Calculation of the Linear-Absorption Spectrum of an Ideal Two-Dimensional System of MoS_2

Presenter
Vo Chau Duc Phuong [1]

Supervisors
Dr. Huynh Thanh Duc [2]

[1]University of Science, Ho Chi Minh city

[2]Institute of Applied Mechanics and Informatics

December 11, 2024

Table of Contents

Transition Metal Dichalcogenide Monolayer

Transition metal dichalcogenide (TMD) is the compound has the form of MX_2.

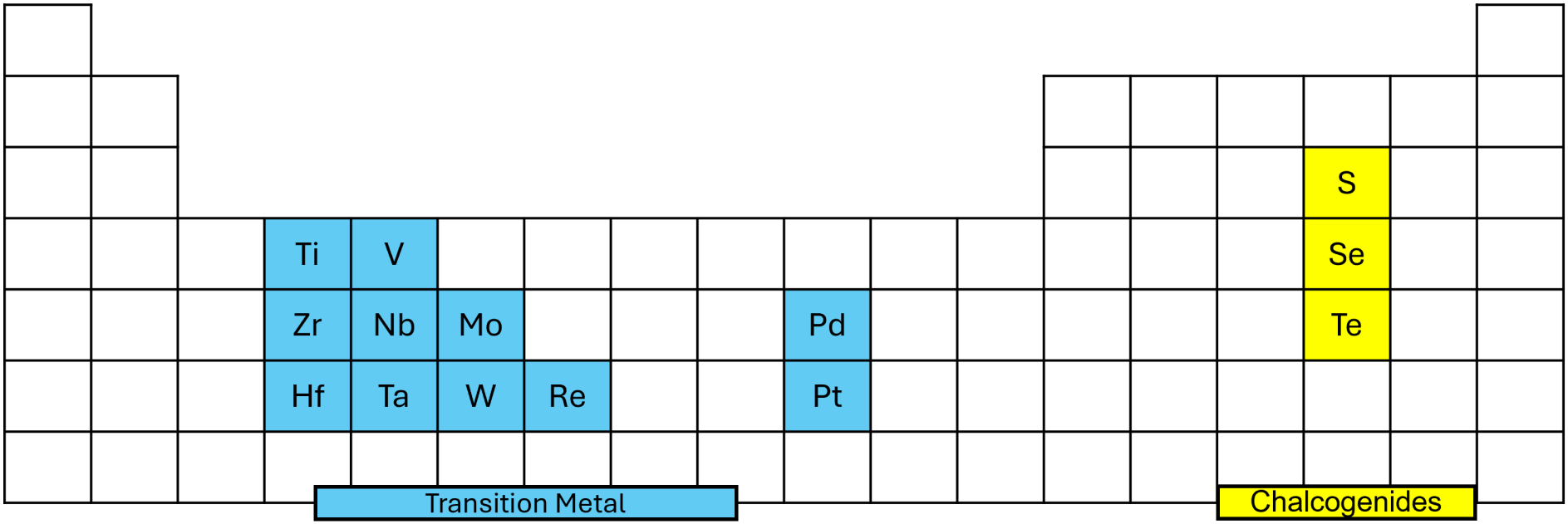


Figure: Transition metal dichalcogenide compound, M is a transition metal atom and X is a chalcogenides atoms

TMD Mono-layer structure

- The M (huge black dots) layer has been sandwiched by two X (small green dots) layers as shown in top view (a) and side view (b).
- They have the inverse asymmetry.
- The symmetry of the lattice results in the hexagon Brillouin Zone (BZ).

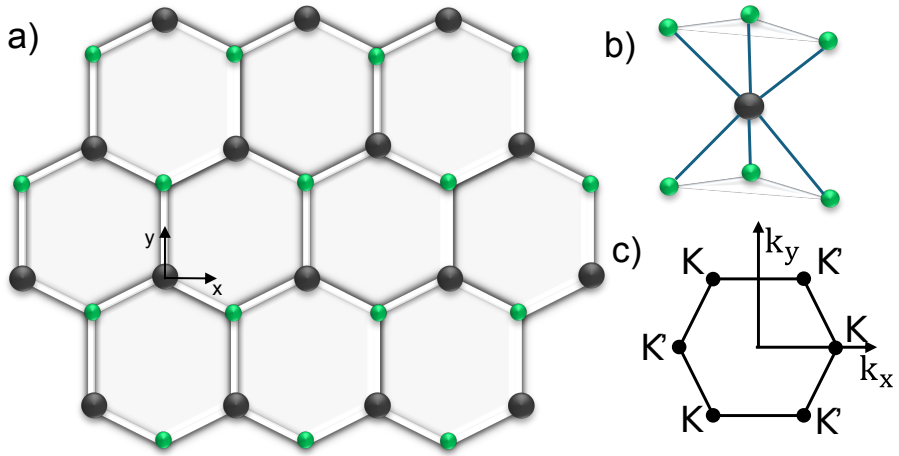


Figure: Structure and Brillouin Zone of Monolayer TMD, redrawing from[1]

My thesis focused on MoS_2 monolayer, has the visible band gap in the band structure, which can be used in creating the transistor devices.[2]

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

[2] Radisavljevic et al., "Single-layer MoS_2 transistors".

