Optical Signatures of Spin-Orbit Interaction Effects in a Parabolic Quantum Dot

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We demonstrate here that the dipole-allowed optical absorption spectrum of a parabolic quantum dot subjected to an external magnetic field reflects the interelectron interaction effects when the spin-orbit (SO) interaction is also taken into account. We have investigated the energy spectra and the dipole-allowed transition energies for up to four interacting electrons parabolically confined, and have uncovered several novel effects in those spectra that are solely due to the SO interaction.

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Far-infrared (FIR) optical absorption spectrum of quantum dots, in particular, dots with a parabolic confinement, has a long and colorful history [1–5]. First of all, there is a very good theoretical and experimental understanding of the single-electron states in a quantum dot with parabolic confinement. The solution of the Schrödinger equation for an electron confined by a harmonic potential, $v_c = \frac{1}{2}m^*\omega_0 r^2$ in the presence of an external magnetic field, is well established [2,6]. The eigenvalues in this case are given by

$$E_{nl} = (2n + |l| + 1)\hbar\Omega - \frac{1}{2}l\hbar\omega_c,$$

where $n=0,1,2,\ldots$ and $l=0,\pm 1\ldots$ are the principal and azimuthal quantum numbers, respectively, $\Omega^2=[\omega_0^2+\frac{1}{4}\omega_c^2]$, and ω_c is the cyclotron frequency. Dipole-allowed transitions among these energy levels will have energies [2-4]

$$\Delta E_{\pm} = \hbar \Omega \pm \frac{1}{2} \hbar \omega_c.$$

This relation has been verified to great accuracy by a variety of experiments [1,2,5]. Interestingly, however, the observed magnetic field dependent FIR absorption in quantum dots with more than one electron was found to be essentially independent of the number of confined electrons and instead was dominated by the above relation for ΔE_{+} [3]. It was a rather puzzling result because according to this, magneto-optics was clearly incapable of providing any relevant information about the effect of mutual interactions of the confined electrons. The puzzle was later resolved by Maksym and Chakraborty [1,2,4,7], who pointed out that for a parabolic quantum dot (QD) in an external magnetic field, the dipole interaction is a function of the center-of-mass (c.m.) coordinate alone and the interelectron interaction does not play any role. Despite this somewhat disappointing performance of a parabolic dot, FIR spectroscopy of QDs (parabolic or otherwise) has generated enormous interest for over a decade that has yet to subside [5]. In this Letter we demonstrate that in the presence of spin-orbit coupling the situation changes considerably which can be exploited to determine optically the unique effect of SO coupling in quantum dots described below.

Interest on the role of the spin-orbit coupling in nanostructured systems is now at its peak, due largely to its relevance to spin transport in low-dimensional electron channels [8,9]. The intriguing possibility of tuning the SO field and thereby coherently manipulate electron spins in quantum dots has sparked a lot of interest in recent years [10]. It is hoped that an improved understanding of spin dynamics in the QDs might pave the way for future electronic and information processing, especially in quantum computing and quantum communication [11]. While the majority of experimental efforts has focused on magnetotransport measurements [12], here we present accurate results for the optical absorption spectra that are experimentally observable and could, in principle, provide an important probe of SO coupling in quantum dots.

The spin-orbit interaction that we are here concerned with is described by the Hamiltonian [13,14]

$$\mathcal{H}_{SO} = \alpha (\vec{k} \times \vec{\sigma})_z = i\alpha \left(\sigma_y \frac{\partial}{\partial x} - \sigma_x \frac{\partial}{\partial y}\right).$$

Here the z axis is chosen perpendicular to the two-dimensional electron gas (2DEG) (in the xy plane), α is the spin-orbit coupling constant, which is sample dependent and is proportional to the interface electric field that confines the electrons in the x-y plane, $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ denotes the Pauli spin matrices, and \vec{k} is the planar wave vector. In this potential, the spin of finite-momentum electrons feels a magnetic field perpendicular to the electron momentum in the inversion plane. This results in an isotropic spin splitting energy Δ_{SO} at B=0 that is proportional to k [8,13].

