Topological Wannier excitons in Bi_2Se_3 nanosheets

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Abstract. We analyze the bulk Wannier excitons in nanosheets of the topological insulator Bi_2Se_3 and find that excitons inherit the topology of the electronic bands. The excitonic spectrum is strongly indirect due to the band inversion of the underlying single-particle model. We predict that the *s*-wave and *d*-wave states of two exciton families are selectively bright under left- or right-circularly polarized light. We furthermore show that every *s*-wave exciton state consists of a quartet with a degenerate and quadratically dispersing nonchiral doublet, and a chiral doublet with one nonanalytic linear mode. Finally, we demonstrate the existence of topological edge states of chiral excitons arising from the bulk-boundary correspondence.

The exciton problem

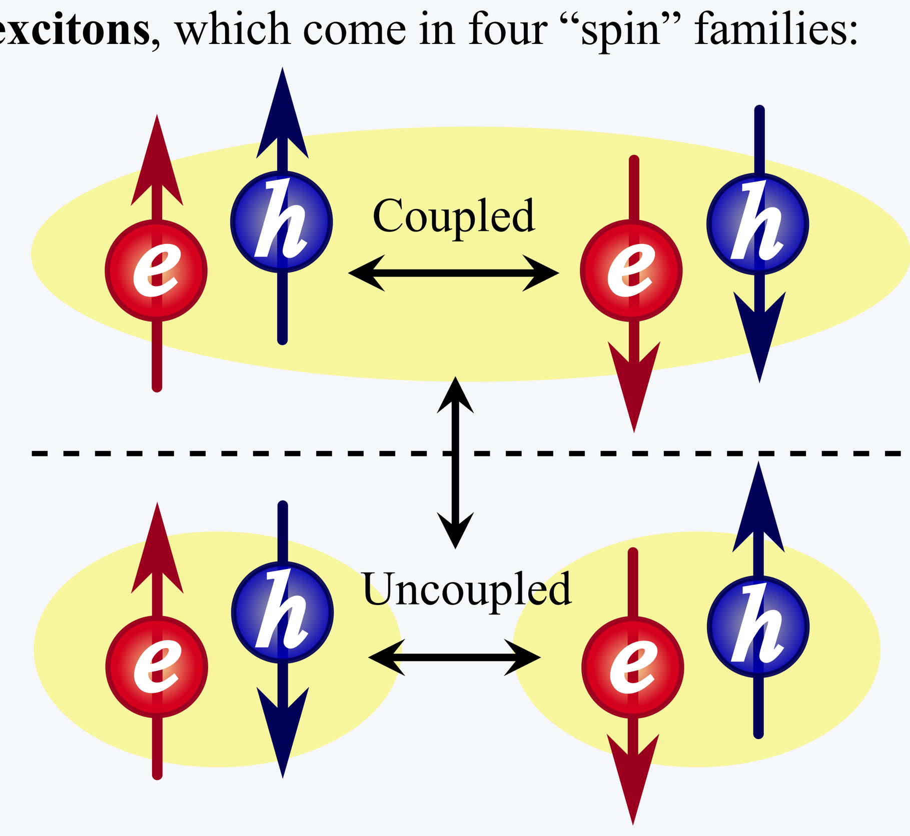
Single electrons and holes are described by a BHZ Hamiltonian:

$$H(\boldsymbol{k}) = \epsilon_0(\boldsymbol{k}) + \mathcal{M}(\boldsymbol{k})\,\tau_z + A_2\,(k_x s_x + k_y s_y)\,\tau_x\,,$$

s : spin
τ : orbital

where $\mathcal{M}(\boldsymbol{k}) = M - B_2\,(k_x^2 + k_y^2)$ and a **topological phase** exists for $M B_2 > 0$.

Adding the Coulomb interaction, we can form bound electron hole pairs or **excitons**, which come in four "spin" families:



A repulsive **exchange interaction** couples two of these families together for nonzero total exciton momentum.

