Inner and outer ring states of MoS ₂ quantum rings: Energy spectrum, charge and spin currents

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ABSTRACT

We investigate the energy levels and persistent currents of MoS_2 quantum rings having different shapes and edge types in the presence of a perpendicular magnetic field by means of the tight-binding approach. We find states localized at the inner and outer boundaries of the ring. These energy levels exhibit different magnetic field dependences for the inner and outer ring states due to their different localization properties. They both exhibit the usual Aharanov–Bohm oscillations but with different oscillation periods. In the presence of spin–orbit coupling, we show distinct spin and charge persistent currents for inner and outer ring states. We find well-defined spin currents with negligibly small charge currents. This is because the local currents of spin-up and -down states flow in opposite directions.

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I. INTRODUCTION

Monolayer transition metal dichalcogenides (TMDs) are newly emerged members of the 2D crystal family.¹ These TMD monolayers exhibit fascinating physical properties resulting from their reduced dimensionality and crystal symmetry and provide excellent platforms for fundamental studies of novel 2D material systems. TMD monolayers have the combined properties of excellent electrostatic control, large direct bandgap, and high carrier mobility making them well suited for low power electronics and optoelectronic applications.²⁻⁴ Moreover, electrons and holes in TMD monolayers have coupled spin and valley degrees of freedom and, in this context, TMD monolayers are particularly suitable for studying spin and valley related physics such as spin and valley Hall effect. In addition, strong light-matter interaction in TMD monolayers provides a unique optical means to manipulate the spin- and valley-dependent properties. These results suggest that TMD monolayers could also be promising for integrated spintronic and valleytronic applications.⁵

Quantum confinement effects occurring in low-dimensional systems lead to strong modifications of the electronic, optical, and transport properties when compared with conventional bulk systems. Quantum dots (QDs) are an important class of low-dimensional systems. QDs are also sometimes referred to as artificial atoms,¹¹ having discrete electronic states, similar to real atoms or molecules. To date, QDs in novel 2D materials, such as graphene,¹²⁻¹⁶ phosphorene monolayer and bilayer,¹⁷⁻²¹ and TMD monolayers,²²⁻²⁵ are actively studied.

Recently, quantum rings (QRs) have also been fabricated from 2D materials, which display unique electronic properties different from QDs. For example, the Aharanov–Bohm (AB) effect was observed in graphene quantum rings $(GQRs)^{26-29}$ and predicted for phosphorene quantum rings (PQRs).^{19,30} The necessary condition to observe the AB oscillations is that the phase coherence length of carriers in these QRs is larger than the ring circumference. Another striking property of quantum rings is the persistent current, which can be driven by an external magnetic flux.³¹ In GQRs, the states localized at the inner edge exhibit different behaviors as a function of the magnetic flux threading the ring when compared to those localized at the outer edges.²⁹ More recently, monolayer MoS₂ QRs have gained increased interest. Oliveira *et al.* used a two-band model³² to investigate monolayer MoS₂ QRs.^{33,34} They found that the valley Zeeman energy in

monolayer MoS₂ QRs exhibits an oscillatory dependence on the magnetic flux Φ with a possible vanishing valley Zeeman effect even for nonzero magnetic flux, and the valley Zeeman energy can be tuned by either magnetic flux or ring confinement or both of them.³³ In addition, the magneto-optical absorption spectrum undergoes a transition from the AB-like quantum interference to aperiodic oscillation with changing magnetic field.³⁴ Experimentally, there are several strategies for the preparation of MoS₂ QDs, such as lithium intercalation,³⁵ liquid exfoliation in organic solvents,³⁶ hydrothermal synthesis,³⁷ electrochemical etching,³⁸ electro-Fenton reaction processing,³⁹ and grinding exfoliation.⁴⁰

In this paper, we investigate the electronic properties of MoS₂ QRs with different shapes and edge types in the presence of a perpendicular magnetic field by means of the tight-binding (TB) approach. We find localized states (localized at the inner and outer boundaries of the ring) that are mainly induced by the d orbitals of the Mo atoms (the p orbitals of the S atoms contribute little). The energy levels of the inner and outer ring states show different magnetic field dependence due to their different localization properties. They both exhibit the usual AB oscillations but with different oscillation periods. In the presence of spin-orbit coupling (SOC), which is typically strong in TMD monolayers, we show spin and charge persistent currents of the inner and outer ring states in MoS2 QRs. We find well-defined spin currents with negligibly small charge currents. This is because the local currents of spin-up and spin-down states flow in the opposite directions.