Several experimental groups [12] investigating the Shubnikov-de Haas (SdH) oscillations in a 2DEG confined at the heterojunctions with a narrow-gap well (e.g., InGaAs/InAlAs, InAs/GaSb, etc.) have already established that lifting of spin degeneracy results from inversion

asymmetry of the structure which invokes an electric field perpendicular to the layer. Experimentally observed values of the SO coupling strength α lie in the range of 5–45 meV nm [12]. Energy levels of two interacting electrons confined in a parabolic quantum dot in an external magnetic field were recently reported by us for this range of SO coupling strength [14]. In the absence of the SO coupling, electron-electron interaction causes the ground state energy to jump from one angular momentum value to another as the magnetic field is increased [2,4]. The influence of the SO coupling is primarily to move the energy level crossings to weaker fields [14].

The reason why dipole-allowed transitions in a parabolically confined quantum dot can be very different in the presence of SO interaction is explained as follows. When subjected to the radiation field with amplitude a and polarization $\vec{\epsilon}$, the vector potential \vec{A} in the single particle Hamiltonian

$$\mathcal{H}_0 = \frac{1}{2m} \left(\vec{p} - \frac{e}{c} \vec{A} \right)^2 + \frac{1}{2} m \omega_0^2 r^2 + \frac{\alpha}{\hbar} \left[\vec{\sigma} \times \left(\vec{p} - \frac{e}{c} \vec{A} \right) \right]_z + \frac{1}{2} g \mu_B B \sigma_z$$

must be replaced with the potential

$$\vec{A} \rightarrow \vec{A} + \vec{A}_{\omega}, \qquad \vec{A}_{\omega} = \vec{\epsilon} a e^{i\vec{k}\cdot\vec{r} - i\omega t}.$$

In the dipole approximation we assume that

$$A_{\omega} \approx \vec{\epsilon} a e^{-i\omega t}$$

and correspondingly the Hamiltonian will be [15]

$$\mathcal{H} \approx \mathcal{H}_0 - \mathcal{H}' e^{-i\omega t}$$

where

$$\mathcal{H}' = \frac{ea}{mc} \vec{\epsilon} \cdot \left(\vec{p} - \frac{e}{c} \vec{A} \right) + \frac{\alpha ea}{\hbar c} [\vec{\sigma} \times \vec{\epsilon}]_z.$$

In a many-body system when $\alpha=0$ the first term generates the c.m. density excitations where mutual interactions play no role. Consequently (in dipole approximation), only transitions between these modes are possible. When α is different from zero, the second term $(\propto \sigma_x \epsilon_y - \sigma_y \epsilon_x)$ in \mathcal{H}' can create spin-density oscillations and interactions have effect on their properties. It is to be noted that, in SO coupled systems, the dipole operator still retains its familiar form, $\hat{Q} = \frac{ea}{c} \vec{\epsilon} \cdot \vec{r}$, as is easily verified by evaluating its commutator with the Hamiltonian \mathcal{H}_0

$$[\hat{O}, \mathcal{H}_0] = i\hbar \mathcal{H}'$$
.

Dipole operator is independent of the electron spin. The dipole-allowed optical transitions are always from the same spin states, but the angular momenta must differ by unity. In the presence of SO coupling, neither the dipole operator nor the selection rule changes, but the SO interaction mixes the neighboring angular momentum values (l and l+1) as well as the spin and hence the selection rule now applies to the total angular momentum J as well.

Therefore, transitions from other states that are not allowed without the SO coupling are now allowed [16].

For numerical evaluation of the optical absorption spectrum, we have considered a InAs quantum dot where most of the spin-related phenomena have been studied [12]. We have considered up to four interacting electrons in the quantum dot. Evaluation of the transition energies of a quantum dot containing more than two electrons is quite challenging. First, since we work in the occupation space spanned by direct antisymmetrized products of the spinors

$$|\lambda_l\rangle = \left(egin{array}{c} \sum\limits_{n=0}^{n} u_n^{\lambda_l} f_{nl} e^{il heta} \ \sum\limits_{n=0}^{n} d_n^{\lambda_l} f_{n,l+1} e^{i(l+1) heta} \end{array}
ight),$$

