $\omega_-$ can be excited for right hand polarization. By increasing the RSO coupling, new possible excitations appear below and above the $\omega_-$ mode. In particular the one below increases markedly in intensity when the magnetic field increases. We have shown that it goes almost soft at the crossover to the fully spin polarized state for the dot [14, 15]. This is the collective spin excitation which recalls the skyrmion ($\Delta S = 0$) of a Ferromagnetic Quantum Hall disk at filling close to one. Inspection of the intensities in Fig.(2a,b,c) shows that, by increasing the RSO, the intensity of the Kohn mode drops down and the lost spectral weight is transferred to the newly emergent modes (the colors correspond to the $\omega_0$ reported in Fig.(2d,e)). In fact, we have verified that the optical sum rule holds, as customary in atoms and solids [16]. The optical sum rule in this case, reads:

$$\sum_\lambda \omega_0 \left| \langle \lambda | \rho_+^\dagger | 0 \rangle \right|^2 = 0 = \left| \left[ \rho_+^\dagger, [H, \rho_+] \right] \right| 0 \rangle = N \omega_-$$

(6)

where $|0\rangle$ is the GS. The sum rule does not depend on the interaction term, nor, remarkably, on the RSO, because $[\rho_+^\dagger, [V^\text{RSO}, \rho_+]] = 0$. At zero magnetic field $\omega_- = \omega_d$, so that Eq. (6) sums up to $N \omega_d$ only. This can be easily checked analytically for non interacting particles, by using a single Slater determinant for $|0\rangle$. The sum rule is plotted vs. $\omega_c$ in the top panel of Fig.2a, left (N = 2) and Fig.2a, right (N = 3). Only few terms were included in the summation over $\lambda$, because strict selection rules limit the number of states contributing, up to a relatively high energy. The curves for $\alpha = 0$ and $25 \text{meV}$ almost coincide, except for the neighborhood of $\omega_c \sim 4 \text{meV}$, where levels cross and a larger computational Hilbert space in the calculations would be desirable. Of course, only the CM transition contributes for $\alpha = 0$.

In summary, the inclusion of a spin orbit interaction invalidates Kohn’s theorem for FIR absorption in the dipole approximation, even for parabolically confined dots. The possibility to excite non-center of mass modes makes the optical response of QDs more rewarding. As in atoms and solids, the total sum of the oscillator strengths depends on the number of particles in the dot. The optical sum rule is a precious tool to extract valuable information on correlation effects in QDs by using the FIR spectroscopy. Here we have considered a top gate controlled RSO coupling and circularly polarized radiation. While the relative weight of the intensities of the absorption peaks depends on the strength of the Rashba spin-orbit coupling, the total sum rule for the circularly polarized light is insensitive to it. We suggest that this fact allows to discriminate the amount of SO coupling present, other than the RSO term $V^\text{RSO}$ given by Eq.(2).

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[21] At $B = 0$ ($\alpha \neq 0$) we find that the total spin differences of the excitations, $\Delta S_{\lambda 0}$ are 1, 0, 0 for $\lambda = 1, 2, 3$, respectively ($N = 2$) and 0, 1, 0, 1 for $\lambda = 1, 2, 3, 4$, respectively ($N = 3$). At larger $\omega_c > 4meV$, $\Delta S_{\lambda 0}$ changes because a fully spin polarized GS sets in.