Magnetic dipole and electric quadrupole responses of elliptic quantum dots in magnetic fields

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Abstract

The magnetic dipole (M1) and electric quadrupole (E2) responses of two-dimensional quantum dots with an elliptic shape are theoretically investigated as a function of the dot deformation and applied static magnetic field. Neglecting the electron-electron interaction we obtain analytical results which indicate the existence of four characteristic modes, with different $B$-dispersion of their energies and associated strengths. Interaction effects are numerically studied within the time-dependent local-spin-density theory, assessing the validity of the non-interacting picture.

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I. INTRODUCTION

The electric dipole (E1) response of quantum dots has deserved much attention in recent years, mainly motivated by the measurements of far-infrared absorption in these systems [1,2]. The manifestation of the so called magnetoplasmons in a perpendicularly applied magnetic field constitutes an example of collective oscillation in finite Fermi systems, physically analogous to those existing in metal clusters, atoms or nuclei. In parabolically confined dots magnetoplasmons are understood as rigid motions of the electronic center of mass, a result that stems from the generalized Kohn’s theorem [3–7]. However, deviations from parabolicity, such as angular deformations or non-quadratic radial behaviour, may result in more complicated absorption patterns which are currently being much investigated [8–10].

The understanding of other excitation modes of quantum dots are also essential for a proper characterization of these systems. Techniques based on resonant inelastic light scattering have already proved extremely useful to this purpose [11–14]. In fact, using polarization selection rules they permit to disentangle charge-density from spin-density and single-particle excitations, as well as to discern different multipolarity peaks in each channel. The momentum transfer and magnetic field dependence of the different excitations of a single sample have been recently reported using this technique [14]. It is worth to mention that theoretical analysis of the Raman spectra in circularly symmetric quantum dots have been presented in Refs. [15–17].

For elliptical quantum dots orbital-current modes and their relationship with the quadrupole response were analysed by us in Ref. [18]. A characteristic low energy mode, depending on deformation and with a conspicuous signal in the magnetic dipole (M1) channel was found in Ref. [18], while the relevance of orbital excitations in the build-up of the electronic moment of inertia was discussed in Ref. [19]. In this paper we focus on the magnetic field dependence of the orbital and quadrupole modes, a necessary step to understand the M1 and E2 responses in deformed dots and towards the description of Raman scattering in symmetry unrestricted nanostructures. It will be shown that four excitation modes with $B$-dependent energies and strengths characterize both M1 and E2 responses in elliptic dots. This result follows from analytical calculations in the so-called non-interacting deformed-harmonic-oscillator (NIDHO) model, as well as for interacting electrons in the local-spin-density approximation (LSDA). Therefore, it constitutes a robust picture against interactions in a somewhat similar way as Kohn’s modes are.

This paper is organized as follows: Sec. II is devoted to the NIDHO model for M1 and E2 responses; in Sec. III we present the time-dependent LSDA results for the same channels; finally, Sec. IV presents the conclusions.

II. THE NIDHO MODEL

A. The analytic solution of the ground state

We consider a system of non-interacting electrons, confined to the $xy$ plane by an anisotropic parabola [20]

$$v^{\text{conf}}(x, y) = \frac{1}{2}(\omega_x^2 x^2 + \omega_y^2 y^2).$$

(1)
The mean parabola coefficient \( \omega_0 = (\omega_x + \omega_y)/2 \) is parametrized as usual, in terms of the Wigner-Seitz radius \( r_s \) and electron number \( N \) as \( \omega_0^2 = 1/r_s^3 \sqrt{N} \). In the following we shall label the dot deformation with the parameter \( \delta = \omega_y/\omega_x \) (ranging from 0 to 1). Taking into account a uniform magnetic field \( B = Be_z \), the system Hamiltonian reads

\[
H = \sum_{i=1}^{N} \left[ \frac{1}{2} (p_i^2 + \gamma A(r_i))^2 + U^{(conf)}(r_i) \right] + g^* \gamma BS_z ,
\]