Splitting In The Band Structure

Huge split Δ (hundreds of meV) in valley (K and -K points) of the band structure caused by the strong spin-orbit coupling (SOC) and the inversion asymmetry.
$\Rightarrow$ Applications in spintronic and optoelectronics[3].

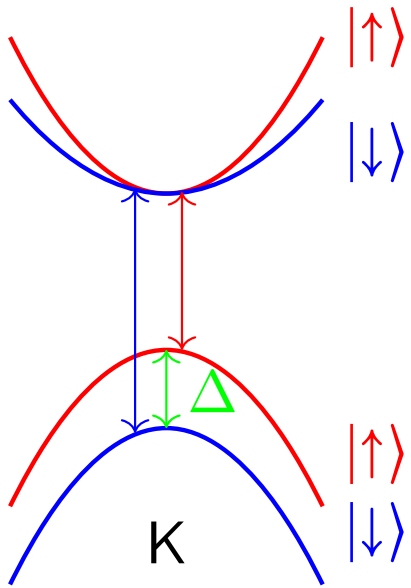


Figure: The allowed optical transition

[3] Liu et al., "Electronic structures and theoretical modelling of two-dimensional group-VIB transition metal dichalcogenides".

Binding Energy of Exciton

When an electron has been excited, it create a hole at initial position. Interaction between the electron and the hole call "Exciton".

$$-\left[\frac{\hbar^2\nabla^2_{\mathbf{r}}}{2m_r}+V(r)\right]\psi_\nu(\mathbf{r})=E_\nu(\mathbf{r})\psi_\nu(\mathbf{r}), \tag{1}$$

where,

- $V(r)$ is the Coulomb interaction with the form:

$$V(r)=\frac{e^2}{\varepsilon|\mathbf{r}|} \tag{2}$$

- $m_r=\frac{m_h m_e}{m_h+m_e}$ is the effective mass.
- $E_\nu(\mathbf{r})$ is the binding energy of the exciton.

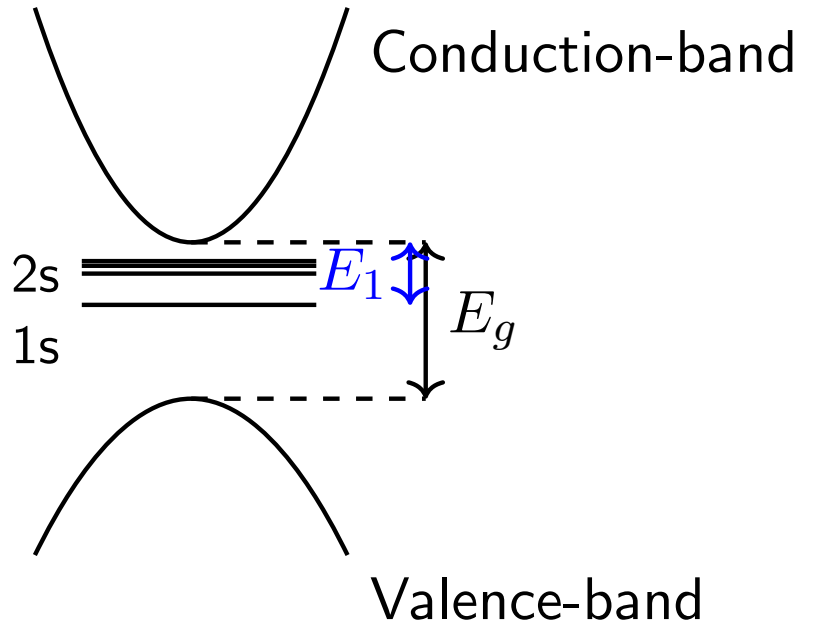


Figure: Binding energy relative to the band gap

Exciton

In the bulk crystals with relative small dielectric constant due to the screening, the exciton have the small binding energy.
Ex: GeAs[4]:

$$E_b \approx 4.8meV \ll E_g = 1.2 - 1.7eV$$

In these materials, the exciton binding energy can be neglected in simulations.

[4] Diakite et al., *Accurate Electronic, Transport, and Bulk Properties of Gallium Arsenide (GaAs)*.

Purpose

So, why need to calculate it in TMD?

- In the 2-D materials, lack of system dimension ⇒ decrease in the dielectric screening.
- Large quantum confinement in nano-material (z-axis).

⇒ Increasing of exciton binding energy $\sim 10^2$ in compared with bulk semiconductor.