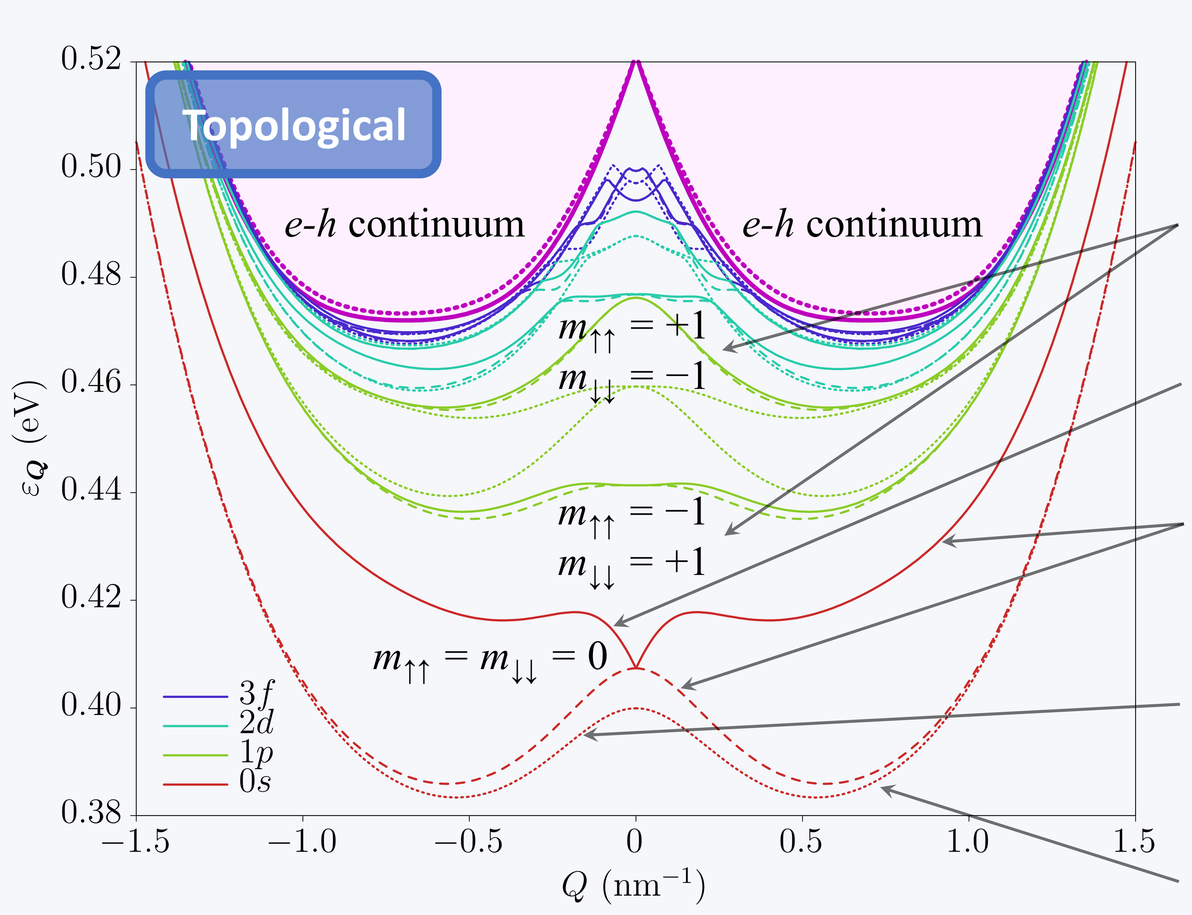
Fig. 1. Exciton families that generalize the singlet and triplet states of normal semiconductors. In Bi_2Se_3 nanosheets the relevant degree of freedom the so-called *spin-orbit parity*. It is analogous to the spin degree of freedom, and we can still talk about "up" and "down" states.

In Ref. [1], we analyze the bound exciton states with total momentum $\boldsymbol{Q}$:

- Dispersion and wave functions
- Optical selection rules
- **What effects does the topology have?**

Exciton dispersion relation

The exciton band structure strongly depends on whether the single-particle Hamiltonian is in the **topological regime** (top) or in the **trivial regime** (bottom):