where \( \gamma = e/c \) (we assume Gaussian magnetic fields) and within the symmetric gauge \( A(r) = B/2(-y,x) \). The last piece is the Zeeman term, depending on the total spin \( S_z \) and the effective gyromagnetic factor \( g^* \) \([21]\). Obviously this is a one-electron picture, in which the relevant one-electron Hamiltonian is \( h = h_{xy} + g^* \gamma BS_z \). Because of the magnetic field, the spatial part \( h_{xy} \) deviates from a simple harmonic oscillator problem. Namely

\[
h_{xy} = \frac{1}{2} \left( p_x^2 + p_y^2 \right) + \frac{\omega_c}{2} (xp_y - yp_x) + \frac{1}{2} \left( \tilde{\omega}_x^2 x^2 + \tilde{\omega}_y^2 y^2 \right) ,
\]

with \( \tilde{\omega}_x^2 = \omega_x^2 + \frac{1}{4}\omega_c^2 \) and \( \tilde{\omega}_y^2 = \omega_y^2 + \frac{1}{4}\omega_c^2 \) the new parabola coefficients, given in terms of the cyclotron frequency \( \omega_c = eB/c \).

The nontrivial problem posed by Eq. (3) has been elegantly solved in an analytical way, by Dippel et al. \([22]\) and Madhav and Chakraborty \([23]\) in the context of atomic physics and quantum dots, respectively. In the following, we will refer to the derivation by Dippel et al. They introduce a similarity transformation to a new Hamiltonian \( h_3 = U^{-1}hU \), where \( U = e^{i\alpha xy}e^{i\beta px} \). The parameters \( \alpha \) and \( \beta \) are chosen in order to obtain two decoupled oscillators in the \( x \) and \( y \) directions

\[
h_3 = \frac{p_x^2}{2M_1} + \frac{p_y^2}{2M_2} + \frac{M_1}{2} \omega_1^2 x^2 + \frac{M_2}{2} \omega_2^2 y^2 .
\]

The reader is addressed to Ref. \([22]\) for the detailed expressions of \( \alpha, \beta, M_1, M_2, \omega_1 \) and \( \omega_2 \) in terms of the original Hamiltonian parameters.

Most importantly, we can now express the eigenstates of \( h_{xy} \) in terms of those of \( h_3 \). The latter are simply products of one-dimensional oscillator functions with a given number of quanta, i.e.,

\[
h_3 \Phi_{n_1n_2}(x,y) = E_{n_1n_2} \Phi_{n_1n_2}(x,y)
\]

\[
\Phi_{n_1n_2}(x,y) = \phi_{n_1}(x)\phi_{n_2}(y) ,
\]

while the eigenstates of \( h_{xy} \) are given by

\[
h_{xy} \Psi_{n_1n_2}(x,y) = E_{n_1n_2} \Psi_{n_1n_2}(x,y)
\]

\[
\Psi_{n_1n_2}(x,y) = U \Phi_{n_1n_2}(x,y) .
\]

Notice that the energy eigenvalues of \( h_{xy} \) coincide with those of \( h_3 \) and that they are

\[
E_{n_1n_2} = (n_1 + \frac{1}{2})\omega_1 + (n_2 + \frac{1}{2})\omega_2 .
\]

Having the one-electron states it is then a simple matter to obtain the \( N \) electron ground state of the NIDHO model just by filling the \( N \) lower energy orbitals.
B. M1 response

The excitations within the NIDHO model will correspond to independent particle-hole (ph) transitions in the level scheme of the ground state. Taking the orbital angular momentum $\ell_z$ as excitation operator the M1 strength function will be given by

$$S_{M1}(\omega) = \sum_{hp} f_h (1 - f_p) \left| \langle n_1^h n_2^h | U^{-1} \ell_z U | n_1^p n_2^p \rangle \right|^2 \times \delta(E_p - E_h - \omega),$$

where we have denoted the electron states $\Phi_{n_1 n_2}$ as $|n_1 n_2\rangle$ and the occupation numbers are given by the $f$ factors.

