Far-infrared absorption of noncenter-of-mass modes and an optical sum rule in a few-electron quantum dot with Rashba spin-orbit coupling

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Spin-orbit interaction in a quantum dot couples far-infrared radiation to noncenter-of-mass excitation modes, even for parabolic confinement and dipole approximation. The intensities of the absorption peaks satisfy the optical sum rule, giving direct information on the total number of electrons inside the dot. In the case of a circularly polarized radiation, the sum rule is insensitive to the strength of a Rashba spin-orbit coupling due to an electric field orthogonal to the dot plane, but not to other sources of spin-orbit interaction, thus allowing one to discriminate between the two.

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Introduction. Semiconducting quantum dots (QD) with few confined electrons are possible candidates for applications in future quantum electronics.[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[2] [e.g., in In QDs (Ref. 3) or field-effect confined GaAs QDs (Ref. 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 (c.m.) 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[5]). Hence, the location of the absorption peaks does not depend on the number of electrons N confined in the dot. Nonparabolic corrections to the confinement potential have been invoked to defeat Kohn's theorem,[2] which would also provide information about e-e correlations by using FIR. Indeed, weak plasma modes have been spotted just below the upper Kohn frequency ω_{+}.[4] Recently, Raman scattering is improving as a tool to probe correlation effects[6] and to prepare spin states in QDs.[7]

Much interest is being focused on the Rashba spin orbit (RSO) interaction,[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.[9] 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.[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.[10,11] In addition, SO affects conductivity directly, by turning weak localization corrections into antilocalization ones, as probed in large QDs.[12]

In the presence of SO coupling, the c.m. dynamics of the electrons and that of their relative coordinates cannot be separated.[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.[14,15] The intensities of the non-c.m. peaks increase with SO coupling at the expenses of the c.m. ones. We find that the absorption intensities satisfy the optical sum rule, encountered in single atoms as well as in solids.[16] In particular, the total intensity is proportional to the number of electrons N confined in the dot.[17] 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.[18]

Center-of-mass excitations in the quantum dot. The electrons are confined in the (x,y) plane by a parabolic potential of characteristic frequency ω_d, in the presence of an uniform orthogonal magnetic field $\vec{B}=-B\hat{z}$. 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

$$H=\sum_{i}^{N}\left[\frac{1}{2m_e^*}\left(\vec{p}_i+\frac{e}{c}\vec{A}_i\right)^2+\frac{1}{2}m_e^*\omega_d^2\vec{r}_i^2\right]+\sum_{\substack{i,j=1\\ i<j}}^{N}\frac{U}{|\vec{r}_i-\vec{r}_j|}, \tag{1}$$

with $\vec{A}_i=B/2(y_i,-x_i,0)$. 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 $\omega_c=eB/m_e^*c$), the characteristic length due to the lateral geometrical confinement $l=\sqrt{\hbar/m_e^*\omega_o}$ depends on the frequency $\omega_o=\sqrt{\omega_d^2+\omega_c^2/4}$.

The ratio $v=U/\omega_o$ gives an estimate of how strong the correlations are. By tuning U and ω_o, one can range from a Fermi liquid behavior ($v\sim 1$), up to very strongly correlated

regimes ($v \sim 5-7$), in which cristallized phases appear, the so-called Wigner molecule.[19] 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.[20] We use exact numerical diagonalization as done previously.[21]

The Hamiltonian of Eq. (1) separates as $H=H_{\text{c.m.}}+H_r$, with $[H_{\text{c.m.}},H_r]=0$. Here $H_{\text{c.m.}}$ is the Hamiltonian for the c.m. coordinates $\vec{R}=\frac{1}{N}\Sigma_i\vec{r}_i$, $\vec{P}=\Sigma_i\vec{p}_i$, with total mass $M^*=Nm_e^*$ and H_r involves only the relative coordinates $\vec{p}_{ij}\equiv\vec{p}_i-\vec{p}_j$, $\vec{r}_{ij}\equiv\vec{r}_i-\vec{r}_j$.

