The effect of valley, spin and band nesting on the electronic properties of gated quantum dots in a single layer of transition metal dichalcogenides (TMDCs)

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We present here results of atomistic theory of electrons confined by metallic gates in a single layer of transition metal dichalcogenides. The electronic states are described by the tight-binding model and computed using a computational box including up to million atoms with periodic boundary conditions and parabolic confining potential due to external gates embedded in it. With this methodology applied to MoS2, we find a twofold degenerate energy spectrum of electrons confined in the two non-equivalent K-valleys by the metallic gates as well as six-fold degenerate spectrum associated with Q-valleys. We compare the electron spectrum with the energy levels of electrons confined in GaAs/GaAlAs and in self-assembled quantum dots. We discuss the role of spin splitting and topological moments on the K and Q valley electronic states in quantum dots with sizes comparable to experiment.

I. INTRODUCTION

There is currently interest in electron spin based qubits1–6 and circuits realized in field-effect transistors (FET)7–10. Since the first localization of a single electron in a GaAs/GaAlAs FET by metallic gates3, circuits in GaAs and silicon have been realized11–15. A similar effort was directed towards understanding electronic states of electrons confined in self-assembled quantum dots16–18. In both cases the single particle spectrum was understood in terms of a spectrum of two harmonic oscillators and directly observed in InAs/GaAs quantum dots18. In these structures electrons are localised in a volume containing millions of atoms, hence nuclear spins and atomic vibrations contribute to decoherence of electron spins. Recent realization of semiconductor layers with atomic thickness19–23 opens the possibility of confining single electrons to few atom thick layers potentially significantly increasing operating temperature and coherence of electron spin qubits. The conduction band minima in both graphene and transition metal dichalcogenides (TMDCs) are localized in two non-equivalent valleys opening the possibility of using the valley degree of freedom as additional variable24–29. The low energy conduction and valence band states in TMDCs can also be approximated by massive Dirac Fermion Hamiltonian with resulting nontrivial valley and topological properties29–31. The potential of massive Dirac Fermions as qubits has been recognized by a number of theoretical32–40 and experimental41–43 works. Much of this interest in TMDCs based qubits is the possibility of manipulation of the ‘valley’ degree of freedom, with oppositely circularly polarised light25,26,34. In addition to the massive Dirac Fermion physics and the two K-valleys, TMDCs exhibit 3 additional minima per valley in the conduction band at Q points. The presence of Q points24,29,35 results in the band nesting and strong coupling to light. Even though all TMDCs share a honeycomb crystal structure, direct bandgaps at K and -K valleys, strong excitonic effects and different metal atoms (Mo or W) change the spin ordering and dispersion of conduction bands at K and Q points, allowing for nontrivial spin dependence of confined electrons. Moreover, the electronic properties of TMDCs can be engineered with, e.g., composition46–49, strain50,51, substrate51,52 or external electromagnetic fields53–57, facilitating their application in spin- and valley- based electronics.

Recently, quantum dots (QDs) in graphene, bilayer graphene and TMDCs have been realized as either finite size clusters with different edge termination41,58–62 or by electrostatic confinement with lateral metal electrodes41,62–66. QDs are also formed by combining different TMDC crystals in the plane, which form a potential well67.

Gate defined quantum dots avoid the need for atomistic control of the edges. Several groups reported on the creation of finite size electron droplets using metallic gates and observed Coulomb blockade in transport41,43,62. Gated quantum dots combined with large trion binding energies allowed for optical probing of excitons in TMDC QDs41,43,62,68. Gerardot and co-workers demonstrated single electron and hole transfer into WSe2 QDs43 and Srivatsava and co-workers estimated long valley lifetimes of localised holes in these QDs due to excess charge42. Charged excitons have also been proven to suppress valley scattering by Vamivakas and co-workers69. Moreover, local tunable confinement potential has been realized by Kim and co-workers52 and gate tuning of QD molecules have been shown by Guo and co-workers69.

There has been significant progress in theoretical understanding of TMDC QDs. Stability and electronic properties of small QDs with various composition, orientation and edge type have been studied within DFT theory70–75. Galli and coworkers studied the electronic properties of triangular MoS2 quantum dots as a function of the number of layers. The results demonstrated
that while bulk MoS$_2$ is an indirect gap semiconductor, a single atomic layer of MoS$_2$ becomes a truly two-dimensional direct gap semiconductor.

