Hofstadter butterfly in transistion metal dichalcogenide monolayers

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Overview

Group VI-B Transition Metal Dichalcogenides (TMD) are compound semiconductors of the type MX_2

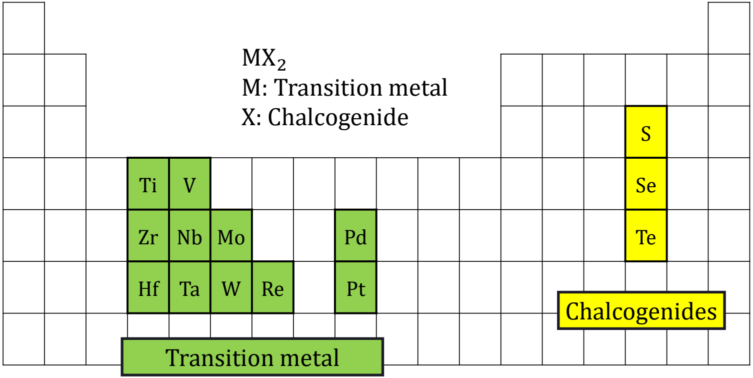


Figure: Transition metal dichalcogenides compound.

Transition Metal Dichalcogenides Monolayers

- One M layer sandwiched by two X layers as show in top view (a) and side view (b).
- Crystal structure has no central inversion symmetry.
- The symmetry of the lattice results in the hexagon Brillouin Zone (BZ).

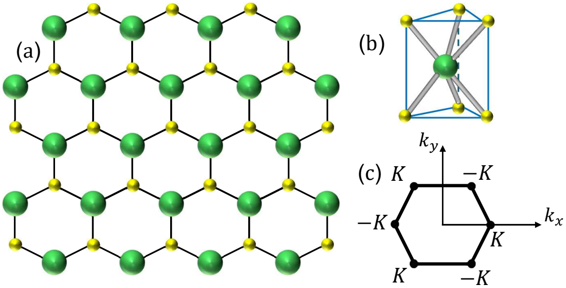


Figure: Structure and Brillouin Zone of Monolayer TMD, redrawing from[1].

[1] Liu et al., "Three-band tight-binding model for monolayers of group-VIB transition metal dichalcogenides".

Transition Metal Dichalcogenides Monolayers

Properties

- Both mono-layer and few-layers remain stable at room temperature.
- TMD monolayer has the visible band gap in the ban structure, which can be used in creating the transistor devices[2].
- Strong spin-orbit coupling (SOC) in TMD monolayers lead to spin splitting of hundres meV.

$\Rightarrow$ Promising material in electronic and optoelectronic applications.

[2] Radisavljevic et al., "Single-layer MoS2 transistors"

Three-band tigh-binding model without magnetic field

Time-independent Schrödinger equation for an electron in the crystal

$$\left[-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m}+U_0(\mathbf{r})\right]|\psi_{\lambda,\mathbf{k}}(\mathbf{r})\rangle=\epsilon_{\lambda,\mathbf{k}}\,|\psi_{\lambda,\mathbf{k}}(\mathbf{r})\rangle\,. \tag{1}$$

Tight-binding (TB) wave function

$$|\psi_{\lambda,\mathbf{k}}(\mathbf{r})\rangle=\sum_j C_j^{\lambda}(\mathbf{k})\sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}}\,|\phi_j(\mathbf{r}-\mathbf{R})\rangle\,. \tag{2}$$

The basis consists of three d-orbitals of the M atom:

$$|\phi_1\rangle=|d_{z^2}\rangle\,,|\phi_2\rangle=|d_{xy}\rangle\,,|\phi_3\rangle=\left|d_{x^2-y^2}\right\rangle\,. \tag{3}$$

The coeffcents $C_j^{\lambda}(\mathbf{k})$ are the solutions of the eigenvalue equation

$$\sum_{jj'}^{3}\left[H_{jj'}^{\mathsf{TB}}(\mathbf{k})-\varepsilon_{\lambda}(\mathbf{k})S_{jj'}(\mathbf{k})\right]C_j^{\lambda}(\mathbf{k})=0. \tag{4}$$

Three-band tigh-binding model without magnetic field

Overlap matrix elements

$$S_{jj'}(\mathbf{k}) = \sum_{\mathbf{R}} \left\langle \phi_j(\mathbf{r}) \middle| \phi_{j'}(\mathbf{r} - \mathbf{R}) \right\rangle \approx \delta_{jj'}. \quad (5)$$

TB Hamiltonian matrix elements

$$H^{\text{TB}}_{jj'}(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \phi_j(\mathbf{r}) \right| \left[-\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} + U_0(\mathbf{r}) \right] \left| \phi_{j'}(\mathbf{r} - \mathbf{R}) \right\rangle. \quad (6)$$