To evaluate the matrix element in Eq. (8) we first need to obtain the transformed operator. This can be accomplished by using the Baker-Haussdorf lemma for unitary transformations [24], which introduces a nested commutators expansion. A straightforward calculation yields

$$U^{-1} \ell_z U = (1 - 2\alpha\beta)\ell_z + \beta(1 - \alpha\beta)(p_x^2 - p_y^2) + \alpha(x^2 - y^2).$$

Position and momentum operators may now be transformed to creation and annihilation ones

$$x = \left(\frac{1}{2M_1\omega_1}\right)^{\frac{1}{2}} (a_1^+ + a_1),$$

$$p_x = \left(\frac{M_1\omega_1}{2}\right)^{\frac{1}{2}} (a_1^+ - a_1),$$

with similar relations for $y$ and $p_y$ in terms of $a_2$ and $a_2^+$. The matrix elements are therefore written in terms of the creation and annihilation operator ones

$$\langle n_\alpha | a_1^+ | n_\beta \rangle = \sqrt{n_\beta + 1} \delta_{n_\alpha n_\beta + 1}$$

$$\langle n_\alpha | a_1 | n_\beta \rangle = \sqrt{n_\beta} \delta_{n_\alpha n_\beta - 1}.$$  

From the calculation it emerges that there are only four allowed transition energies: $\omega_{11} = 2\omega_1$, $\omega_{22} = 2\omega_2$, $\omega_+ = \omega_1 + \omega_2$ and $\omega_- = |\omega_1 - \omega_2|$ whose M1 strengths are

$$S_{M1}(\omega_{11}) = \frac{(\alpha - \beta)(1 - \alpha\beta)M_2^2\omega_1^2}{4M_1^2\omega_1^2} \sum_{\text{occ. levels}} (1 - f_{n_1 + 2n_2}) (n_1 + 1) (n_1 + 2)$$

$$S_{M1}(\omega_{22}) = \frac{(\alpha - \beta)(1 - \alpha\beta)M_2^2\omega_2^2}{4M_1^2\omega_2^2} \sum_{\text{occ. levels}} (1 - f_{n_1 n_2 + 2}) (n_2 + 1) (n_2 + 2)$$

$$S_{M1}(\omega_+) = \frac{(1 - 2\alpha\beta)^2}{4M_1 M_2\omega_1\omega_2} (M_2\omega_2 - M_1\omega_1)^2 \times \sum_{\text{occ. levels}} (1 - f_{n_1 + 1 n_2 + 1}) (n_1 + 1) (n_2 + 1)$$

$$S_{M1}(\omega_-) = \frac{(1 - 2\alpha\beta)^2}{4M_1 M_2\omega_1\omega_2} (M_2\omega_2 + M_1\omega_1)^2 \times \sum_{\text{occ. levels}} (1 - f_{n_1 + 1 n_2 - 1}) (n_1 + 1) n_2.$$  

(12)
Result (12) provides a clear interpretation of the different modes: \( \omega_{11} \) corresponds to the absorption of two \( x \)-oscillator quanta, \( \omega_{22} \) absorbs two \( y \) quanta while \( \omega_{+} \) takes one quantum in each oscillator. By contrast, \( \omega_{-} \) is associated with the absorption of one \( x \) quantum accompanied with the emission of a \( y \) quantum. We remind the reader that our convention \( (\omega_{y} \leq \omega_{x}) \) renders the absorption of a \( y \) quantum accompanied by the emission of an \( x \) quantum energetically forbidden.

Figure 1 depicts the absorption energies and associated intensities \( \omega S(\omega) \) as a function of the magnetic field for different deformations in a quantum dot with \( N = 6 \) electrons and \( r_s = 1.51 \). For \( \delta \geq 0.7 \), when the system is just slightly deformed \((\delta = 1 \) corresponds to the circular case), only the \( \omega_{+} \) mode is active at low \( B \)'s. As the magnetic field is increased, very rapidly the \( \omega_{11} \) and \( \omega_{22} \) modes gain strength and disperse in energy. Eventually, for very large magnetic fields \( \omega_{22} \) becomes the lowest energy mode and carries most of the strength.