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 wave function factorizes, as well as the two-dimensional harmonic oscillator wave function of the c.m. Finally, just a single particle orbital wave function for the relative coordinate is present. The c.m. wave function is always symmetric with respect to the exchange of the two particles. Hence, the requirement of overall antisymmetry for the total wave function, fixes reciprocally the symmetries of the relative motion and of the spin wave functions. The ground state (g.s.), at zero magnetic field, is a singlet of energy $E_0=4.097\omega_o$, for $\omega_o=5$ meV, $U=13$ meV. The c.m. excitations are always equally spaced at each B. Indeed, we find, at $B=0$, the first two c.m. excitations at energies $E_1=5.099\omega_o$ and $E_2=6.100\omega_o$ with a relative error $\sim 2/1000$ with respect to the correct result.

For more than two electrons the analytical factorization of spin and orbital wave function is possible only when the dot is fully spin polarized. This implies that, in the general case, the c.m. modes can be identified only by comparing the energies of the states numerically. In Fig. 1(a) we have plotted a few low lying energy levels for $N=3$ vs ω_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 g.s., 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 $E_1-E_{\text{g.s.}}$ (red circles), E_2-E_1 (green triangles) and the expected difference ω_- (black line) are reported in units of ω_o.

The RSO coupling, included in Fig. 1(b), adds to the noninteracting Hamiltonian of Eq. (1) the potential

$$V^{\text{RSO}}=\frac{\alpha}{\hbar}\hat{z}\times\sum_i^N\left(\vec{p}_i+\frac{e}{c}\vec{A}_i\right)\cdot\vec{\sigma}_i. \tag{2}$$

Here $\vec{\sigma}$ are the Pauli matrices and α 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 $\omega_d=5$ meV and $U=13$ meV, we choose α in the range 0–25 meV nm. In the presence of the term of Eq. (2) in the Hamiltonian, the orbital angular momentum 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 c.m. levels in Fig. 1(b) keeps being the same as that of the g.s. Nevertheless, S of the g.s. increases with ω_c due to crossings.

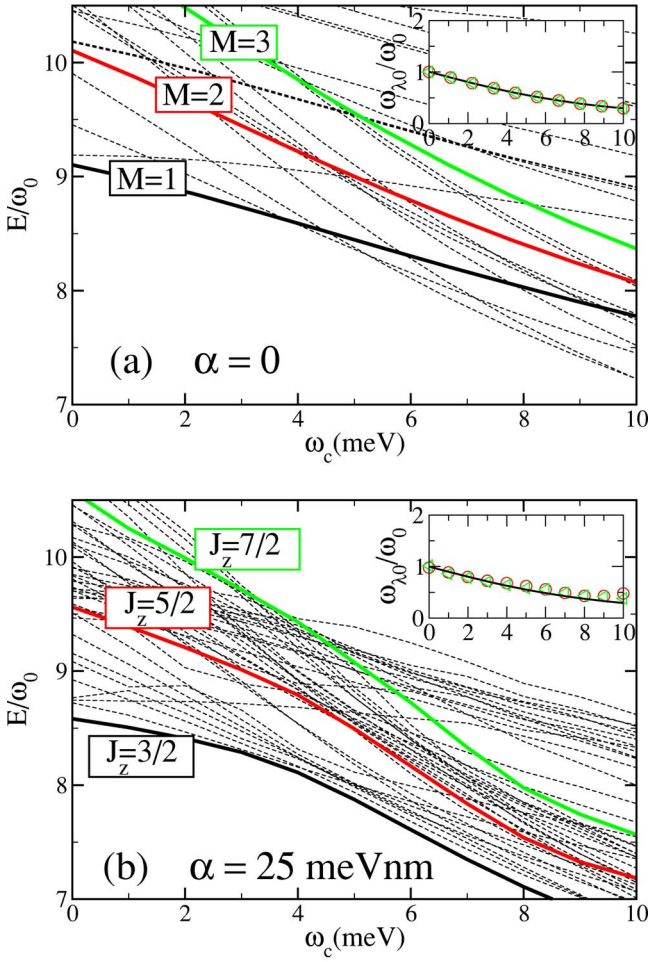

FIG. 1. (Color online) Low lying energy spectrum for a three electron QD as a function of ω_c in the absence of RSO $\alpha=0$ (top panel) and with RSO $\alpha=25$ meV nm (bottom panel) ($\omega_d=5$ meV, $U=13$ meV). Main panels: the low lying levels are thin dashed lines, the g.s. and the first two c.m. excitations ($S=1/2$) are singled out of the plotted levels with heavy lines of different colors. The total M (top) or J_z (bottom) are indicated. Inset: the energy difference between successive c.m. excitation energies vs ω_c showing equal spacing, which are equal to ω_- (plotted as a black curve) for $\alpha=0$, but not for $\alpha\neq 0$.