This paper is organized as follows. In Sec. II, we present the TB Hamiltonian of MoS_2 quantum rings in the presence of a perpendicular magnetic field. In Sec. III, we present and discuss the energy levels and the persistent currents of the inner and outer ring states in the absence/presence of SOC. Finally, we conclude with a summary in Sec. IV.

II. MODEL AND THEORY

The electronic properties of a monolayer MoS₂ can be described using various multiband Slater–Koster tight binding schemes derived from first-principle calculations.^{41–45} The most comprehensive model involves 11 bands corresponding to the *d* orbitals of Mo atom and the *p* orbitals of the S atom. By performing an appropriate unitary transformation, the *p* orbitals of the top and bottom S atoms can be cast into symmetric and antisymmetric combinations with respect to the z axis. Therefore, the 11-band model can be decoupled in six bands with even symmetry with respect to $z \rightarrow -z$ inversion and five bands with odd symmetry.⁴⁴ Low-energy excitation bands belong exclusively to the first block, so that we can restrict ourselves to the six bands model. In this model, we have the reduced Hilbert space with general wave function

$$\psi = (d_{3z^2 - r^2}, d_{x^2 - y^2}, d_{xy}, p_x^S, p_y^S, p_z^A),$$
(1)

where $p_i^S = 1/\sqrt{2}(p_i^t + p_i^b)$ and $p_i^A = 1/\sqrt{2}(p_i^t - p_i^b)$, and t and b refer to the top and bottom S layers, respectively. The tight-

binding Hamiltonian of monolayer MoS₂ can be written as^{46,47}

$$H = \sum_{i,\mu} \varepsilon^{M}_{i,\mu} c^{\dagger}_{i,\mu} c_{i,\mu} + \varepsilon^{S}_{i,\mu} b^{\dagger}_{i,\mu} b_{i,\mu}$$
$$+ \sum_{\langle \langle ij \rangle \rangle \mu \nu} (t^{MM}_{ij,\mu\nu} e^{i\phi_{ij}} c^{\dagger}_{i,\mu} c_{j,\nu} + t^{SS}_{ij,\mu\nu} e^{i\phi_{ij}} b^{\dagger}_{i,\mu} b_{j,\nu})$$
$$+ \sum_{\langle ij \rangle \mu \nu} t^{MS}_{ij,\mu\nu} e^{i\phi_{ij}} c^{\dagger}_{i,\mu} b_{j,\nu} + H.c., \qquad (2)$$

where i, j and μ, ν run over the lattice sites and atomic orbits, respectively. $c_{i,\mu}^{\dagger}$ and $c_{i,\mu}$ ($b_{i,\mu}^{\dagger}$ and $b_{i,\mu}$) are the creation and annihilation operators for Mo(S) atoms. The on-site energies of Mo and S atoms are given by

$$\boldsymbol{\varepsilon}_{i}^{M} = \begin{bmatrix} \Delta_{0} & 0 & 0\\ 0 & \Delta_{2} & -is\lambda_{M}\\ 0 & is\lambda_{M} & \Delta_{2} \end{bmatrix}$$
(3)

and

$$\boldsymbol{\varepsilon}_{i}^{S} = \begin{bmatrix} \Delta_{p} + t_{xx}^{\perp} & -\frac{i}{2}s\lambda_{S} & 0\\ -\frac{i}{2}s\lambda_{S} & \Delta_{p} + t_{yy}^{\perp} & 0\\ 0 & 0 & \Delta_{z} - t_{zz}^{\perp} \end{bmatrix},$$
(4)

where $\lambda_M = 0.075 \text{ eV}$ and $\lambda_S = 0.052 \text{ eV}$ represent the strength of the spin-orbit interactions for Mo and S,⁴⁸ respectively. The other parameters are given in Table I. Since all the hopping terms $t_{ij,\mu\nu}^{MM}$, $t_{ij,\mu\nu}^{SS}$, and $t_{ij,\mu\nu}^{MS}$ within a Slater–Koster tight-binding model are given in Ref. 44, we will not repeat them here.

