Valley and spin polarized broken symmetry states of interacting electrons in gated MoS₂ quantum dots

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Understanding strongly interacting electrons enables the design of materials, nanostructures and devices. Developing this understanding relies on the ability to tune and control electron-electron interactions by, e.g., confining electrons to atomically thin layers of 2D crystals with reduced screening. The interplay of strong interactions on a hexagonal lattice with two nonequivalent valleys, topological moments, and the Ising-like spin-orbit interaction gives rise to a variety of phases of matter corresponding to valley and spin polarized broken symmetry states. In this work we describe a highly tunable strongly interacting system of electrons laterally confined to monolayer transition metal dichalcogenide MoS₂ by metallic gates. We predict the existence of valley and spin polarized broken symmetry states tunable by the parabolic confining potential using exact diagonalization techniques for up to \( N = 6 \) electrons. We find that the ground state is formed by one of two phases, either both spin and valley polarized or valley unpolarised but spin intervalley antiferromagnetic, which compete as a function of electronic shell spacing. This finding can be traced back to the combined effect of Ising-like spin-orbit coupling and weak intervalley exchange interaction. These results provide an explanation for interaction-driven symmetry-breaking effects in valley systems and highlight the important role of electron-electron interactions for designing valleytronic devices.

I. INTRODUCTION

The role of electron-electron (e-e) interactions in determining the many-electron ground and excited states in different materials is controlled by the ratio of Coulomb energy \( V \) to kinetic energy \( T \) as \( V/T = r_s \) where \( \pi r_s^2 \) is an area per electron\(^1\). For small \( r_s \) electrons in 2D are well described by the Fermi liquid theory but as \( r_s \) increases, density decreases, and the spin polarised and Wigner crystal phases follow\(^2,3\). In the 2D Hubbard model the electronic phases are controlled by the ratio of on-site Coulomb energy \( V \) to the tunneling matrix element \( U/t \). On a hexagonal lattice, calculations predict a semimetallic phase followed by the anti-ferromagnetic and Mott-insulating phase\(^4–6\). The \( U/t \) can be tuned by controlling screening \( (U) \) or controlling \( t \). Recent work on twisted bilayer graphene (BG) showed that \( t \) can be significantly reduced by twisting layers in BG\(^7\). The quenching of tunneling results in strongly correlated system with Mott-insulating and superconducting phases\(^8,9\). Recent experiments in BG\(^10,11\) and transition metal dichalcogenides (TMDCs) point to potential existence of spin\(^12\) and valley polarized\(^13\) interaction driven broken symmetry valley and spin polarised states.

In this work we focus on a new emerging highly tunable strongly interacting system of \( N \) electrons laterally confined to monolayer 2D crystal, such as MoS₂\(^14–19\) by metallic gates\(^20–34\). The confinement to a single atomic layer leads to reduced screening and enhanced e-e interactions manifested in large, \( \sim 300 \) meV, exciton binding energies\(^16,32,35–37\). Metallic gates can be used to define quantum dots (QDs) with discrete levels with spacings \( \omega \) and enable a controlled charging of the QDs with \( N \) electrons. The ratio \( V/T \) scales with \( \omega \) as \( V/T = 1/\sqrt{\omega} \). In small GaAs QDs at large \( \omega \), the ground state (GS) is well approximated by configurations minimizing single particle (SP) energy\(^38\), but in large QDs, for small \( \omega \), spin polarised\(^38–40\) and correlated phases emerge\(^38,41\). Here we combine the atomistic multimillion atom description of SP states, lateral confining potential and realistic e-e interaction matrix elements with accurate exact diagonalization techniques to determine GS and excited states of electrons in MoS₂ QDs.

II. MODEL

Fig. 1a shows the top view of a monolayer MoS₂ lattice. The blue (yellow) atoms correspond to Mo metal (S) atoms with 3 \( d \)-orbitals (3 \( p \)-orbitals) as described in detail in Ref.\(^33\). The single particle (SP) Hamiltonian describes the tunneling of electrons between Mo \( d \)-orbitals and S \( p \)-orbitals. The conduction band (CB) wavefunctions are expanded in Mo and S orbitals and computed for a large computational box with \( \sim 10^6 \) atoms and periodic boundary conditions. The SP states are hence characterised by a band index and a wavevector \( k \), free from edge states present in a finite computational box. The relevant band structure consists of valence band (VB) and conduction band (CB), with the smallest energy gap at the two non-equivalent CB minima at \( +K \) and \( -K \) points of the Brillouin zone, and of six additional minima (3 per \( K \)-point), at the Q-points.