Nonhydrogenic **splitting** between opposite angular momenta

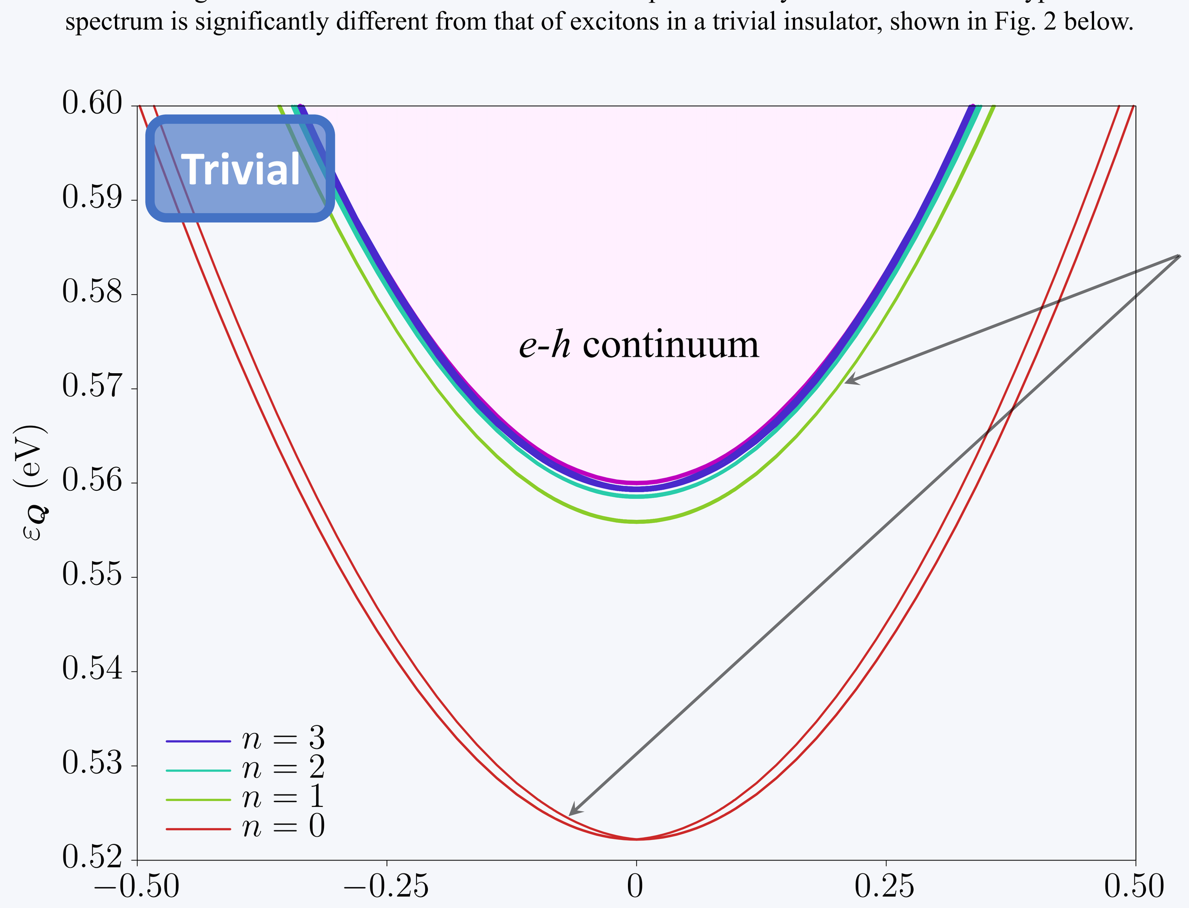
Linear mode

Coupled $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ states

Uncoupled $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ states (degenerate)

Indirect dispersion (long radiative lifetimes)

Fig. 2. Exciton energy levels as a function of the total exciton momentum $\boldsymbol{Q}$ in the topological insulator regime. The four exciton families are represented by the different line types. The spectrum is significantly different from that of excitons in a trivial insulator, shown in Fig. 2 below.



Each level n contains angular momenta $m \in \{-n, \ldots, 0, \ldots, n\}$

At $\boldsymbol{Q} = \boldsymbol{0}$ we recover the 2D Rydberg series

$$\varepsilon_n \propto (n + 1/2)^{-1}$$

with degeneracies

$$g_n = 4 \times (2n + 1)$$

(4 pseudospin families!)

Fig. 3. Exciton energy levels in the trivial insulator regime.

