Spin-related phenomena have attracted great attention recently as they are the key ingredient in the emerging field of spintronics[1]. Among these, spin-orbit (SO) coupling mechanisms in semiconductors provide a basis for device applications, and a source of interesting physics, especially in systems with reduced dimensionality. Transport through chaotic quantum dots in the presence of SO interaction has been studied both experimentally[2] and theoretically[3, 4], while the effect of SO coupling on the spin lifetime has been investigated in Ref. [5]. Here, we are interested in how the electronic properties of few-electron quantum dots, such as the addition energy[6, 7] or the spin properties of the dot ground state[8], are affected by Rashba SO interaction[9, 10]. These questions are interesting from the theoretical point of view for the following reasons. First, the Rashba effect has a different form than the usual SO coupling term in real atoms. Second, the tunability of the Rashba effect[11, 12, 13] allows a more complicated electronic structure.

We start by describing the physics of a quasi zero-dimensional system with Rashba SO at the non-interacting electron level, providing analytical results for the single-particle spectrum when the SO coupling can be treated as a perturbation. Then, we introduce the electron-electron interaction in the framework of Spin Density Functional Theory (SDFT)[14]. This allows us to study how the addition spectrum is modified by varying the strength of SO coupling. Studying the spin properties of the many-particle ground state, we find a suppression of Hund’s rule when the SO coupling can still be treated as a perturbation for the single-particle problem. For higher strengths it affects the single-particle spectrum so strongly that it gives rise to a completely different addition spectrum. The introduction of an in-plane magnetic field, leads to a paramagnetic behavior of the dot in a closed shell configuration, and to spin texture in space.

Quantum dots are often realized by lateral confinement of a two dimensional electron gas (2DEG) obtained in a heterostructure. Due to the lack of inversion symmetry along the growth direction $z$ of the heterostructure[1, 15], the electrons in the 2DEG are subject to the Rashba spin-orbit coupling Hamiltonian

$$H_{so} = \frac{\hbar k_{so}}{m} (\sigma_x p_y - \sigma_y p_x) .$$

The strength of the SO coupling, here denoted as $k_{so}$, can be tuned by changing the asymmetry of the quantum well via externally applied voltages, as shown in several experimental studies[11, 12, 13].

It is interesting to study the effect of the SO coupling term Eq. (1) on the quantum mechanics of a quasi zero-dimensional system[13]. To this end, we consider a two-dimensional quantum dot defined by a parabolic confining potential

$$V_{conf}(x, y) = \frac{m}{2} \omega^2 (x^2 + y^2) .$$

Thus, the single-particle Hamiltonian in the effective-mass approximation reads

$$H = \frac{p^2}{2m} + V_{conf}(x, y) + H_{so} .$$

In the absence of SO coupling the eigen-energies are

$$E_M^{(0)} = \hbar \omega (M + 1) ,$$

with $M$ being a non-negative integer. A degenerate subspace $S_M$ of dimension $D_M = 2(M + 1)$, where the factor 2 is due to spin, is associated to each energy $E_M^{(0)}$.

We will now treat $H_{so}$ as a perturbation. This is valid as long as $k_{so} \omega \ll 1$, where $\omega$ is the oscillator length $\sqrt{\hbar/(m \omega)}$. We obtain for the second-order eigen-energies

$$\tilde{E}_{M,i,\sigma} = E_M^{(0)} + \hbar \omega (k_{so} \omega)^2 [2(i - 1) - (M + 1)] ,$$

where $i = 1, \cdots , M + 1$, and $\sigma = \pm 1$ is the quantum number relative to $\sigma_z$, i.e. the spin projection along $z$. As the single-particle levels will play an important role in the following, we show an example of the low-energy part of the spectrum calculated using Eq. (6) together with the results of numerical diagonalization in the upper panel.