The \( \omega_{-} \) mode deserves a special discussion. Deformed dots at low deformation and magnetic field are characterized by the same oscillator occupancy numbers of the corresponding circular limit. In the case of magic number dots \((N = N(N + 1) \) with \( N \) an integer number specifying the last occupied shell) the \( \Delta n_{1} = 1, \Delta n_{2} = -1 \) ph transitions are Pauli-blocked thus completely inhibiting the \( \omega_{-} \) mode. This excitation is switched on (with a sudden increase in strength) only when the deformation or \( B \) are high enough to break the closed shell structure, which takes place in first instance when

\[
\frac{\omega_{2}}{\omega_{1}} = \frac{N}{N + 1}.
\]

Figure 2 displays the regions in the \((\delta, B)\) plane in which the \( \omega_{-} \) mode is active, for different dot sizes. This effect is absent for non-magic electron numbers since there is no Pauli blocking for these systems and, as a consequence, \( \omega_{-} \) is active at all \( \delta \) and \( B \). For \( N = 12, 20, \ldots \), subsequent changes in the ground state level structure give also rise to enhancements of the \( \omega_{-} \) strength by allowing an increasing number of ph transitions. The mechanism discussed here is also responsible for strong enhancements of the moment of inertia in these systems.

The general situation in Fig. 1 is qualitatively very similar for the deformations \( \delta = 0.9 \) and 0.7, we remark however that for \( \delta = 0.7 \) the splitting \( \omega_{11} - \omega_{22} \) is higher at low \( B \) and the \( \omega_{-} \) mode switches on at a smaller magnetic field. For large deformations \((\delta = 0.4)\) the \( \omega_{-} \) mode is active even at \( B = 0 \). Notice also that the splitting \( \omega_{11} - \omega_{22} \) is so high that \( \omega_{22} \) approaches \( \omega_{-} \) at vanishing magnetic fields. A common feature to all deformations is that \( \omega_{22} \) dominates the response at high \( B \)'s. Altogether, the NIDHO model provides a quite interesting scenario of the M1 channel, with the emergence of novel modes and big strength transfers between them as a function of the magnetic field and deformation.

### C. E2 response

The E2 strength is given in terms of the quadrupole operator \( xy \) by

\[
S_{E2}(\omega) = \sum_{hp} f_{h}(1 - f_{p}) \left| \langle n_{1}^{p}n_{2}^{h}|U^{-1}xyU|n_{1}^{p}n_{2}^{h}\rangle \right|^{2} \times \delta(E_{p} - E_{h} - \omega).
\]
In a way similar to the M1 analysis we may obtain the E2 matrix elements. After a straightforward calculation one finds the same four modes of the M1 channel manifesting in the E2 spectra, although with different strengths (see third column in Fig 1). The detailed expressions are

\[ S_{E2}(\omega_{11}) = \frac{\beta^2}{4} \sum_{\text{occ. levels}} (1 - f_{n_1 + 2n_2})(n_1 + 1)(n_1 + 2) \]

\[ S_{E2}(\omega_{22}) = \frac{\beta^2}{4} \sum_{\text{occ. levels}} (1 - f_{n_1 + 2n_2})(n_2 + 1)(n_2 + 2) \]

\[ S_{E2}(\omega_+) = \frac{(1 - \beta^2 M_1 M_2 \omega_1 \omega_2)^2}{M_1 M_2 \omega_1 \omega_2} \times \sum_{\text{occ. levels}} (1 - f_{n_1 + n_2 + 1})(n_1 + 1)(n_2 + 1) \]

\[ S_{E2}(\omega_-) = \frac{(1 + \beta^2 M_1 M_2 \omega_1 \omega_2)^2}{M_1 M_2 \omega_1 \omega_2} \times \sum_{\text{occ. levels}} (1 - f_{n_1 + n_2 - 1})(n_1 + 1)n_2 . \]  

We notice that the share of strength as a function of the magnetic field and deformation is similar to the magnetic dipole case. Several differences may, however, be remarked. Firstly, the \( \omega_+ \) mode is relatively enhanced for all \( \delta \) and \( B \) as compared to the results for the M1 channel. For instance the intensity ratio \( I_{E2}(\omega_+)/I_{E2}(\omega_-) \) is enhanced by a factor \( \approx 4 \) at \( \delta = 0.4 \) and \( B = 0 \). It is also worth to point out that the \( \omega_{11} \) and \( \omega_{22} \) intensities are reverted with respect to the M1 result. Finally, at large magnetic fields the low energy \( \omega_{22} \) mode is no longer the dominant one since both \( \omega_{11} \) and \( \omega_- \) show a higher intensity.