Optical selection rules

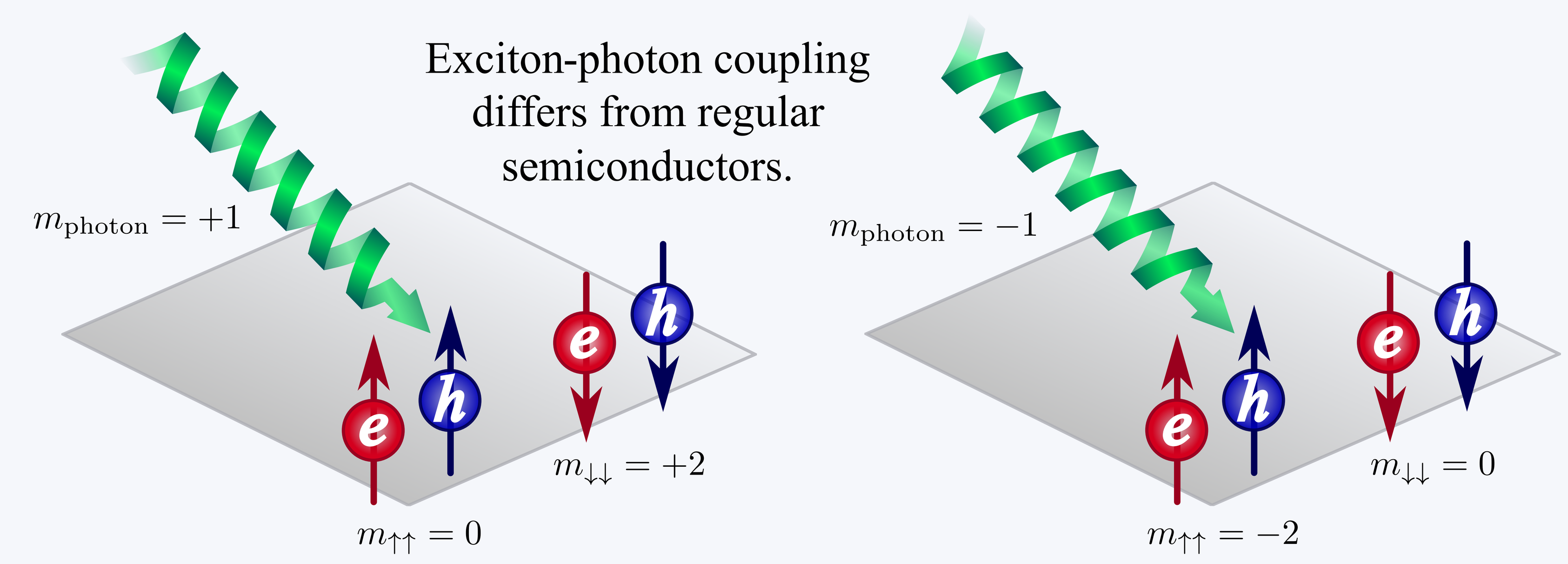


Fig. 4. Optical selection rules under circularly polarized light. The $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ *s*-wave and *d*-wave states selectively couple to left- or right-circular photons in a time-reversal-symmetric fashion. By contrast, all $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ states are dark.

Effects of the topology

The **Berry curvature** $\boldsymbol{\Omega}(\boldsymbol{k})$ gives an anomalous contribution to the velocity [2]:

$$\boldsymbol{v}_\alpha(\boldsymbol{k}) = \boldsymbol{\nabla}_{\boldsymbol{k}}\,\varepsilon_\alpha(\boldsymbol{k}) - q\boldsymbol{E} \times \boldsymbol{\Omega}_\alpha(\boldsymbol{k})$$

$$(\text{with } \boldsymbol{\Omega}_\alpha(\boldsymbol{k}) = i\,\langle \boldsymbol{\nabla} u_\alpha | \times | \boldsymbol{\nabla} u_\alpha \rangle)$$

This acts as a **momentum-space magnetic field** that splits the states with angular momenta m and $-m$.

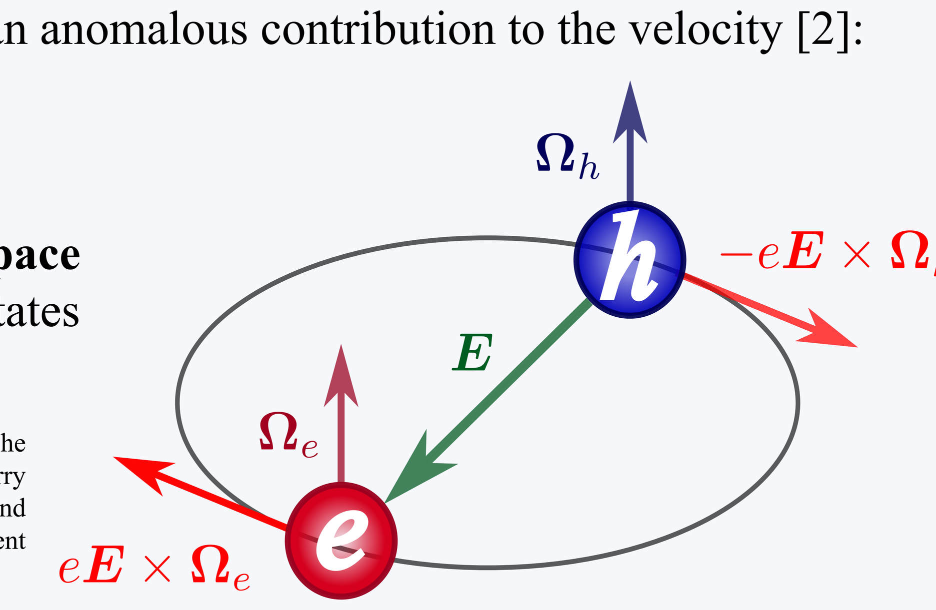
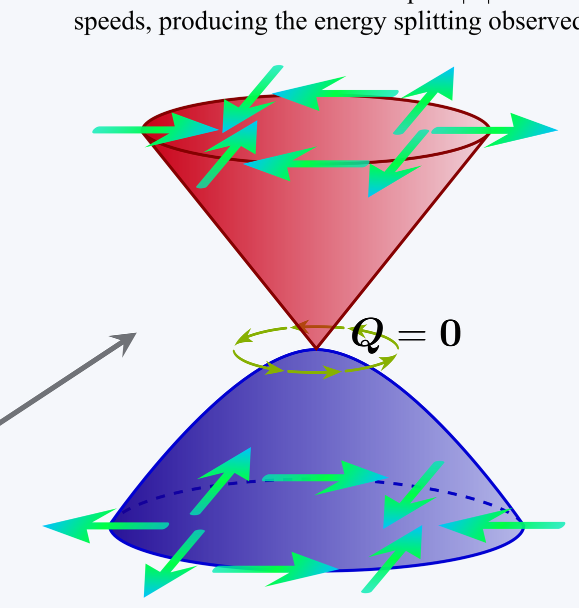