The ab-initio approaches have been extended to tight binding models capable of describing quantum dots in the tens of nanometer lateral sizes. Using a 3-band tight-binding model limited to metal orbitals Peeters and co-workers$^{33-36,38,40}$ analyzed the effect of quantum dot shape and external magnetic field on the single particle energy spectrum. Using atomistic tight binding approach spin-valley qubits have been described by Bednarek and co-workers$^{33}$. In order to understand size dependence of the electronic states in quantum dots for realistic sizes involving millions of atoms, $k \cdot p$ and effective massive Dirac fermion models were applied$^{34-36,38-40}$. In this work, the states of electrons in multi-million atom quantum dots are described by the ab-initio based computational box, periodic boundary conditions are used. This allows a study of electrically confined processes, including mixing by the confining potential has also been analyzed by Yao and co-workers$^{35}$. Magnetic control of the spin-valley coupled states in TMDC QDs has been shown by Qu and co-workers$^{36,39}$. Lateral QD molecules have also been studied by several groups$^{53,80}$.

In this work, the states of electrons in multi-million atom quantum dots are described by the ab-initio based tight-binding Hamiltonian including 3 d-orbitals of metal atoms and 3 p-orbitals of sulfur dimers, made even with respect to the plane of the quantum dot$^{33}$. The effect of metallic electrodes is simulated by the parabolic external potential with finite depth and radius, embedded in a computational box with up to million atoms. To avoid edge states associated with a particular termination of the computational box, periodic boundary conditions are used. This allows a study of electrically confined circular quantum dots in TMDCs of experimentally realizable sizes up to 100 nm in radius$^{41,62}$. We find the ladder of degenerate harmonic oscillator states derived from K-valleys, and, as expected and noticed already by Chirolli et al.$^{33}$, two three-fold degenerate harmonic oscillator shells originating from Q points. We also find the splitting of excited harmonic oscillator shells due to the topological moments, opposite for the two valleys$^{33-36,38-40}$. We find the splitting to increase for higher angular momentum shells and to be of order of magnitude higher in Q-derived shells. We also discuss the shell ordering due to negative spin orbit coupling (SOC) as well as due to interplay of inter-shell and SOC splitting. These topological and spin splittings together with shell spacing result in the interplay between the K- and Q-derived states which could allow for exploration of the exotic physics of SU(3) symmetry in condensed matter systems$^{85}$.

The paper is organized as follows. In Chapter 2 we describe the tight binding model and the conduction band states of MoS$_2$. In Chapter 3 we describe the confining potential and the model of MoS$_2$ QD. In Chapter 4 we present results on the K-derived and Q-derived spectrum, shell and spin orbit splitting as well as size-dependent ordering of states in MoS$_2$ QDs. We end with conclusions in Chapter 5.

II. THE TIGHT BINDING MODEL AND CONDUCTION BAND OF MoS$_2$

We describe here our tight binding model and electronic properties of a single layer of MoS$_2$. Dirac fermion models were applied$^{34-36,38-40}$. Lateral QD molecules have also been studied by several groups$^{53,80}$. We find the splitting to increase for higher angular momenta.

\[ H_0 = \sum_{ir} \varepsilon_{ir} c_{ir}^+ c_{ir} + \sum_{<ir,jp>} t_{ir,jp} c_{ir}^+ c_{jp}, \]  

where $c_{ir}^+$ describes creation of electron on atom $i$ and orbital $r$ and $t_{ir,jp}$ are tunneling matrix elements between atoms $i$ and $j$ and orbitals $r$ and $p$, determined by the Slater-Koster rules. For metal atom sublattices A and sulfur dimer sublattices B we construct matrix elements $t_{ir,jp}$ of the Hamiltonian for nearest neighbour tunneling $\langle \Psi_{A,m}^k | H | \Psi_{B,m'}^{k'} \rangle$ and next nearest neighbour tunneling processes, $\langle \Psi_{A,m}^k | H | \Psi_{A,m}^{k'} \rangle$ and $\langle \Psi_{B,m}^k | H | \Psi_{B,m}^{k'} \rangle$, forming a $6 \times 6$ matrix in the basis of Mo and $S_2$ Bloch functions $\Psi_{A,m}^k = e^{ikr} u_{A,m}^k (r)$ and $\Psi_{B,m}^k = e^{ikr} u_{B,m}^k (r)$ of the form:

\[ H (\vec{k}) = \begin{bmatrix} H_{Mo-Mo} & H_{Mo-S_2} \\ H_{Mo-S_2}^T & H_{S_2-S_2} \end{bmatrix} \]

\[ H_{Mo-Mo} = \begin{bmatrix} E_{m_1=0} W_{3g_2} (\vec{k}) & W_{4g_1} (\vec{k}) \\ +W_{3g_1} (\vec{k}) & E_{m_2=0} W_{3g_2} (\vec{k}) \end{bmatrix} + W_{2g_0} (\vec{k}) \]