PACS numbers: 73.21.La, 71.15.Mb, 75.75.+a

Quantum dots with Rashba spin-orbit coupling

M. Governale

Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe, Germany

(Dated: March 22, 2022)
of Fig. 1. From the perturbative treatment the following conclusions can be drawn: 1) Each degenerate level \( E_{M}^{(0)} \) is split in \( M \) sublevels, each of which is double degenerate due to Kramers theorem; 2) Spin rotational invariance is broken but still the eigenstates are (to this order in perturbation theory) eigenstates of \( \sigma_z \). From conclusion 1) we can infer that SO coupling changes the addition spectrum of the dot, while conclusion 2) tells us that the Rashba effect will not influence the lifetime of the eigenstates of \( \sigma_z \). For values of \( k_{\text{so}} \) for which perturbation theory breaks down, the eigen-energies are of course still grouped in Kramers-degenerate sublevels [as shown in the inset of Fig. 1(a)], although it can happen that different sublevels have almost the same energy.

To introduce the Coulomb interaction between the electrons we use spin density functional theory (SDFT), in the local density approximation [14]. We write the density of states of the dot, calculated both by perturbation theory (dots) and by numerical diagonalization (squares) for \( k_{\text{so}} \omega = 2.633 \) [this value corresponds to the data for \( k_{\text{so}} = 0.01 \, \text{nm}^{-1} \) for the addition energies of the realistic dot shown in panel (b)]. The label \( p \) is an index that enumerates the eigenstates in order of ascending energy. Inset: Low-energy part of the single-particle spectrum calculated numerically for \( k_{\text{so}} \omega = 0.7896 \) [this value correspond to \( k_{\text{so}} = 0.03 \, \text{nm}^{-1} \) in panel (b)] In this case the SO coupling dominates the single-particle spectrum. (b) Addition energy vs number of electrons in the dot for different values of the SO coupling strength. In this figure and in the following ones the dot is defined by a confining potential of strength \( h \omega = 5 \, \text{meV} \).

FIG. 1: (a) Low-energy part of the single-particle spectrum for the dot, calculated both by perturbation theory (dots) and by numerical diagonalization (squares) for \( k_{\text{so}} \omega = 0.2633 \) [this value corresponds to the data for \( k_{\text{so}} = 0.01 \, \text{nm}^{-1} \) for the addition energies of the realistic dot shown in panel (b)]. The label \( p \) is an index that enumerates the eigenstates in order of ascending energy. Inset: Low-energy part of the single-particle spectrum calculated numerically for \( k_{\text{so}} \omega = 0.7896 \) [this value correspond to \( k_{\text{so}} = 0.03 \, \text{nm}^{-1} \) in panel (b)] In this case the SO coupling dominates the single-particle spectrum. (b) Addition energy vs number of electrons in the dot for different values of the SO coupling strength. In this figure and in the following ones the dot is defined by a confining potential of strength \( h \omega = 5 \, \text{meV} \).

Now, we focus on realistic dots obtained in an InAs heterostructure, where the Rashba effect can be quite large [3]. We use for the electron effective mass the value \( m = 0.022 \, m_0 \), with \( m_0 \) being the free-electron mass; and for the dielectric constant \( \epsilon = 14.6 \, \epsilon_0 \), being \( \epsilon_0 \) the one of vacuum.

In a quantum dot without SO interaction we expect peaks in the addition energy when the number of electrons \( N \) equals a magic number, i.e. at those integer values which correspond to a closed shell configuration. For a parabolic dot the first magic numbers are 2, 6, 12, see Eq. (4) and the discussion below it. Besides these peaks for \( N \) coinciding with a magic number, some additional peaks are expected for a number of electrons correspond-
spectrum, peaks tend to be present for even number of electrons in the dot. The fact that a degenerate level $E_M^{(0)}$ is split in $M$ Kramers-degenerate sublevels (in the perturbative regime), leads to a suppression of the Hund’s rule: in a half-filled level to maximize the total spin the electrons should be allocated one per sublevel, but this has an energy cost equal to the sublevel splitting; if the sublevel splitting is larger than the gain in exchange energy, then the spin polarization for a half-filled level is suppressed. This is indeed what we see by analyzing the spin properties of the SDFT ground-state wave-function. At this point it is important to stress that due to the tunability of the SO coupling strength $\text{(11, 12, 13)}$, it is possible to investigate experimentally the effect of the Rashba term on the addition spectrum of few-electrons quantum dots (addition spectra were measured by Tarucha et al.$^{[6]}$), and the transition from weak ($k_{so}l_\omega \ll 1$) to strong SO coupling.