Fig. 5. Effect of the Berry curvature on an exciton state. The electric field between both particles couples to the Berry curvature giving an anomalous velocity. Thus, clockwise and counterclockwise states of equal $|m|$ will rotate at different speeds, producing the energy splitting observed in Fig. 2.

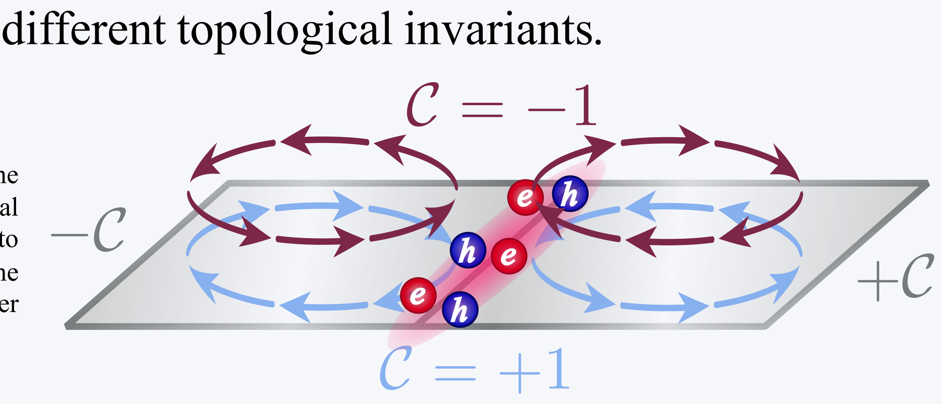


When m is even, we identify a **pseudospin vector** that **winds** twice around itself as one circles around the origin of the total exciton momentum. The winding direction is opposite for the upper and lower eigenstates of each doublet. Thus, they have **chirality** +2 and −2, respectively.

Fig. 6. Pseudospin winding around the origin of $\boldsymbol{Q}$ for the *s*-wave ground state of the coupled exciton pair. This winding is the origin of the chirality of these excitonic states.

The **effective Hamiltonian** 2×2 for the *s*-wave ground state is topological when time-reversal symmetry is broken. We obtain **chiral exciton boundary states** at the interface of two regions with different topological invariants.

Fig. 7. Chiral boundary modes of excitons localized at the interface between two regions with opposite topological invariants $\mathcal{C}$ (right) and $-\mathcal{C}$ (left). These states arise due to the **bulk-boundary correspondence**. Depending on the sign of $\mathcal{C}$, the excitons flow in one direction or the other along this boundary.



Summary and outlook

- Excitonic spectra are strongly dependent on the topological character of Bi_2Se_3.
- The Berry curvature has observable effects on the exciton bands.
- Optical selection rules differ from those in normal semiconductors.
- Topological exciton states are chiral and can give rise to boundary modes.
- Bulk excitons can couple to plasmons on the surfaces of the nanosheet.
- The topological character of excitons may be preserved in their recombination.

References

[1] L. Maisel Licerán et al. *arXiv* 2102.06781
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Acknowledgments

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