\[ H_{S_2-S_2} = \begin{bmatrix} E_{m_1=0} & 0 \\ +W_{5g_0} (\vec{k}) & E_{m_2=1} \end{bmatrix} \]

\[ H_{Mo-S_2} = \begin{bmatrix} V_{f-1} (\vec{k}) & -V_{5f_1} (\vec{k}) & V_{5f_0} (\vec{k}) \\ -V_{4f_0} (\vec{k}) & -V_{5f_1} (\vec{k}) & -V_{2f-1} (\vec{k}) \\ -V_{3f_1} (\vec{k}) & -V_{2f-1} (\vec{k}) & V_{5f_0} (\vec{k}) \end{bmatrix} \]

where the amplitudes $V$, $W$ and k-dependent functions $f$, $g$ are given in the Appendix A of Ref. 81. The diagonal $3 \times 3$ blocks correspond to next nearest neighbour...
Mo-Mo and S$_2$-S$_2$ tunneling while the off-diagonal block translates into Mo-S$_2$ nearest-neighbour tunneling processes.

![Fig. 1](image)

**FIG. 1:** (a) CB energy $E_c(k)$ in the BZ consists of K and -K valleys and 6 secondary minima at Q points. The red line shows the path along which the CB and VB edges are shown in (b). (c) Two schemes showing possible spin ordering in the conduction and valence bands. The low energy bands are mainly composed of $d$ orbitals, with the red line being responsible for nesting of conduction and valence bands for MoS$_2$.

We diagonalize the Hamiltonian in Eq. 2 for each k-point in the basis of Bloch functions $\Psi^k_{A,m,u}$ and $\Psi^k_{B,m,v}$ and obtain 3 conduction and 3 valence band states. The parameters of the Hamiltonian, Eq. 2, are obtained from the fitting of energy levels to results of ab-initio derived energy bands.

The lowest energy conduction band (CB) dispersion $E_c(k)$ in the first Brillouin zone (BZ) is shown in Fig. 1a. The Brillouin zone is hexagonal, with 6 K points at the six corners, with 3 of them being equivalent up to reciprocal lattice vector translation in both K and -K valleys. The lack of inversion symmetry in the unit cell leads to K and -K points being non-equivalent. A single layer of TMDCs has a direct band gap, located in the vicinity of both K and Q points, when the spin up states at K and spin down states at Q become degenerate (Fig. 1c left). This scheme prevails in materials with tungsten as a metal. For compounds with molybdenum (Fig. 1c right) gap between K- and Q- points spin-split bands is larger. In this work we focus on MoS$_2$, but we explore the physics of QD states built from K- and Q-points, which may be equally relevant for low energy spectra in different MX$_2$ materials.

### III. THE MODEL OF A QUANTUM DOT

We now discuss our model of a quantum dot. We start with a rectangular computational box of a single plane of MoS$_2$ with periodic boundary conditions as described in Section 2 and shown in Fig. 2a. We then introduce a parabolic potential generated by metallic gates as shown in Fig. 2b. The total Hamiltonian of the parabolic QD (Fig. 2a) with radius $R_{QD}$ is given by:

$$H = H_0 + \sum_{ir} V_i c_{ir}^+ c_{ir},$$

where $V_i$ is the external potential on atom $i$ generated by metallic gates. For gated quantum dots the potential $V(r)$ is largely parabolic and given by:

$$V_i = V(r_i) = \begin{cases} \frac{1}{2} \omega^2 r_i^2 - V_{\text{max}}, & \text{for } r_i < R_{QD} \\ 0, & \text{for } r_i > R_{QD}. \end{cases}$$

The parabolic confining potential can be expressed by corresponding harmonic oscillator level spacing $\omega = 2|V_{\text{max}}|/R_{QD}^2$ defined by electrostatic potential with depth $V_{\text{max}}$ and radius $R_{QD}$. For definiteness, we keep $V_{\text{max}}$ at -300 meV throughout this work. At the boundary of the dot confining potential goes to 0. Dot edges are kept sufficiently far from computational box edges, connected by periodic boundary conditions (BC). We have confirmed that in our model states localized inside the dot are not influenced by choice of BC. The sizes of the computational domain studied are up to $\sim 220 \times 220$. 

![Fig. 2](image)
nm, which corresponds to $\sim 1.1 \times 10^6$ atoms, and up to 100 nm dot radii, corresponding to experimentally studied systems\textsuperscript{41,69}.

Diagonalization of such large, sparse Hamiltonian matrices, is performed using FEAST algorithm\textsuperscript{91} as well as with sparse matrix diagonalization routines within PETSC library\textsuperscript{92}.