where $f_{nl} = \sqrt{n!/(n+|l|)!} x^{|l|/2} e^{-x/2} L_n^l(x)$, $u_n^{\lambda_l}$ and $d_n^{\lambda_l}$ are the expansion coefficients [14], the two-body matrix elements are composed of Coulomb matrix elements expressed in a parabolic quantum dot as finite sums [2]. In this case, however, the expansions can extend to Laguerre polynomials of large degree and large angular momenta which leads to well-known numerical instabilities [17]. To avoid these, we had to resort to multiple precision arithmetics (but, in order to circumvent the resulting extremely long computation times, we had to tabulate selected subsummations). Second, since in the presence of the spinorbit interaction all possible spin configurations need to be considered, the dimension of the Hilbert space required for convergence can easily become huge (of the order of 10⁶ for four electrons). To diagonalize these "monster matrices" we implemented the Davidson-Liu algorithm [18] that is very suitable for this task.

Our numerical results for energy spectra and absorption spectra (dipole-allowed) are presented in Figs. 1–3, for 2–4 electrons and for various values of the SO coupling strength α . We have considered the following parameters for the InAs quantum dot: $m^*/m_0 = 0.042$, $\epsilon = 14.6$, g = -14, and $\hbar\omega_0 = 3.75$ meV. The dipole matrix elements are evaluated from

$$\begin{split} d_{\lambda_1\lambda_2} &= \langle \lambda_1|re^{i\theta}|\lambda_2\rangle \\ &= \delta_{l_1,l_2+1} \underset{n}{\sum} [\sqrt{n+l_1}u_n^{\lambda_1}u_n^{\lambda_2} - \sqrt{n}u_{n-1}^{\lambda_1}u_n^{\lambda_2} \\ &+ \sqrt{n+l_1+1}d_n^{\lambda_1}d_n^{\lambda_2} - \sqrt{n}d_{n-1}^{\lambda_1}d_n^{\lambda_2}] \end{split}$$

when $l_1 \ge 0$ and a similar type of equation for $l_1 < 0$. The intensity is obtained from $I \propto |d_{\lambda_1 \lambda_2}|^2$ [19]. In our plots for the absorption spectra (the right panels of the figures), the size of the points is proportional to the calculated intensity.

A striking feature visible in the absorption spectra (right-hand panels of the figures) is the appearance of discontinuities, anticrossings, and new modes in addition to the two main ($\alpha=0$) absorption lines. These optical signatures of the SO interaction are consequences of the multitude of level crossings and level repulsions that occur in the energy spectra (left-hand panels of Figs. 1–3). The latter

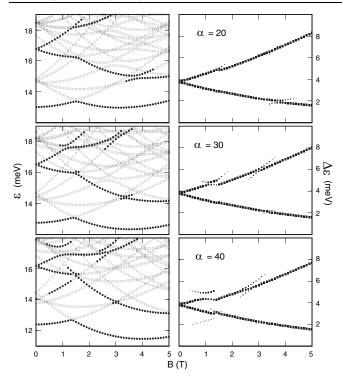


FIG. 1. Energy spectra (left panel) and dipole-allowed transition energies (right panel) for two interacting electrons confined in an InAs quantum dot and for various values of the SO coupling strength α [meV nm]. The solid dots in the energy spectrum identify the energy levels involved in transitions that correspond to the lowest branches of the absorption spectra (in the right panel). In the right panels, the size of the points in the figures is proportional to the calculated intensity.

ones can be attributed to an interplay between SO and Zeeman couplings. In order to understand their origin, let us first examine the case of the two-electron system. In our spinor notation the main contribution to the ground state at zero magnetic field comes from the two-electron state $|\lambda_{l_1}, \lambda_{l_2}\rangle = |\lambda_0, \lambda_{-1}\rangle$, where $|\lambda_{l_1}\rangle$ is a spinor with $J_1 = l_1 + 1/2 = 1/2$, $d_n^{\lambda_1} = 0$, and $|\lambda_{l_2}\rangle$ a spinor with $J_2 = 1/2$ -1/2 and $u_n^{\lambda_2} = 0$; i.e., both electrons have zero orbital angular momenta with opposite spins (corresponding to $J = J_1 + J_2 = 0$). Now when we increase the magnetic field the spin triplet configuration will become, due to the interaction, energetically more favorable. If the Landé factor is negative then the electrons would like to occupy states with orbital angular momenta 0 and -1 with both spins up. In the spinor picture this means that $|\lambda_{l_2}\rangle$ still has $l_2=-1$ (J=0) but now $u_n^{\lambda_2}\neq 0$ and $d_n^{\lambda_2}=0$. The SO interaction mixes these two configurations which results in a level repulsion. On the other hand, when the strength of the SO coupling is further increased, the relative significance of the Zeeman contribution to \mathcal{H}_0 decreases. The energy shifts to states with $J \neq 0$ will then become energetically feasible and we have again crossings of levels. For increasing number of electrons in the dot, the energy spectra are more dense and exhibit additional level crossings (Figs. 2 and 3). As a consequence, the ground state