The perpendicular applied magnetic field is included by Peierls substitution by adding $e^{i\phi_{ij}}$ to the hopping terms, where $\phi_{ij} = \frac{2\pi e}{h} \int_{\mathbf{r}_i}^{\mathbf{r}_j} \mathbf{A} \cdot d\mathbf{l}$, where *h* is Planck's constant and **A** is the vector potential induced by the magnetic field **B**. We use the Landau gauge with the vector potential $\mathbf{A} = (0, Bx, 0)$. The magnetic flux threading the ring is defined as $\Phi = BS$ in units of the flux quantum $\Phi_0 = h/e$, where *S* is the area enclosed by the outer edges of the monolayer MoS₂ QRs.

The energy levels and wave functions of monolayer MoS_2 QRs subjected to a perpendicular magnetic field are obtained by solving the TB model. All numerical TB calculations are performed using the recently developed <code>PyBINDING⁴⁹</code> and <code>KWANT⁵⁰</code> packages. In electronic density of states (DOSs), we add a Gaussian broadening to

TABLE I. The parameters in units of eV of the Slater–Koster tight-binding parameters from the first-principle calculation band structure of monolayer MoS_2 .

Symbol	Value	Symbol	Value
$\Delta_0 \Delta_p \Delta_M t_{\pm}^{\pm}$	-1.094 -3.560 0.075 -0.467	$\Delta_2 \ \Delta_z \ \lambda_S \ t_z^+$	-1.512 -6.886 0.052 1.225
		~~	

the discrete energy levels E_n which gives

$$DOS(E) = \frac{1}{\sqrt{2\pi\Gamma^2}} \sum_{n} \exp\left[-\frac{(E-E_n)^2}{2\Gamma^2}\right],$$
 (5)

where Γ is the broadening. The local current flowing from site *i* to site *j* for eigenfunction *n* is defined as

$$\boldsymbol{I}_{ij}^{n} = 2Im[(\boldsymbol{\Psi}_{i}^{n})^{\dagger}\boldsymbol{H}_{ij}\boldsymbol{\Psi}_{j}^{n}]\boldsymbol{d}_{ij}, \qquad (6)$$

where Ψ_i^n is the *n*th wave function on site *i*, H_{ij} is the Hamiltonian element between *i*th and *j*th atoms, and \mathbf{d}_{ij} is a unit vector between the two neighboring atoms.

III. RESULTS AND DISCUSSIONS

In this paper, we consider triangle zigzag QRs (TZQRs), hexagonal zigzag QRs (HZQRs), and hexagonal armchair QRs (HAQRs). We use the number of atoms along each side N_{out} and N_{in} (as shown in Fig. 1) to describe the size of QRs.

A. Triangular quantum rings

First, for simplicity, we consider the spinless model first, and the SOC is omitted, i.e., $\lambda_M = 0$ and $\lambda_S = 0$. We calculate the DOS of MoS₂ triangle zigzag quantum dot (TZQD) and triangle zigzag quantum ring (TZQR) which are shown in Fig. 2. As can be seen from Fig. 2, the DOS of TZQR is larger than the DOS of TZQD in the gap region (green box), which is dominated by the edge states. However, the DOS of TZQR is smaller than the one of TZQD in valance band and conduction band, which is dominated by the bulk states. The enhanced confinement effect in the TZQR due to the presence of the antidot gives additional edge states, including inner edge states and outer edge states. In addition, the number of bulk states is smaller due to the presence of the antidot. In order to investigate the behavior of the inner edge states and the outer edge states, we calculate the energy spectrum of TZQR in the presence of a magnetic field which is shown in Fig. 3(a). Most of the edge states in TZQR show threefold oscillating behavior in the presence of the magnetic field due to these edge states which are distributed



FIG. 1. Schematics of monolayer MoS_2 QRs. Blue (orange) dots indicate Mo (S) atoms. $N_{out}(N_{in})$ is the number of atoms along the outer (inner) side. (a) Triangle zigzag quantum ring (TZQR) and (b) hexagonal armchair quantum ring (HAQR).



FIG. 2. DOS of the TZQD and TZQR in the absence of magnetic field using a broadening of $\Gamma = 0.05 \text{ eV}$. The insets are the corresponding model of TZQD ($N_{\text{out}} = 21$) and TZQR ($N_{\text{out}} = 21$, $N_{\text{in}} = 9$).