FIG. 3: (a) Ladder of QD K-derived states. Harmonic oscillator shells are doubled due to valley and due to spin. Inter-shell spacing is labeled with $\Delta E_{0,1}^K$, while the intra-shell splitting is labeled with $\Delta E_{0,1}^K$. (b) Fourier composition of the two states from the lowest shell marked with A & B.

IV. RESULTS

A. K-point-derived and Q-point-derived spectrum of electronic states

We start with a parabolic QD defined electrostatically on representative TMDC, MoS$_2$ as shown in Fig. 2b. For clarity, we first neglect spin-orbit coupling in the tight-binding Hamiltonian in Eq. 1. The results of diagonalization of the quantum dot Hamiltonian with $V_{\text{max}} = 300$ meV and variable $R_{\text{QD}} = \{1.2, 1.5, 1.8, 2.0\}$ nm are shown in Fig. 4. We see that electronic states are arranged into almost equally spaced electronic shells. Each shell consists of states derived from K and -K points, doubly degenerate due to spin, as schematically shown on Fig. 3a. Fig. 3b shows the Fourier composition of the first 2-level shell of the QD. With very small spin-orbit splitting one can attribute each of these 2 states to either +K or -K valley. In each valley there are equally spaced electronic shells with degeneracies identical to the spectrum of two harmonic oscillators as observed directly in self-assembled quantum dots\textsuperscript{18}. However, unlike in GaAs or self-assembled quantum dots, the degeneracy of each electronic shell is removed, an effect discussed below. Fig. 4 shows the evolution of the energy levels with increasing dot radius $R_{\text{QD}}$ while keeping the depth of potential fixed. We see that with increasing $R_{\text{QD}}$ more electronic shells are confined within the dot. However, in contrast with gated quantum dots in GaAs, for all studied QD sizes we always find, in addition to K derived electronic shells, perfectly 6-fold degenerate shells, emerging at higher energy and marked with rectangular boxes in Fig. 4.

FIG. 4: QD states for increasing QD radius $R_{\text{QD}}$. K-derived harmonic oscillator ladder of states is interrupted by the Q-derived states marked with boxes higher in the spectrum.

The 6-fold degeneracy of new electronic shells stems from 3 non-equivalent Q points around K valley and 3 non-equivalent Q points around -K valley, as shown schematically in Fig. 5a and 5b. Fig 5c shows the Fourier composition of the first shell of 6 degenerate Q-derived states. For very small spin orbit coupling two sets of 3 states can be attributed to the mixture of 3 Q points around K and -K valley. Interestingly, these Q-derived shells can be understood as condensed matter physics analogue of flavour SU(3) symmetry\textsuperscript{85}, describing quarks in high energy physics.

FIG. 5: (a) Ladder of QD Q-derived states. Harmonic oscillator shells are sixfold multiplied due to K and -K points and 3 Q points around each valley as shown in matching colours in (b). Inter-shell spacing is labeled with $\Delta E_{0,1}^Q$, while the intra-shell splitting is labeled with $\Delta E_{1,1}^Q$. (c) Fourier composition of the two sets of states from the lowest shell is marked with A & B.
B. Topological splitting of electronic shells

In spectra shown in Fig. 4 we observe intra-shell splitting despite cylindrical symmetry of confining potential. The splitting appears to depend on the angular momentum of harmonic oscillator states in degenerate electronic shell. As shown experimentally in Ref.\(^\text{18}\) the application of external magnetic field removes the degeneracy of harmonic oscillator states. Hence, this splitting can be understood as resulting from the Berry’s curvature analogous to magnetic field acting on finite angular momentum states, in opposite directions in K and -K valleys\(^\text{83,84}\).

As shown schematically in Fig. 3a and Fig. 5a, this splitting is observed for both K- and Q-derived harmonic oscillator shells. We note that for the same \(R_{QD}=30\) nm, intra-shell ”topological” splitting grows with shell number and, importantly, is an order of magnitude stronger for Q-point states, reaching up to 8 meV. We note that the smaller the dot, the larger splitting is observed. We notice also that angular momentum \(L=\pm2\) state splitting around \(L=0\) state for K-point series, is not symmetric, pointing that Berry’s curvature might influence also \(L=0\) states, as in s-series of excitons in TMDC’s materials\(^\text{93,94}\).