As remarked above the number of electrons in Fig. 1 (\( N = 6 \)) corresponds at low deformations \( \delta \rightarrow 1 \) to a closed shell quantum dot. When analysing the M1 and E2 responses of dots that correspond to open shells in the circular limit the results are quite similar to those in this Figure, but with the important difference that the \( \omega_- \) mode is already active at \( B = 0 \) since Pauli blocking is not effective in this case.

**III. THE LSDA APPROACH**

**A. The method**

To analyze the role of electron-electron interactions in a microscopic formalism we resort to the LSDA version of density functional theory. This theory provides a practical way to include electronic exchange and correlation effects by relying on exact calculations for the uniform electron gas. At different levels, density functional theory has been applied by many authors to describe the ground state [25-29] and excitations of quantum dots [1,30]. The most refined version is the so-called current-density functional, first applied to quantum dots by Ferconi and Vignale [25], that was recently used to describe the edge reconstruction in these systems for large magnetic fields [31]. Nevertheless, current terms are known to be rather small for moderate magnetic fields and will be neglected in this work in which we shall resort to the approach of Ref. [8], developed for the treatment of noncircular nanostructures.
The description of excitations in deformed nanostructures constitutes a highly nontrivial task, mainly because of the lack of symmetry not allowing the analytic integration of angular variables as in circular systems. For this reason we shall use the time-dependent LSDA to obtain the time evolution, following an initial perturbation, of relevant expectation values. The set of single-particle orbitals \( \{ \varphi_i(r) \} \) evolves in time as

\[
i \frac{\partial}{\partial t} \varphi_{i\eta}(r, t) = h_{\eta}[\rho, m] \varphi_{i\eta}(r, t),
\]

where \( \eta = \uparrow, \downarrow \) is the spin index, and total density and magnetization are given in terms of the spin densities \( \rho_{\eta}(r) = \sum_i |\varphi_{i\eta}(r)|^2 \), by \( \rho = \rho_{\uparrow} + \rho_{\downarrow} \) and \( m = \rho_{\uparrow} - \rho_{\downarrow} \), respectively. The Hamiltonian \( h_{\eta} \) in equation (16) contains, besides of kinetic energy, the confining \( v^{(\text{conf})}(r) \), Hartree \( v^{(H)}(r) = \int d\mathbf{r}' \rho(\mathbf{r}')/|\mathbf{r} - \mathbf{r}'| \) and exchange-correlation \( v^{(xc)}_{\eta}(r) = \frac{\partial}{\partial \rho_{\eta}} E_{xc}(\rho, m) \) potentials. The exchange-correlation energy density \( E_{xc}(\rho, m) \) has been described as in Refs. [7–9,30]. This technique was already used by us in Ref. [18] to describe orbital (\( \omega_- \)) excitations in quantum dots at zero magnetic field.

An initial perturbation of the orbitals \( \varphi'(r) = \mathcal{P} \varphi(r) \) models the interaction with the external field. The unitary operator \( \mathcal{P} \) is given in terms of a displacement field \( \mathbf{u}(r) \) as

\[
\mathcal{P} = \exp \left[ i \mathbf{u}(r) \cdot \mathbf{p} \right].
\]

The appropriate fields for the M1 and E2 channels are \( \mathbf{u}_{M1} = \lambda r e_{\theta} \) and \( \mathbf{u}_{E2} = \lambda \nabla(x y) \), where \( \lambda \) is a small parameter that guarantees the linear regime. Actually, these operators correspond to a rigid rotation (M1) and a quadrupole distortion (E2) of the electronic orbitals. After the initial distortion we keep track of \( \langle \sum_i \ell_z^{(i)}(t) \rangle \) or \( \langle \sum_i x_i y_i \rangle(t) \) and a subsequent frequency analysis of the signal provides the absorption energies and their associated strengths [8].