FIR absorption, Kohn modes, and optical sum rule. The FIR interaction in the dipole approximation can be written as

$$H_{\text{FIR}}=\mathcal{A}_0(\omega)\hat{\epsilon}\cdot\vec{P}e^{i\omega t}+\text{H.c.} \tag{3}$$

where $A_0(\omega)$ is the envelope function of the FIR wave packet in ω space, which we suppose to be almost monochromatic and $\hat{\epsilon}$ 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 c.m. 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

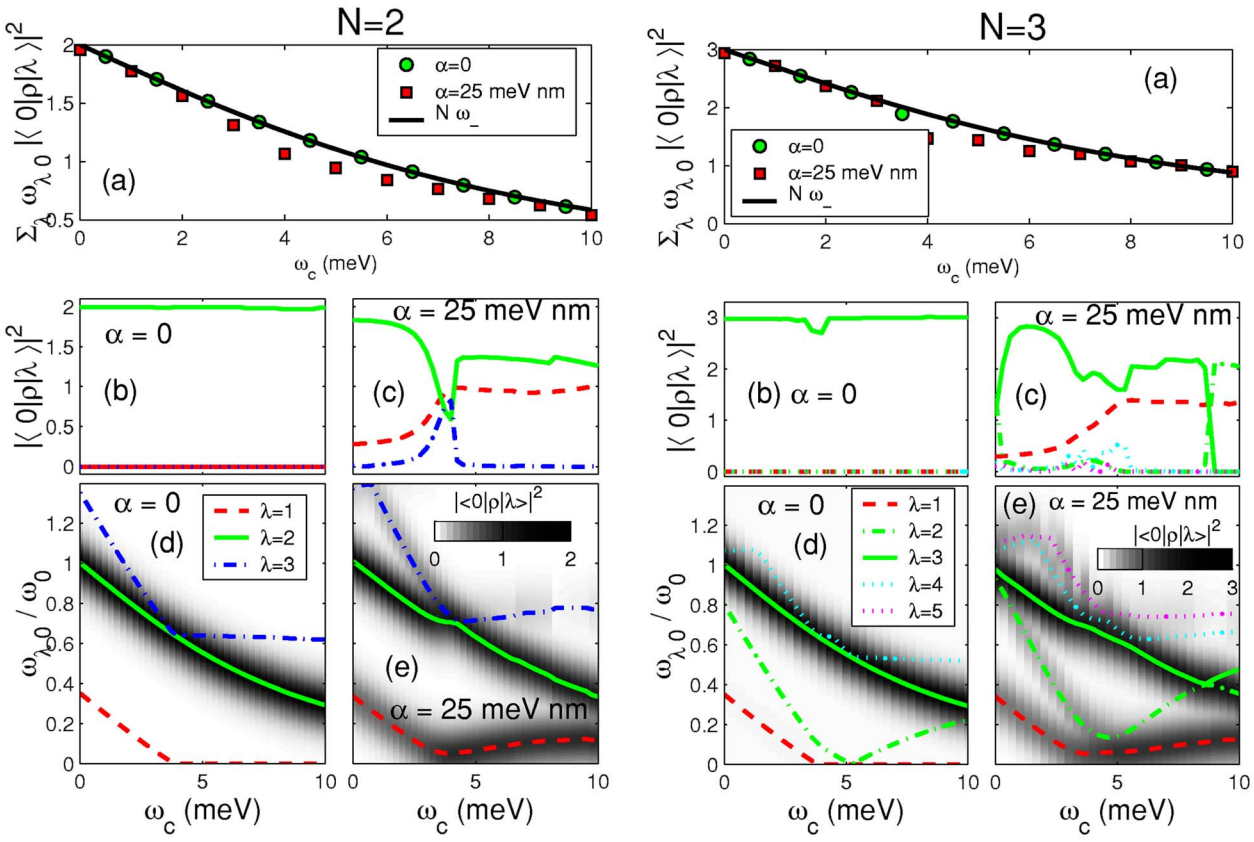

FIG. 2. (Color online) $N=2$ (left) and $N=3$ (right). Bottom panels: the excitation modes energies $\omega_{\lambda 0} \equiv E_\lambda - E_{\text{g.s.}}$ vs ω_c, in units of ω_o, for $\alpha=0$ (d) and 25 meV nm (e). The intensities of their FIR absorption peaks are represented by a greyscale plot underlying the heavy lines. At $\alpha=0$ a single peak appears, corresponding to the c.m. 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 (Ref. 22). 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 ω_c in units of ω_o. The plotted sum is independent of the RSO interaction. Numerical discrepancy occurs in the neighborhood of a level crossing ($\omega_c \sim 4$ meV), due to the truncation of the Hilbert space.

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 $\hat{\epsilon}_R = \hat{x} + i\hat{y}$, the radiation transfers one unity of angular momentum to the dot, $H_{\text{FIR}} \propto \rho_+^\dagger + \text{H.c.}$, where

$$\rho_+^\dagger = \sum_{nm\sigma}{}' \frac{m}{|m|} (c^\dagger_{n-1m+1\sigma} c_{nm\sigma} + c^\dagger_{n+1m+1\sigma} c_{nm\sigma}). \tag{4}$$

The operators $c_{nm\sigma}$ correspond to the single particle Darwin-Fock orbitals ϕ_{nm}.[14] These are the eigenfunctions of the 2D harmonic oscillator with frequency ω_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 $[m \in (-n, -n+2, \ldots, n-2, n)$ with $n \in (0,1,2,3,\ldots)]$ and σ is the spin projection along the $\hat{z}$ 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. $\rho_+^\dagger$ is the operator creating an excitation which increases $M = \Sigma_i^N m_i$ 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 ω_c for $\alpha=0$ (d), and $\alpha=25$ meV nm (e) and their intensity