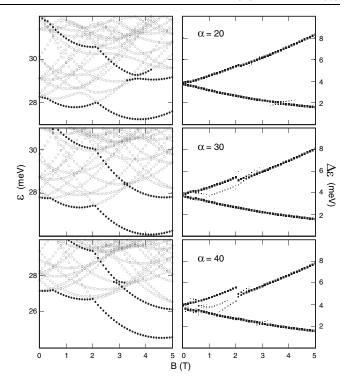


FIG. 2. Same as in Fig. 1, but for three interacting electrons in a quantum dot.

momentum also changes more frequently as compared to that of the two-electron case.

At moderate SO coupling strengths, the absorption spectra do not essentially differ from the single particle spec-

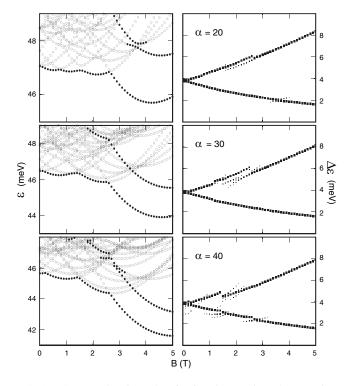


FIG. 3. Same as in Fig. 1, but for four interacting electrons in a quantum dot.

trum. But when the coupling strength increases the deviation from the pure parabolic confinement also increases which in turn implies that the lowest final states of dipoleallowed transitions are not any more achievable by adding $\hbar\Omega \pm \frac{1}{2}\hbar\omega_c$ to the initial state energies. In particular, this results in discontinuities and anticrossing behaviors as well as appearance of new modes. As an illustration, let us consider the absorptions that at the magnetic field B =1 T take the two-electron system from the ground state to excited states. In the absence of the SO coupling the ground state is a spin singlet state S = 0 with total angular momentum J = 0. According to the dipole selection rules absorptions cause transitions to states $J = \pm 1$ and S = 0with energies ΔE_{\pm} above the ground state. Looking at the bottom right panel of Fig. 1, we note that in addition to the two main lines there are now two additional lines (at B =1 T) of appreciable intensity at the SO coupling strength $\alpha = 40$. Further analysis reveals that the ground states still have J=0 and that the expectation value of the spin z component is $\langle \sigma_z \rangle = 0$. The excited states also have J = ± 1 , as before. However, the final spin states can no longer be classified as singlets: the expectation values $\langle \sigma_z \rangle$ vary between -0.03 and 0.39. When the number of electrons increases the number of these additional modes also increases but at the same time the relative intensities decrease (at each B we have normalized the total intensity to unity). On the other hand, the discontinuities as consequences of deviations from a parabolic confinement become more pronounced (Figs. 2 and 3).

In conclusion, the calculated optical absorption spectra of up to four interacting electrons in a parabolic quantum dot subjected to an externally applied perpendicular magnetic field exhibit new modes that are a direct consequence of the SO coupling effects. These are manifested in the energy spectra as multiple level crossings and level repulsions that are attributed to an interplay between the Zeeman and SO couplings present in the system Hamiltonian. Experimental observation of these features will provide a unique signature on the nature of SO coupling effects in nanostructured systems.

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- [1] T. Chakraborty, Comments Condens. Matter Phys. **16**, 35 (1992); V. Gudmundsson, A. Manolescu, R. Krahne, and D. Heitmann, in *Nano-Physics & Bio-Electronics: A New Odyssey*, edited by T. Chakraborty, F. Peeters, and U. Sivan (Elsevier, New York, 2002).
- [2] T. Chakraborty, Quantum Dots (North-Holland, Amsterdam, 1999).
- [3] C. Sikorski and U. Merkt, Phys. Rev. Lett. **62**, 2164 (1989).