![Diagram of the spin ordering of levels from K-derived and Q-derived ladder. Spins order oppositely in levels from around K and -K valley. Spin splittings of K-derived (Q-derived) shells are marked with \(\Delta_{SOC}^K\) (\(\Delta_{SOC}^Q\)).](Image)

FIG. 6: Diagram of the spin ordering of levels from K-derived and Q-derived ladder. Spins order oppositely in levels from around K and -K valley. Spin splittings of K-derived (Q-derived) shells are marked with \(\Delta_{SOC}^K\) (\(\Delta_{SOC}^Q\)).

C. Spin-orbit coupling vs. shell splitting

We now turn on the spin-orbit coupling (SOC) in the TB Hamiltonian given by Eq. 1, which induces a splitting between spin up and spin down states in all shells, as shown schematically in Fig 6. The splitting \(\Delta_{SOC}\) changes sign when going from K and -K valley. It increases with QD radius \(R_{QD}\) and for the K-derived states it reaches value close to the bulk value of 4.2 meV\(^\text{24,81}\) for \(R_{QD}=100\) nm.

![Graph showing inter-shell, intra-shell and SO splittings as a function of quantum dot radius in MoS\(_2\) QDs. (a) Inter-shell spacing decreases with QD radius \(R_{QD}\). (b) Intra-shell topological splitting increases for higher shells and for Q-derived shells it reaches 6 meV for \(R_{QD}=30\) nm. (c) SOC splitting increases for larger dots and saturates close to bulk value of 4.2 meV for QDs larger than \(R_{QD}=100\) nm. For \(R_{QD}=100\) nm the SOC splitting is higher than the inter-shell splitting, which affects the order of levels.](Image)

FIG. 7: Inter-shell, intra-shell and SO splittings as a function of quantum dot radius in MoS\(_2\) QDs. (a) Inter-shell spacing decreases with QD radius \(R_{QD}\). (b) Intra-shell topological splitting increases for higher shells and for Q-derived shells it reaches 6 meV for \(R_{QD}=30\) nm. (c) SOC splitting increases for larger dots and saturates close to bulk value of 4.2 meV for QDs larger than \(R_{QD}=100\) nm. For \(R_{QD}=100\) nm the SOC splitting is higher than the inter-shell splitting, which affects the order of levels.

Importantly, the QD energy spectrum also depends heavily on the SO splitting. As shown in Fig. 7c the SO splitting in the first K-derived shell of states grows with QD size and saturates for systems close to bulk size value of 4.2 meV, marked with grey line in Fig. 7c). This interplay of splittings will determine the order of shells for TMDC QDs and therefore, the shell filling in a many-electron system.

In Fig. 8 we show two scenarios of the order of K-derived shells for \(\Delta_{SOC}^K > 0\) and \(\Delta_{SOC}^K < 0\) type of materials. When \(\omega > \Delta_{SOC}\) (Fig. 8a), the lower energy shells are ordered according to angular momentum \(L\). First two energies are doubly degenerate, and fifth state belongs to the next \(L=1\) shell. However, when \(\omega < \Delta_{SOC}\) (Fig. 8b), the energy of the third state already reaches the energy of the \(L=1\) shell. Interestingly, this reordering can be also observed for MoS\(_2\) QDs, if the \(R_{QD}\) can be varied. As can be seen from Fig. 7a and Fig. 7c, for MoS\(_2\) QDs with radii larger than 100 nm the inter-shell splitting of the lowest K-derived shell \(\Delta E_{K0}\) is lower than its SO splitting \(\Delta_{SOC}^K\), which mixes order of the shell spectrum, like in \(\Delta_{SOC}^K < 0\) type of TMDCs. By fabricating QDs with two sizes it is possible to realize the scenarios described in Fig. 8, mimicking two distinct TMDC compounds.
FIG. 8: 2 regimes for inter-shell spacing $\omega_0$ relative to the SOC splitting $\Delta_{\text{SOC}}$. (a) If $\omega_0$ is large comparing to $\Delta_{\text{SOC}}$, the shells stay separate. (b) If $\omega_0$ is small comparing to $\Delta_{\text{SOC}}$, the shells intertwine.

V. CONCLUSIONS

In this work we presented atomistic theory of electrons confined by metallic gates in a single layer of transition metal dichalcogenides. The electronic states were described by the tight-binding model including metal and sulfur orbitals and computed using a computational box including up to million atoms with periodic boundary conditions and with embedded in it parabolic confining potential due to external gates. This allowed to determine the energy spectrum in quantum dots with experimentally relevant sizes. We found a twofold valley - degenerate energy spectrum and a six-fold degenerate spectrum associated with Q-valleys. We discussed the role of spin splitting and topological moments on the K and Q valley electronic states. We pointed out importance of SU(3) flavor Q point states for low lying QD states. Future work will determine means of controlling valley degree of freedom and the role of electron - electron interactions.

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