In such a realistic computational box we add a gate-defined parabolic confining potential \( V(r) \) (described in \( V \)), as shown in Fig. 1b. The confining potential mixes the CB states, lowers their energy into the energy gap of MoS₂ and confines electrons to the center of a QD.
A schematic picture of a typical low energy SP spectrum is presented in Fig. 1c. It is doubly degenerate due to the valley index $+K, -K$. In each valley the spectrum resembles that of a 2D harmonic oscillator (HO), consisting of shells of states separated by the spacing $\omega$, which can be tuned by the depth of the confining potential or the radius of the QD. A separate six-fold degenerate HO-like spectrum originating from $Q$ points is present at higher energies (not shown). These states are not occupied by electrons for the range of $\omega$ considered here and are not considered in what follows. The SP levels are labelled with quantum numbers $p, \sigma$, where $p = [(n, m), K]$ contains state index $(n, m)$ and valley index $+K, -K$, and $\sigma$ denotes spin. The $(n, m)$ are HO quantum numbers, where $n + m$ determines the shell index and $L = n - m$ is the angular momentum of the state in valley $+K$ (left) or $-K$ (right). The spin-orbit induced Zeeman splitting $\Delta_{SO}$ between spins ($\uparrow$ and $\downarrow$ shown in red and blue respectively in Fig. 1c) is opposite for both valleys.

A further modification of a simple HO level structure is a topological splitting $\delta$ proportional to $\omega$, exhibited by all electronic shells. This splitting arises from the valley topological moments in each valley. This results in opposite angular momentum $L$ states as the lowest energy states in $+K$ and $-K$ valleys.

\[ H = \sum_{p\sigma} e_{p\sigma} c_{p\sigma}^\dagger c_{p\sigma} + \frac{\eta}{2} \sum_{pqst\sigma\sigma'} \langle pq | V | st \rangle c_{p\sigma}^\dagger c_{q\sigma'}^\dagger c_{s\sigma} c_{t\sigma}, \]  

where the first term describes energies $e_{p\sigma}$ of the SP HO states $p\sigma$ shown in 1c) and the second term describes interaction energy, with Coulomb matrix elements describing scattering between pairs of states. The Coulomb matrix elements $\langle pq | V | st \rangle$ are computed using atomistic million atom orbitals and with both bare Coulomb and Keldysh-screened interaction, accounting for reduced screening by 2D materials [see V for details]. The parameter $\eta$ allows us to turn the e-e interaction on and off.

The $N$-electron configurations are constructed as $|x\rangle = \prod_{p,\sigma} c_{p\sigma}^\dagger |0\rangle$, and the wavefunction of $N$-electron system is expanded in all possible electronic configurations $|x\rangle$. The Hamiltonian matrix in the space of configurations $|x\rangle$ is constructed and diagonalized giving exact eigenstates and eigenvalues. For example, for $N = 6$ we find up to $\sim 5 \cdot 10^7$ configurations for $M = 60$ SP orbitals.

We now turn to discuss the properties of $N$-electron systems. We focus here on $N = 2, 4$ and $N = 6$ electrons. This is because in a non-interacting system filling the first $s$-shell requires $N = 4$ electrons. Half filling of the $s$-shell is realised with $N = 2$ electrons and to obtain half filling of the first 2 shells $N = 6$ electrons are needed.

### III. RESULTS

#### A. N=2 electron complex

In order to build the understanding of the role of interactions in MoS$_2$ QDs, it is instructive to first focus on $N = 2$ electrons on the first 4-fold degenerate $s$-shell of SP states. In the absence of SO splitting $\Delta_{SO}$, this system describes the half-filled lowest energy shell of BG QD$^{20,31,34}$ or a half-filled $p$-shell of a self-assembled QB$^{38}$. As we will see the GS is determined by the exchange interaction and can be understood in terms of spin singlets and triplets.