Three-band tigh-binding model without magnetic field

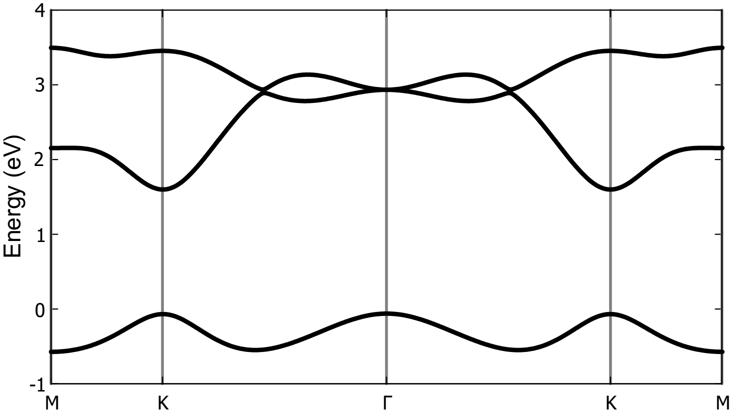


Figure: Band structure of MoS_2 monolayer[3].

[3] Liu et al., "Three-band tight-binding model for monolayers of group-VIB transition metal dichalcogenides".

Three-band tigh-binding model under a magnetic field

TB Hamiltonian matrix elements change to

$$H = \frac{(-i\hbar\boldsymbol{\nabla} + e\mathbf{A}(\mathbf{r}))^2}{2m} + U_0(\mathbf{r}) + g^*\mu_B\mathbf{B}\cdot\mathbf{L}, \tag{7}$$

It is possible to add a phase factor to the basis functions

$$\psi_{\lambda,\mathbf{k}}(\mathbf{r}) = \sum_{j=1}^{3} C_j^{\lambda}(\mathbf{k}) \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} e^{i\theta_{\mathbf{R}}(\mathbf{r})}\phi_j(\mathbf{r}-\mathbf{R}). \tag{8}$$

By choosing $\theta_{\mathbf{R}} = -\frac{e}{\hbar}\int_{\mathbf{R}}^{\mathbf{r}} \mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'$ as Peierls substitution, the Hamiltonian matrix elements as the form

$$\begin{aligned} H_{jj'}^{\text{TB}}(\mathbf{k}) &= \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} e^{\frac{ie}{\hbar}\int_{\mathbf{0}}^{\mathbf{R}}\mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'} \left\langle \phi_j(\mathbf{r}) \right| \left[-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + U_0(\mathbf{r}) \right] \left| \phi_{j'}(\mathbf{r}-\mathbf{R}) \right\rangle \\ &+ g^*\mu_B\mathbf{B}\cdot\sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}+\frac{ie}{\hbar}\int_{\mathbf{0}}^{\mathbf{R}}\mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'} \left\langle \phi_j(\mathbf{r}) \right| \mathbf{L} \left| \phi_{j'}(\mathbf{r}-\mathbf{R}) \right\rangle . \end{aligned} \tag{9}$$

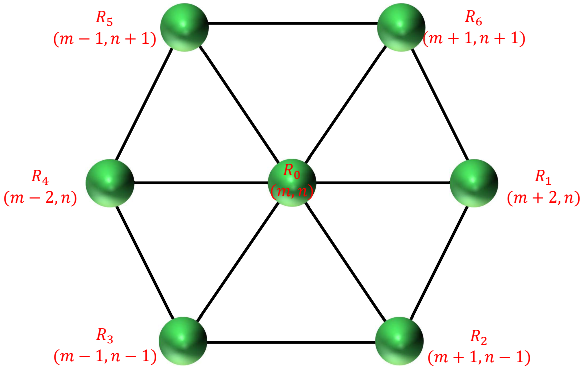


Figure: The TB model of TMDC with six neighbors atom M.

Three-band tigh-binding model under a magnetic field

The Eq (9) is consist only 1-atom M in the unit cell, and the Hamiltonian does not invariant under the expansion of lattice vector along the x axis. In order to restore this invariance, we expanded the origin unit cell into a magnetic unit cell, which now contains q-atoms M.

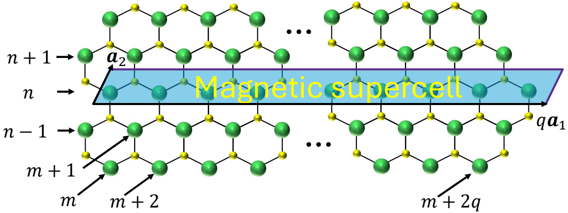


Figure: Magnetic unit cell for TMD monolayers.