B. LSDA results and discussion

Figure 3 summarizes the M1 and E2 spectra of the \( N = 6 \) electron dot within time-dependent LSDA. Quite remarkably many features of the NIDHO model are also present in the LSDA spectra. In fact we can identify the four modes, labeled in Fig. 3 by analogy with the NIDHO results, although in general they lie at different energies because of the interactions.

Focusing on the M1 channel, we notice for \( \delta = 0.9 \) the emergence of the low energy mode \( \omega_- \) and its crossing with the \( \omega_{22} \) mode. This crossing takes place at \( B \approx 1.5 \) T for both \( \delta = 0.9 \) and \( \delta = 0.7 \) and at \( B \approx 1 \) T for \( \delta = 0.4 \). The dominance of \( \omega_{22} \) at large \( B \)'s is also in very good agreement with the NIDHO prediction. Quite remarkably, for \( \delta = 0.7 \) the \( \omega_- \) mode is switched on even at \( B = 0 \) as a result of the interactions. At \( \delta = 0.4 \) the closeness of \( \omega_{22} \) and \( \omega_- \) at low magnetic fields predicted in the non-interacting case is nicely seen in Fig. 3. It is also worth to mention the strong quenching of the \( \omega_{11} \) mode within LSDA.

The E2 results also reflect to a great extent the systematics predicted by the NIDHO model. In general the high energy modes \( \omega_+ \) and \( \omega_{11} \) are more important in the E2 spectra than in the M1 ones, especially at large magnetic fields. In some cases the LSDA strengths show some small fragmentations that we attribute to ph effects (Landau damping). For instance, this is quite clear in the \( \omega_{11} \) mode at 3 and 4 teslas.
IV. SUMMARY AND CONCLUSIONS

The M1 and E2 channels of elliptic quantum dots are characterized by four modes whose energies and strengths vary with magnetic field and deformation. Their main characteristics are already seen in a non-interacting model, although interactions shift the mode energies and introduce several minor differences. The main trends seen in Figs. 1-3 may be summarized as follows:

a) Three modes $\omega_{11}$, $\omega_+$ and $\omega_-$ have a positive dispersion relation with $B$ while the other $\omega_{22}$ exhibits a negative one. At low magnetic fields and deformations $\omega_{11}$, $\omega_+$ and $\omega_{22}$ are very close, while $\omega_-$ lies at a much lower energy. As the deformation is increased the three upper modes separate in energy (at $B \approx 0$), the lower of them $\omega_{22}$ coming close to $\omega_-$. 

b) At low $B$’s the M1 strength of closed shell dots is exhausted by $\omega_+$ while, when increasing the deformation $\omega_-$ is also active. This mode is also switched on when increasing the magnetic field for a fixed deformation as a consequence of the Pauli blocking mechanism. Generally, a crossing between $\omega_-$ and $\omega_{22}$ occurs for intermediate magnetic fields. At large magnetic fields the low energy $\omega_{22}$ mode eventually takes all the strength.

c) The E2 spectra are similar to the M1 ones, although an important amount of strength shifts to the high energy modes $\omega_+$, $\omega_-$ and $\omega_{11}$ as compared to the magnetic dipole channel. Contrary to the M1 case the E2 absorption does not show a clear dominant peak at high $B$’s.

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FIGURES

FIG. 1. Results within the NIDHO model for a $N = 6$ electron dot with $r_s = 1.51$. Left panels display the mode energies in $H^*$ while central and right ones show the M1 and E2 absorption cross sections $\omega S(\omega)$ as a function of the magnetic field. Each row corresponds to a different dot deformation.

FIG. 2. The lines show the boundary between regions for $\omega_-$ mode in the NIDHO model and different dot sizes. Left and right of each curve correspond to $\omega_-$ being active or non-active (Pauli blocked) respectively.

FIG. 3. M1 an E2 absorption intensities within LSDA for different magnetic fields and deformations. The results correspond to a dot with $N = 6$ electrons and $r_s = 1.51$. 
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