We now investigate the effect of an in-plane magnetic field. Due to the fact that the system is invariant under rotation around the $z$-axis, we can choose the direction of the in-plane magnetic field arbitrarily without losing any generality. We introduce a magnetic field $B$ along $x$, which does not affect directly the orbital motion, but couples to the $x$-component of the total spin, giving rise to a Zeeman term, $H_z = \hbar \omega_z S_z/2$, where $S_z = \sum_{i=1,N} \sigma_z^{(i)}$, and $\hbar \omega_z = \mu_B g^* B$, with $\mu_B$ being Bohr’s magneton, and $g^*$ the g-factor. We consider now a dot in a closed-shell configuration, namely we take $N = 2$ and $N = 6$. In the case of vanishing SO coupling and in the independent-electron picture, such a system does not respond to the in-plane magnetic field for Zeeman splitting smaller than the level splitting ($\omega_z < \omega$). The situation changes when the Rashba term is introduced; the ground state of the dot exhibits now some net-spin polarization. In the upper panel of Fig. 2, the average value of $S_z$ is plotted vs magnetic field, showing how the system gets magnetized even in a closed-shell configuration due to the interplay of SO coupling and Zeeman splitting. The average values of $S_x$ and $S_z$ remain equal to zero. In the lower panel of Fig. 2, the variation of the ground state energy with magnetic field is plotted vs magnetic field. It shows a decrease with increasing field (which is well fitted by a parabola), yielding a positive susceptibility $\chi = -\partial^2 E/\partial B^2$. Thus, we can conclude that the dot in a closed shell configuration exhibits a paramagnetic behavior. This is in contrast to what happens in real atoms, where a closed shell gives a diamagnetic response due to orbital degrees of freedom (Larmor diamagnetism)$^{[19]}$, while in our case the Larmor term is suppressed by the two-dimensionality of the dot. This paramagnetic behavior$^{[20]}$ is due to the single-particle eigen-states (see below), but it persists when the electron-electron interaction is present (it is enhanced by it), as shown in Fig. 2.

In the limit of $k_{so}l_\omega \omega_z \ll 1$, and $w_z < w$, it is possible to obtain a perturbative expression in $H_{so}$ for the single-particle eigen-energies:

$$E_{M,i,\sigma} = E_{M}^{(0)} + \sigma \frac{\hbar \omega_z}{2} - \frac{\hbar \omega_1}{2}(k_{so}l_\omega)^2 \left\{ 1 + \frac{\omega^2}{\omega_z^2 - \omega^2} \left[ 1 + \sigma(2i-1)\frac{\omega_z}{\omega} \right] \right\},$$

(7)

where $i = 1 \cdots M + 1$, $\sigma = \pm 1$ is the quantum number relative to the projection of spin in the direction of the magnetic field, i.e $\sigma_z$, and $E_{M}^{(0)}$ are the energies given in Eq. (5). In the independent-electron approximation, the energy of a closed shell $E_{cs}(M) = \sum_{i,\sigma} E_{M,i,\sigma}$ reads

$$E_{cs}(M) = 2(M + 1)E_{M}^{(0)} - (M + 1)\hbar \omega(k_{so}l_\omega)^2 \left[ 1 + \frac{\omega^2}{\omega_z^2 - \omega^2} \right].$$

(8)

Expanding Eq. (8) in $\omega_z/\omega$ we get for the magnetic-field dependent part of the closed-shell energy $-(M +
closed-shell parabolic behavior seen in Fig. 2. From Eq. (8) we get a

tion of 1¯

corresponding total-spin components.

of visualization, we plot electrons, χ

computed by means of SDFT, for a dot with N = 6 electrons, ks = 0.02 nm

-1, and hωz = 1 meV. In (a), for ease of visualization, we plot n_x instead of n_x. Spatial integration of n_y and n_z gives zero, yielding a zero average for the corresponding total-spin components.