Three-band tigh-binding model under a magnetic field

The new basis set of $3q$ atomic orbitals is defined as

$$\psi_{\lambda,\mathbf{k}}(\mathbf{r}) = \sum_{j,i} C_{ji}^{\lambda}(\mathbf{k}) \sum_{\mathbf{R}_\alpha}^{N_{UC}} e^{i\mathbf{k}\cdot(\mathbf{R}_\alpha+\mathbf{r}_i)} \phi_j(\mathbf{r}-\mathbf{R}_\alpha-\mathbf{r}_i), \tag{10}$$

in which $\mathbf{r}_i$ is the position of an atom in a unit cell, while $\mathbf{R}_\alpha$ is the position of different unit cells. The Hamiltonian matrix elements in the new basis is written as

$$H_{ii'}^{jj'}(\mathbf{k}) = \sum_{\mathbf{R}_\alpha}^{N_{\text{UC}}} \sum_{\mathbf{R}_\beta}^{N_{\text{UC}}} e^{i\mathbf{k}\cdot(\mathbf{R}_\beta-\mathbf{R}_\alpha+\mathbf{r}_{i'}-\mathbf{r}_i)} \left\langle \phi_j(\mathbf{r}-\mathbf{R}_\alpha-\mathbf{r}_i) \right| \left[-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + U_0 \right] \left| \phi_j(\mathbf{r}-\mathbf{R}_\beta-\mathbf{r}_{i'}) \right\rangle . \tag{11}$$

Now we center our system at $\mathbf{r}' = \mathbf{r}-\mathbf{R}_\alpha-\mathbf{r}_i$ and define $\mathbf{R}_\gamma = \mathbf{R}_\alpha - \mathbf{R}_\beta$. This lead us to

$$H_{ii'}^{jj'}(\mathbf{k}) = \sum_{\alpha}^{N_{\text{UC}}} \sum_{\gamma}^{N_{\text{UC}}} e^{-i\mathbf{k}\cdot(\mathbf{R}_\gamma+\mathbf{r}_i-\mathbf{r}_{i'})} \left\langle \phi_j(\mathbf{r}) \right| \left[-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + U_0 \right] \left| \phi_j(\mathbf{r}+\mathbf{R}_\gamma+\mathbf{r}_i-\mathbf{r}_{i'}) \right\rangle . \tag{12}$$

Three-band tigh-binding model under a magnetic field

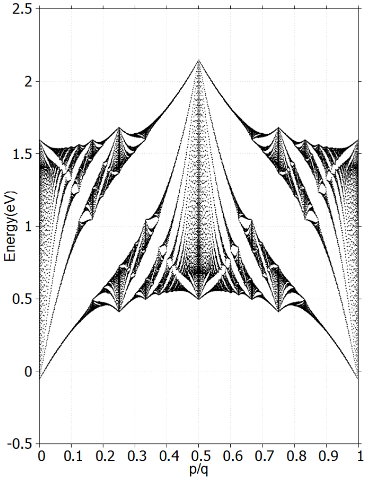
Only considering the nearest-neighbors, we define our hopping terms in the new basis

$$H_{jj'}^{ii'}(\mathbf{k}) = \sum_{\alpha}^{N_{\text{UC}}} \sum_{\gamma}^{N_{\text{UC}}} e^{-i\mathbf{k}\cdot\mathbf{R}_\gamma} \left\langle \phi_j(\mathbf{r}) \right| \left[-\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} + U_0(\mathbf{r}) \right] \left| \phi_{j'}(\mathbf{r} + \mathbf{R}_\gamma) \right\rangle \delta_{i,i'}. \tag{13}$$

Note that $i = (m, n)$, taking the sum over $\mathbf{R}$ and plugging the Peierls phase into Eq. (13), we get the Hamiltonian under a magnetic field

$$H_{jj'}^{ii'}(\mathbf{k}) = e^{i\theta_{m,n}^{m,n}} e^{i\mathbf{k}\cdot(\mathbf{0}-\mathbf{R})} \left\langle \phi_j(\mathbf{r}) \right| \left[-\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} + U_0(\mathbf{r}) \right] \left| \phi_{j'}(\mathbf{r} - \mathbf{R}) \right\rangle \delta_{m,m'}^{n,n'}. \tag{14}$$

Three-band tigh-binding model under a magnetic field



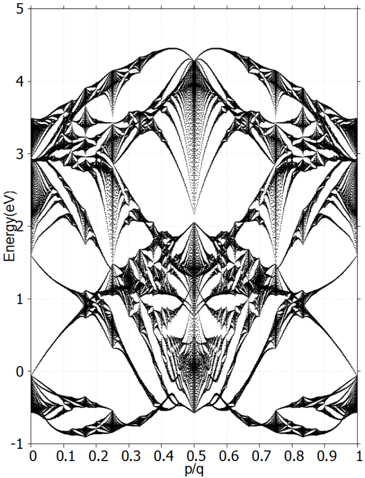


Figure: Hofstadter butterfly for single-band $|dz\rangle \equiv \left|\phi_1^1(x,y)\right\rangle$(left) and three-band(right) with $q = 797$ with field strength $B_0 = 4.6928 \times 10^4$ T.