With $N = 2$ electrons on $s$-shell orbitals in opposite valleys the $N = 2$ electron spin states can be classified into three spin triplets $|T_2^+\rangle = |\uparrow\rangle |\uparrow\rangle$, $|T_2^-\rangle = |\downarrow\rangle |\downarrow\rangle$, $|T_2^\sigma\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle |\downarrow\rangle + |\downarrow\rangle |\uparrow\rangle)$, or $|T_2^\pi\rangle = |\sigma\rangle |\sigma\rangle$. The total wavefunction is therefore simultaneously a valley singlet $|S^\sigma\rangle = \frac{1}{\sqrt{2}} (|K\rangle |K\rangle - |\bar{K}\rangle |\bar{K}\rangle)$. The spin triplet valley singlet state $|S^\pi\rangle |T_2^\pi\rangle$ is shown schematically in Fig. 2A. In the absence of $\Delta_{SO}$, the energy of the spin triplet configuration $E_T$ is composed of the sum of SP energies of $s$-type $(0, 0)$ orbitals, the direct interaction $V_{20}$ and intervalley exchange $V_{2X}(+K, -K)$ to give
$E_T = \epsilon_{00} + \epsilon_{00,1} + V_{D}^0(+K,-K) - V_{D}^0(+K,-K)$. The exchange interaction lowers the energy of $|T^*\rangle$ compared to $|S^*\rangle$. Exact diagonalisation of the $N = 2$ electron system on the s-shell with $\Delta_{SO} = 0$ gives $|S^*\rangle = |T^*\rangle$ as the triply degenerate GS, due to the intervalley exchange $V_{D}^0(+K,-K)$. This is in accordance with what has been found for half filled p-shell of QDs\textsuperscript{45} and for BG QDs\textsuperscript{31}, a two valley system with negligible SO.

In TMDCs the Ising-like SO interaction leads to spin splitting in the CB ranging from $\sim 3\text{meV}$ in Mo-based material to $\sim 30\text{meV}$ in W-based material\textsuperscript{13,17}. Turning on $\Delta_{SO}$ leads to a decrease in the energy of spin-down states in valley $K$ as well as of spin-up states in valley $-K$. For the case of $N = 2$ electrons this means that the spin triplets $|T^*\rangle$ and spin singlets $|S^*\rangle$ mix and the three-fold degeneracy of the $|S^*\rangle$ $|T^*\rangle$ GS is broken by the $\Delta_{SO}$. The splitting $\Delta_{SO}$ competes with intervalley exchange $V_{D}^0(+K,-K)$. For weak intervalley exchange $\Delta_{SO} \ll \Delta_{SO}$ the spin unpolarized state, depicted as configuration B in Fig. 2, becomes the lower energy state separated from the spin polarized states, configuration A in Fig. 2. This is shown in Fig. 2 (right) for $\omega = 36\text{meV}$ and varied strength of Keldysh-screened Coulomb interactions $\eta$. Configuration B can be written as a mixture of $|S^*\rangle |T_0^0\rangle$ and $|T_0^0\rangle |S^*\rangle$ and becomes the spin-valley singlet $|S^{sv}\rangle = \frac{1}{\sqrt{2}} (|S^*\rangle |T_0^0\rangle - |T_0^0\rangle |S^*\rangle) = \frac{1}{\sqrt{2}} (|K\downarrow\rangle - |K\uparrow\rangle) - |K\uparrow\rangle |K\downarrow\rangle).

We now lower the level spacing $\omega$ and allow the second shell of p-type single-particle states to be occupied by a second electron, e.g. as shown in Fig. 3D and Fig. 1C in Supplementary Material. The transfer from the s-shell to the p-shell costs SP energy $\omega + \delta/2$ but it is compensated by gain in interaction energy. Instead of $V_{D}^0(+K,-K) - V_{D}^0(+K,-K)$ for configuration A, the interaction is now $V_{D}^0(+K,+K) - V_{D}^0(+K,+K)$ (the superscript denotes $L$ of the second electron). This change lowers the energy of D compared to A and B. This is because of the significantly stronger intra-valley exchange $V_{D}^0(+K,+K)$ compared to inter-valley $V_{D}^0(+K,-K)$. There are two possible p-shell orbitals and two possible $N = 2$ electron configurations, out of which D (with the second electron in $L = +1$ ($L = -1$) orbital at $+K$ ($-K$)) is lower in energy, as discussed in Supplementary Material.

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like configurations $|^s_{0}\rangle$ (valley-spin polarised) compete for the GS with the triplet configurations $|^s_{0}\rangle$ (valley-spin unpolarised).