over the whole edge and are called ring states.⁵¹ However, there are two kinds of oscillations of ring states [marked by 1 and 2 in Fig. 3(a)] having different oscillating periods. The corresponding probability densities in Fig. 3(b) show that the state with smaller period (marked by 1) is the outer ring state, and the state with larger period (marked by 2) corresponds to the inner ring state. Figure 3(c) shows the local currents due to the inner and outer ring states. When electrons are moving along a closed path in the presence of a magnetic field, there is a change in the phase of the electron,

$$\Delta \Phi = \frac{e}{\hbar} \oint \mathbf{A} \cdot d\mathbf{l}.$$

Using the Stokes theorem, the phase change when encircling a close path with surface area S becomes $\Delta \Phi = 2\pi \Phi/\Phi_0$ with $\Phi = BS$ the flux through this surface. Because of the difference in the enclosed surface area between the inner ring and the outer ring, the period of oscillations will be very different. Hence, the period of oscillation of inner ring states is larger than the period of outer ring states. Figure 3(b) shows that the outer ring states should be more delocalized than the inner ring states. Hence, the outer ring states should be more affected by the magnetic field. For a perfect metal ring of zero width, we have $E_i(\Phi) \propto (l - \Phi/\Phi_0)^2$, and the oscillating period is Φ_0 , where *l* is the angular quantum number, which is an integer number. However, the quantum number l is not a good quantum number for our triangular MoS₂ QRs. The coupling between states can change the period of oscillation. Herein, the oscillating period is not Φ_0 . Moreover, the magnitude of local currents in outer ring states is larger than that of inner ring states. The reason is that the atoms at the outer edge are Mo, and the atoms at the inner edge are S. Figure 3(b) shows that the probability densities are distributed mainly over Mo atoms. The edge atoms are S atoms for the inner edge, and the corresponding probability densities are small. From Eq. (5), we see that the local currents are related to the hopping Hamiltonian H_{ij} . Therefore, the electrons can hop from S



FIG. 3. (a) Energy spectrum of a TZQR ($N_{out} = 21$, $N_{in} = 9$) as a function of magnetic field. (b) The corresponding probability densities of states marked in (a) with $\Phi = 0$. (c) The corresponding local currents of the states marked in (a) for $\Phi = 0$. The arrows indicate the directions of local currents.

atoms to Mo atoms and form local currents at the inner edge. The behavior in monolayer MoS₂ QRs is different from graphene rings⁵² and phosphorene rings,¹⁹ where the edge states cannot be distributed over the whole edge.

B. Hexagonal quantum rings

We now turn our attention to MoS₂ hexagonal QRs with different edges, i.e., hexagonal zigzag QRs (HZQRs) and hexagonal armchair QRs (HAQRs). Two kinds of oscillating behavior also emerge in both HZQRs and HAQRs, such as the states which are marked by 1 and 2 in HZQR and the states marked by 3 and 4 in HAQR in Figs. 4(c) and 4(d), respectively. The corresponding probability densities of these states are given in Fig. 4(e). The oscillating periods of inner ring states are also large than the outer ring states due to different path lengths. Comparing 1 and 2 with 3 and 4 in Fig. 4(e), the ring states are distributed more uniformly over the edge in HAQR. In Figs. 4(a) and 4(b), we see that the chemical composition of every edge in HAQR is the same. However, the edge consisting of S atoms and the edge consisting of Mo atoms appear alternately in HZQR. As discussed above, the probability densities are mainly distributed over the Mo atoms. Therefore, probability densities are different in HZQRs and HAQRs. However, the local currents exhibit tiny differences in HAQRs and HZQRs due to the fact that the electrons can jump between neighboring atoms. Circle-like paths emerge in both HZQRs and HAQRs, which lead to the oscillating behavior of the value of energy levels. The number of Mo atoms and S atoms at the edge in both HZQR and HAQR are equal; therefore, the local currents in HZQRs and HAQRs are similar.

C. Spin-orbit coupling

Next, we examine the effect of the spin-orbit coupling (SOC). The strength of SOC is characterized by the parameters

 $\lambda_M = 0.075 \text{ eV}$ for Mo and $\lambda_S = 0.052 \text{ eV}$ for S. In Fig. 5(a), we found that both inner ring states and outer ring states are split into two levels due to the presence of SOC. However, the oscillating behavior(including oscillating period, phase, and amplitude) is not significantly affected by the presence of SOC. Figures 5(b) and 5(d) give the probability densities of inner states [yellow box in Fig. 5(a)] and outer states [green box in Fig. 5(a)] with spin up and spin down. Compared with Fig. 3(b), the inner and outer ring states are robust in the presence of SOC. As can be seen in Figs. 5(a)–5(e), the probability densities of the inner and outer ring states are the same for spin up and spin down, and thus, the magnitudes of the local currents of the spin up and spin down states are also the same, but the directions of the local currents of the spin up and spin down states are opposite.