Hofstadter butterfly

Properties

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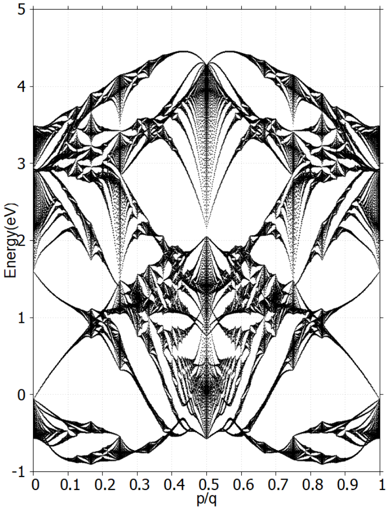
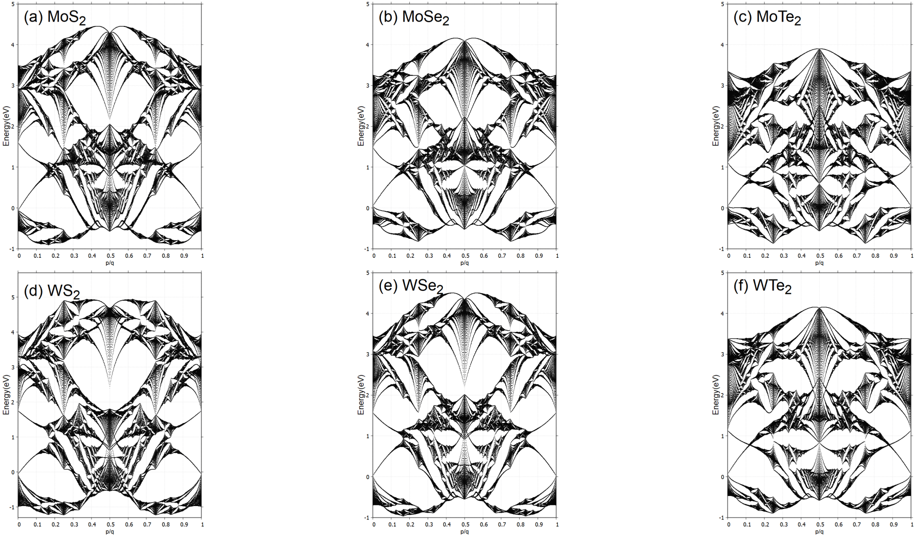
- The spectrum also invariant under reversal of the magnetic field $\frac{p}{q} \rightarrow -\frac{p}{q}$.
- At weak magnetic field, Landau levels can clearly seen from the Hofstadter spectrum.



Hofstadter butterfly in MX_2



Landau levels

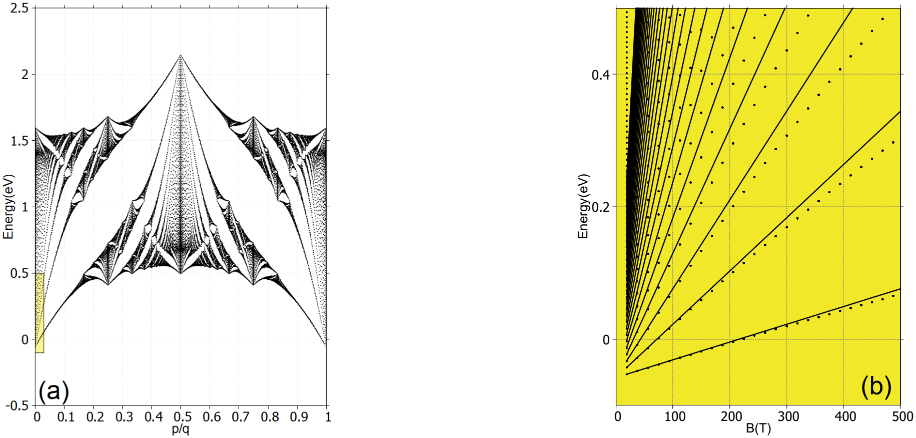


Figure: (a) Same plot as Fig (2.6) but considering a small area and (b) shows superposition of the Landau fan diagram and the Hofstadter butterfly. Display the first $n = 30$ levels near the bottom of the conduction band for a magnetic field up to $B = 500$ T.

Classical Hall effect

Summary:

- We confirm the Hofstadter butterfly in this model corrected compared to previous study.
- From three-band TB $+$ magnetic field $\rightarrow$ QHE.

Further research:

- High Harmonic Generation
- High-order Side-band Generation
- Photovoltaic effect

Thank you for your listening.