**B. GS and excited states of $N \geq 2$ and $M = 60$**

We have so far identified different possible phases of the $N = 2$ electron system and different interactions competing to produce the GS and excited states: SP energies, SO splitting, topological moments, direct and exchange intravalley and intervalley interactions. We now describe results of exact diagonalisation of the $N = 2$ electron problem as a function of $\omega$ for varying number of electronic shells. Converged results for 5 shells per valley ($M = 60$ SP states) for $N = 2$ and $N = 6$ electrons are discussed below and remaining electron numbers are discussed in Supplementary Material. All our numerical results show spin valley locking in the many-body GS, with spin $\uparrow$ (\downarrow) electrons occupying valley $+K$ ($-K$) so that $N_{\uparrow} = N_K$ and $N_{\downarrow} = N_{-K}$, which is in line with our explanation of the GS of the $N = 2$-electron system. This allows us to label the GS with one polarisation quantum number $V = \frac{N_K - N_{-K}}{N}$, denoting total valley polarisation and equal here to the total spin polarisation $\tilde{V} = S_{\uparrow} + S_{\downarrow} = \frac{N_K - N_{-K}}{N}$.

The results for valley and spin polarisation $\tilde{V}$ for $N = 2$ and $N = 6$ electrons are shown in the top panel of Fig. 4 while the corresponding energy gaps, $\Delta E_{X-GS} = E_X - E_{GS}$ where $E_X$ is the first excited state, and schematic electron configurations are shown in the lower panel.

The colors in Fig. 4 (top) denote the degree of polarisation $\tilde{V}$: orange depicts full spin and valley polarisation (SVP) with total $|S_z| = N/2$, while dark green identifies a fully inter-valley anti-ferromagnetic (IVAF) GS with total $S_z = 0$ ($N_{\uparrow} = N_{\downarrow}$) and no net valley polarisation ($N_K = N_{-K}$). Schematic configurations corresponding to IVAF and SVP phases are shown for both $N$. Clear phase transitions from the IVAF GS to the SVP GS accompanying the closure of energy gaps $\Delta E_{X-GS}$ at critical energy spacings $\omega_C \approx 9$meV and $\omega_C \approx 8$meV are visible for $N = 2$ and $N = 6$ electrons respectively. For $N = 2$, the phases IVAF and SVP correspond to the competing triplets $|^s_{0}\rangle$ and $|\sigma_{0}\rangle$ respectively.

In the insets of Fig. 3, we show a schematic representation of the two competing GS phases for $N = 2$ and $N = 6$ electrons with spin $\uparrow$ (\downarrow) electrons shown with red up (blue down) arrows. IVAF (left) involves $N_{\uparrow} = N_{-K} = N_K = 1$ and $N_{\downarrow} = N_{-K} = N_K = 3$ for $N = 2$ and $N = 6$ respectively. The SVP phase (right) is fully polarised with $N = N_{\uparrow} = N_K = 2$ (and a degenerate time-reversed state with $N = N_{\downarrow} = N_{-K} = 2$) and similarly $N = N_{\downarrow} = N_K = 6$ (and a degenerate time-reversed state with $N = N_{\uparrow} = N_{-K} = 6$).

In order to detect the competing GS phases in an experiment, one needs to consider the stability of these phases. It is partly determined by the energy spacing between the GS and excited state $\Delta E_{X-GS}$, which in turn impacts transport measurement. Closing of the energy gaps due to phase transitions would affect the temperature dependence and high-source-drain Coulomb diamonds in transport. The computed energy gaps $\Delta E_{X-GS}$ as a function of $\omega$ for $N = 2$ (black) and $N = 6$ (red) reach several meV. The quantum phase transitions between IVAF and SVP phases occur when $\Delta E_{X-GS} = 0$.

**IV. CONCLUSIONS**

Using atomistic theory combined with exact many-body diagonalisation tools we predict the existence of broken-symmetry Spin and Valley Polarized (SVP) and InterValley AntiFerromagnetic (IVAF) electronic states of interacting electrons electrostatically confined in a parabolic QD in a single layer of MoS$_2$. These results highlight the important role of electron-electron interactions for designing valleytronic devices.