- [4] P. A. Maksym and T. Chakraborty, Phys. Rev. Lett. 65, 108 (1990).
- [5] See, for example, I. Magnusdottir and V. Gudmundsson, Phys. Rev. B 60, 16591 (1999); H. Imamura, P. A. Maksym, and H. Aoki, Phys. Rev. B 53, 12613 (1996); 59, 5817 (1999); R. Krahne et al., ibid. 63, 195303 (2001); E. Lipparini et al., ibid. 56, 12375 (1997); P. A. Maksym, Physica B (Amsterdam) 184, 385 (1993); T. Seki, Y. Kuramoto, and T. Nishino, J. Phys. Soc. Jpn. 65, 3945 (1996); M. Wagner, A. V. Chaplik, and U. Merkt, ibid. 51, 13817 (1995); B. Meurer, D. Heitmann, and K. Ploog, Phys. Rev. Lett. 68, 1371 (1992); T. Chakraborty, V. Halonen, and P. Pietiläinen, Phys. Rev. B 43, R14289 (1991).
- [6] V. Fock, Z. Phys. 47, 446 (1928); C.G. Darwin, Proc. Cambridge Philos. Soc. 27, 86 (1930).
- [7] For a similar result in a parabolic quantum well, see L. Brey, N. F. Johnson, and B. I. Halperin, Phys. Rev. B 40, R10647 (1989).
- [8] Semiconductor Spintronics and Quantum Computation, edited by D.D. Awschalom, D. Loss, and N. Samarth (Springer, New York, 2002); D. Grundler, Phys. World 15, No. 4, 39 (2002); S.A. Wolf et al., Science 294, 1488 (2001); G.A. Prinz, Phys. Today 48, No. 4, 58 (1995).
- [9] Proceedings of the First International Conference on the Physics and Applications of Spin Related Phenomena in Semiconductors, edited by H. Ohno [Physica E (Amsterdam) 10, 1–504 (2001)].
- [10] W. H. Kuan, C. S. Tang, and W. Xu, J. Appl. Phys. 95, 6368 (2004); O. Voskoboynikov, O. Bauga, C. P. Lee, and O. Tretyak, J. Appl. Phys. 94, 5891 (2003); M. Governale, Phys. Rev. Lett. 89, 206802 (2002).
- [11] M. A. Eriksson *et al.*, Quant. Info. Proc. 3, 133 (2004);
 D. Loss, G. Burkard, and D. P. DiVincenzo, J. Nanopart. Res. 2, 401 (2000).
- [12] D. Grundler, Phys. Rev. Lett. 84, 6074 (2000); C.-M. Hu, J. Nitta, T. Akazaki, H. Takayanagi, J. Osaka, P. Pfeffer, and W. Zawadzki, Physica E (Amsterdam) 6, 767 (2000); C.-M. Hu *et al.*, Phys. Rev. B 60, 7736 (1999); Y. Sato, T. Kita, S. Gozu, and S. Yamada, J. Appl. Phys. 89, 8017 (2001); J. Nitta, T. Akazaki, H. Takayanagi, and T. Enoki, Phys. Rev. Lett. 78, 1335 (1997).
- [13] Y. A. Bychkov and E. I. Rashba, J. Phys. C 17, 6039 (1984).
- [14] T. Chakraborty and P. Pietiläinen, Phys. Rev. B 71, 113305 (2005).
- [15] P. Tonello and E. Lipparini, Phys. Rev. B 70, 081201(R) (2004).
- [16] An approximate Hartree-Fock calculation with SO interaction in a parabolic dot was reported in L. Jacak et al., Physica B (Amsterdam) 229, 279 (1997). However, this scheme does not have the correct quantum numbers and is totally inadequate for any correlation-related effects we have investigated here.
- [17] M. Stone, H. W. Wyld, and R. L. Schult, Phys. Rev. B 45, 14156 (1992).
- [18] E. R. Davidson, Comput. Phys. 7, 519 (1993).
- [19] V. Halonen, P. Pietiläinen, and T. Chakraborty, Europhys. Lett. **33**, 377 (1996).