$$I_\lambda = |\langle J_z^{\text{g.s.}} + 1, \lambda | H_{\text{FIR}} | J_z^{\text{g.s.}} \rangle|^2, \tag{5}$$

appears as a grey scale plot in arbitrary units. The broadening of the line shapes is artificial and equal for all the peaks. The excitation energies $\omega_{\lambda 0} \equiv E_\lambda - E_{\text{g.s.}}$, for $\Delta J_z = 1$, are also plotted in units of ω_o vs the magnetic field $\propto \omega_c$ as colored curves in Figs. 2(d) and 2(e)]. λ is a generic label.[22] In the absence of RSO, only the lower Kohn mode ω_- can be excited for right hand polarization. By increasing the RSO coupling, new possible excitations appear below and above the ω_- 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 Figs. 2(b) and 2(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 $\omega_{\lambda 0}$ reported in Figs. 2(d) and 2(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

$$\sum_{\lambda} \omega_{\lambda 0} |\langle \lambda | \rho_+^\dagger | 0 \rangle|^2 = \langle 0 | [\rho_+^\dagger, [H, \rho_+]] | 0 \rangle = N\omega_-, \qquad (6)$$

where $|0\rangle$ is the g.s. The sum rule does not depend on the interaction term nor, remarkably, on the RSO, because $[\rho_+^\dagger, [V^{\mathrm{RSO}}, \rho_+]]=0$. 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 noninteracting particles, by using a single Slater determinant for $|0\rangle$. The sum rule is plotted vs ω_c in the top panel of Fig. 2(a) left ($N=2$) and Fig. 2(a), right ($N=3$). Only a few terms were included in the summation over λ, because strict selection rules limit the number of states contributing, up to a relatively high energy. The curves for $\alpha=0$ and 25 meV nm almost coincide, except for the neighborhood of $\omega_c \sim 4$ 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 noncenter-of-mass modes makes the optical response of QDs more rewarding. As in atoms and solids, the total sum of the oscillator strengths is proportional to 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^{RSO} given by Eq. (2).

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