**V. METHODS**

The hexagonal MoS$_2$ layer consists of two triangular lattices, one of Mo atoms and a second of $S_2$ dimers. We write our Hamiltonian in the basis of $d$ orbitals of Mo atoms and $p$ orbitals of $S_2$ dimers, which are even with...
respect to the metal plane, as

\[ \hat{H}^{TB} = \sum_i E_i c_i^\dagger c_i + \sum_{<i,j>} \left( T_{ij} c_i^\dagger c_j + h.c. \right) 
+ \sum_{<i,j>} \left( W_{ij} c_i^\dagger c_j + h.c. \right), \quad (2) \]

where \( c_i^\dagger \) creates an electron on state \( i \) and \( i \) carries atom unit cell index, orbital index and sublattice index. \( E_i \) are onsite energies and \( T \) (\( W \)) are nearest neighbour (NN) (next nearest neighbour (NNN)) hopping matrices between sites. Energies \( E_i \) include the parabolic potential \( V_i \) generated by the gates (as shown in Fig. 1 b)) on a site corresponding to index \( i \), with \( V_i = V(r_i) = |V_{\text{max}}|/(R_{QD}^2) \cdot r_i^2 - V_{\text{max}} \), for \( |r_i| \leq R_{QD} \) and 0 elsewhere. \( V_{\text{max}} \) is the depth of the potential and \( R_{QD} \) is the radius of the QD.

To avoid edge states in the energy gap we apply periodic boundary conditions, i.e., we wrap the finite computational box on a torus with periodic boundary conditions. The Hamiltonian in Eq. (2) can now be written in the basis of Bloch states as

\[ \hat{H}_{k-\text{basis}}^{TB} = \sum_k \sum_\alpha E_\alpha a_\alpha^\dagger a_\alpha 
+ \sum_k \sum_{<\alpha,\beta>} \left( e^{i(k-d_{\alpha,\beta})} T_{\alpha,\beta} a_\alpha^\dagger a_\beta + h.c. \right) 
+ \sum_k \sum_{<\alpha,\beta>} \left( e^{i(k-d_{\alpha,\beta})} W_{\alpha,\beta} a_\alpha^\dagger a_\beta + h.c. \right) 
+ \sum_{k,k'} \sum_{R_{\alpha}} \left( e^{i((k-k')\cdot R_{\alpha})} V_{R_{\alpha}} a_\alpha^\dagger a_{k'} + h.c. \right), \quad (3) \]

where \( R \) is position of a cell and \( \alpha \) carries orbital and sublattice index. \( d_{\alpha,\beta} \) is the NN or NNN vector between NN or NNN orbitals \( \alpha, \beta \), and only the confining potential \( V_{R_{\alpha}} \) mixes the \( k \)-states\(^ {21} \).

We diagonalize Eq. (3) to obtain valley specific quantum dot states \( p, \sigma \). In the second quantization the many-body Hamiltonian in the basis of SP QD states \( p, \sigma \) reads:

\[ H = \sum_{p\sigma} \epsilon_{p\sigma} c_{p\sigma}^\dagger c_{p\sigma} + \frac{\eta}{2} \sum_{pq\sigma \sigma'} \langle pq | V | st \rangle c_{p\sigma}^\dagger c_{q\sigma'}^\dagger c_{s\sigma'} c_{t\sigma}, \quad (4) \]

where in the first term \( \epsilon_{p\sigma} \) are energies of the SP HO states \( p \) and the second terms includes Coulomb scattering between these states, with \( \eta \) controlling the strength of the interactions. We express the Coulomb matrix elements \( \langle pq | V | st \rangle \) in Eq. (4) in the basis of atomic orbitals as \( \langle pq | V | st \rangle = \sum_{ijkl} A_{pq}^{ij} A_{st}^{kl} \langle ij | V | kl \rangle \), where \( A \) are solutions to the SP Hamiltonian in Eq. (2) and Eq. (3). We include only onsite short-range integrals \( \langle ii | V | ii \rangle \) and the long-range part is taken as a classical Coulomb term. The Coulomb integrals are calculated using Coulomb potential with Keldysh screening, using the 2D Fourier transform, as\(^ {37} \)

\[ V_{K}^{2D}(r-r') = \frac{1}{e^{2}} \int_{-\infty}^{\infty} \frac{1}{|k|} |e^{i(k\cdot(r-r'))}| d^2 k, \quad (5) \]

where \( e^{2} = 2.2 \text{Å} \) is the 2D polarisability and we take \( e^{2} = 2.5 \).

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