The persistent current in quantum rings is dictated by the magnetic flux. In such QRs, the persistent current at zero temperature can be evaluated by taking the derivative of the ground-state energy with respect to the magnetic flux, i.e.,

$$I_{\sigma} = -\frac{\partial E}{\partial \Phi} = -\sum_{n} \frac{\partial E_{n\sigma}}{\partial \Phi},$$

where $E_{n\sigma}$ is the energy of state *n* below the fermi energy and σ represents the spin. The charge current is $I_c = I_{\uparrow} + I_{\downarrow}$, and the spin current is given by $I_s = I_{\uparrow} - I_{\downarrow}$. In Fig. 6, we show the persistent currents in TZQR with SOC. Both the I_{\uparrow} and I_{\downarrow} oscillate with magnetic flux Φ due to the oscillating behavior of the energy levels. However, there is half period phase shift between I_{\uparrow} and I_{\downarrow} , i.e., I_{\uparrow} and I_{\downarrow} move in the opposite directions. This behavior is also shown in Fig. 5 for the local currents. Figure 6(b) shows that the spin current is much larger than the charge current. Therefore, pure spin current can be realized by tuning the magnetic flux. It indicates that the monolayer MoS₂ QRs can be used to act as a



FIG. 4. (a) HZQR with $N_{out} = 7$ and $N_{in} = 5$. (b) HAQR with $N_{out} = 13$ and $N_{in} = 7$. (c) The corresponding energy spectrum of (a) as a function of magnetic field. (d) The corresponding magnetic field dependent energy spectrum of (b). (e) The corresponding probability densities of the states marked by numbers in (c) and (d) in the absence of magnetic field. (f) The corresponding local currents of the states in (e).



FIG. 5. (a) The energy levels of TZQR ($N_{out} = 21$, $N_{in} = 9$) with SOC. (b) The corresponding probability densities of the inner ring states marked by yellow box in (a) for $\Phi = 0$. (c) The corresponding local currents of the inner ring states marked by yellow box in (a) for $\Phi = 0$. (d) The corresponding probability densities of the outer ring states marked by green box in (a) for $\Phi = 0$. (e) The corresponding local currents of the outer ring states marked by green box in (a) for $\Phi = 0$.



FIG. 6. The persistent current of TZQR ($N_{out} = 21$, $N_{in} = 9$) with SOC, and the fermi energy $E_F = 0.32 \,\text{eV}$. $I_0=eV/\Phi_0$ is set as the unit for current. (a) The persistent current with spin up and spin down. (b) The corresponding charge current and spin current. (c) The spin current and charge current caused by the inner ring states. (d) The spin current and charge current caused by the outer ring states.

spin-splitter. Figures 6(c) and 6(d) give the contributions from inner and outer ring states, respectively. Both the charge and spin current caused by inner ring states show fluctuations, but the oscillations are less periodic and notice that the magnitude of the spin current is similar to that of the charge current. The spin and charge currents of outer ring states also exhibit oscillations; however, the magnitude of the spin current is much larger than that of the charge current. In addition, the spin current caused by the outer ring states is larger than that of the inner ring states. The magnitude of charge current caused by the inner ring states is similar to that of outer ring states, but they move in opposite direction. Therefore, the total charge current is very small. From Fig. 5(a), we can find that the number of inner ring states is small, and some inner ring states couple with the outer ring states. The coupling between inner ring states and outer ring states has a great influence on the persistent current of the inner ring states. However, it has faint influence on the persistent current of the outer ring states.

IV. SUMMARY

We investigated the electronic properties of monolayer MoS₂ QRs with different shapes and edge types in the presence of a perpendicular magnetic field. The TB approach is used to calculate the energy levels and the electron probability density. We found localized states at the inner and outer edges of the quantum ring. When compared to edge states in graphene and phosphorene QRs, edge states in monolayer MoS_2 QRs are predominantly induced by the d orbitals of Mo atoms and distributed almost over the entire ring boundaries. Both inner and outer ring states exhibit the usual AB oscillations but with different oscillation periods due to the different encircled surface areas. The influence of the ring shape and its edge type on the inner and outer ring states was also investigated. In the presence of SOC, which is typically strong in monolayer MoS₂, distinct spin and charge persistent currents of the inner and outer ring states are found. We found well-defined spin currents with negligibly small charge currents at the outer edge. This is because the local currents of spin-up and spin-down states flow in the opposite directions.

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