1)hω(k_s l_ω)^2(ω_z/ω)^2 + O[(ω_z/ω)^4], which explains the parabolic behavior seen in Fig. 2. From Eq. (8) we get a paramagnetic contribution to the susceptibility due to a closed-shell

\[ \chi_M = 2(M + 1)\omega_0^2(k_s l_ω)^2 - \frac{2\omega_0^4}{h(\omega_0^2 - \omega_z^2)^2} \] (9)

which in the limit of ω_z/ω ≪ 1 is just a positive constant: \[ \chi_M = 2(M + 1)(k_s l_ω)^2/hω. \]

It is interesting to have a closer look at the spin-density for the magnetized dot. In Fig. 3 the projections of the spin density along the x-, y-, and z-axis are shown for a dot containing six electrons in the presence both of SO coupling and of a Zeeman field. As it is clearly visible, the system shows spin texture in space, this is due to the fact that no common spin-quantization axis exists anymore (a similar situation occurs in quantum wires with strong spin-orbit coupling[21].)

In conclusion, we have studied the effect of Rashba spin-orbit interaction on the addition energy, and on the spin properties of a few-electron quantum dot by means of spin density functional theory. In particular, we have found a suppression of Hund’s rule, for small ks values, for which perturbation theory in H_so still holds. An additional in-plane magnetic field (Zeeman field) leads to a paramagnetic behavior of the dot in a closed shell configuration, and to spin texture in space.

This work was supported by the Center for Functional Nanostructures at the University of Karlsruhe. We thank J. C. Cuenas, M. Macucci, and U. Zülicke for useful discussions.

1] S. A. Wolf et al, Science 294, 1488 (2001).
2] J. A. Folk et al., Phys. Rev. Lett. 86, 2102 (2001)
3] B. I. Halperin et al., Phys. Rev. Lett. 86, 2106 (2001).
4] I. L. Aleiner, and V. I. Fal’ko, Phys. Rev. Lett. 87, 256801 (2001)
5] A. V. Khaetskii, and Y. V. Nazarov, Phys. Rev. B 61, 12639 (2000).
6] S. Tarucha, D. G. Austing, T. Honda, R. J van der Hage, and L. P. Kouwenhoven, Phys. Rev. Lett. 77, 3613 (1996).
7] M. Macucci, K. Hess, and G.J. Iafrate, Phys. Rev. B 55, R4879 (1997).
8] M. Koskinen, M. Manninen, and S. M. Reimann, Phys. Rev. Lett. 79, 1389 (1997).
9] E. I. Rashba, Fiz. Tverd. Tela (Leningrad) 2, 1224 (1960), [Sov. Phys. Solid State 2, 1109 (1960)].
10] G. Lommer, F. Malcher, and U. Rössler, Phys. Rev. Lett. 60, 728 (1988).
11] J. Nitta, T. Akazaki, H. Takayanagi, and T. Enoki, Phys. Rev. Lett. 78, 1335 (1997).
12] T. Schäpers et al., J. Appl. Phys. 83, 4324 (1998).
13] D. Grundler, Phys. Rev. Lett. 84, 6074 (2000).
14] U. von Barth and L. Hedin, J. Phys. C 5 1629 (1972).
15] The effect of the spin-orbit interaction arising from lateral confinement in the dot on the single-particle spectrum has been discussed by O. Voskoboynikov, C. P. Lee, and O. Tretyak, Phys. Rev. b 63, 165306 (2001).
16] W. Kohn and L. J. Sham, Phys. Rev 140, A1133 (1965).
17] B. Tanatar and D. M. Ceperley, Phys. Rev. B 39, 5005, (1989).
18] J. P. Perdew and A. Zunger, Phys. Rev. B 23, 5048 (1981).
19] For a closed atomic shell Van Vleck paramagnetism is absent.
20] The magnetic susceptibility of free electrons subject
to Rashba spin-orbit coupling has been discussed by I. I. Boiko, E. I. Rashba, Fiz. Tverd. Tela Sov. (Leningrad) 2, 1874 (1960), [Phys. Solid State 2, 1692 (1960)]; Y. A. Bychkov and E. I. Rashba, J. Phys. C 17, 6039, (1984).

[21] M. Governale, and U. Zülicke, cond-mat/0201164 (2002).