- Previous theories predict binding energy too large[5], precisely experiment shows significant smaller binding energy[6].
- Find a model not only simple but also precise enough for further research and application.

⇒ Look like enough for my bachelor's thesis ☺.

[5] Ramasubramaniam, "Large excitonic effects in monolayers of molybdenum and tungsten dichalcogenides"; Qiu, Jornada, and Louie, "Optical Spectrum of MoS_2".

[6] Zhang et al., "Absorption of light by excitons and trions in monolayers of metal dichalcogenide MoS_2".

Tight-binding Model

Start from the Hamiltonian for an independence electron:

$$H_{1e}(\mathbf{r}) = -\frac{\hbar^2\nabla^2}{2m} + \sum_{\mathrm{i}} V(\mathbf{r} - \mathbf{R}_{\mathrm{i}} - \mathbf{r}_c), \tag{3}$$

where $\mathbf{R}_i$ is the Bravais lattice position, $\mathbf{r}_c$ is the relative position of atom inside unit cell. We neglected the motion of nucleus because in this case, the nucleus (Transistion metals and Chalcogenides) are very heavy in compare with the electron (Born-Oppenheimer approximation).

Assuming that the electron stay close to its atom and have little overlap on the neighboring sites. Therefore the wave function of each electron can be described by the linearly combination of atomic orbitals (LCAO).

$$\psi(\mathbf{r}) = \sum_{n=1}^{N}\sum_{c=1}^{N_c}\sum_{\alpha=1}^{N_{orbital}} c_{\alpha c}(\mathbf{R}_n)\phi_\alpha(\mathbf{r} - \mathbf{R}_n - \mathbf{r}_c) \tag{4}$$

$N, N_c,$ and N_α is number of unit lattice of the system, number of atom in a basis and number of orbital of an atom, respectively.

From LCAO wavefunctions, Bloch wavefunction can be constructed as:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_{c=1}^{N_c} \sum_{\alpha=1}^{N_{orb}} c_{\alpha c}(\mathbf{k}) e^{i\mathbf{k}(\mathbf{R}_n + \mathbf{r}_c)} \sum_{n=1}^{N} \phi_\alpha(\mathbf{r} - \mathbf{R}_n - \mathbf{r}_c). \tag{5}$$

Substituting (5) into Schrödinger equation with Hamiltomian (3), multiply with $e^{-i\mathbf{k}\mathbf{r}_c}\phi^*_{\alpha'}(\mathbf{r} - \mathbf{r}_{c'})$ and taking the integral on $\mathbf{r}$:

$$\sum_{c=1}^{N_c} \sum_{\alpha=1}^{N_{orb}} (H_{\alpha' c', \alpha c}(\mathbf{k}) - \varepsilon(\mathbf{k}) S_{\alpha c, \alpha' c'}(\mathbf{k})) C_{\alpha c}(\mathbf{k}) = 0, \tag{6}$$

In which

$$H_{\alpha' c', \alpha c} = \sum_{n=1}^{N} e^{i\mathbf{k}(\mathbf{r} + \mathbf{r}_c - \mathbf{r}_{c'})} \left\langle \phi_\alpha(\mathbf{r} - \mathbf{r}_{c'}) \right| H_{1e} \left| \phi_{\alpha'}(\mathbf{r} - \mathbf{R}_n - \mathbf{r}_c) \right\rangle \tag{7}$$

$$S_{\alpha' c', \alpha c} = \sum_{n=1}^{N} e^{i\mathbf{k}(\mathbf{r} + \mathbf{r}_c - \mathbf{r}_{c'})} \left\langle \phi_\alpha(\mathbf{r} - \mathbf{r}_{c'}) \middle| \phi_{\alpha'}(\mathbf{r} - \mathbf{R}_n - \mathbf{r}_c) \right\rangle \tag{8}$$

If we approximate the overlapping matrix elements $S_{\alpha c,\alpha' c'}(\mathbf{k}) \approx \delta_{\alpha\alpha'}\delta_{cc'}$ (no overlapping between two difference atoms), we have (6) in the form of:

$$\sum_{c=1}^{N_c}\sum_{\alpha=1}^{N_{orb}} H_{\alpha' c',\alpha c}(\mathbf{k})C_{\alpha c}(\mathbf{k}) = \varepsilon(\mathbf{k})C_{\alpha c}(\mathbf{k}) \tag{9}$$

In semi-empirical formalism, Hamiltonian matrix elements are defined by the phenomenological "On-site energy" and "Hopping energy" parameters.

So, if we have the Hamiltonian matrix, we can solve it for eigenvalues and corresponding eigenvectors.

But, how to use it?

Second Quantization Hamiltonian

The second quantization Hamiltonian in basis of Bloch function $\{|\psi_{\lambda\mathbf{k}}\rangle\}$ for many electrons system with Coulomb interaction in the electromagnetic field in velocity gauge ($\phi = 0$)

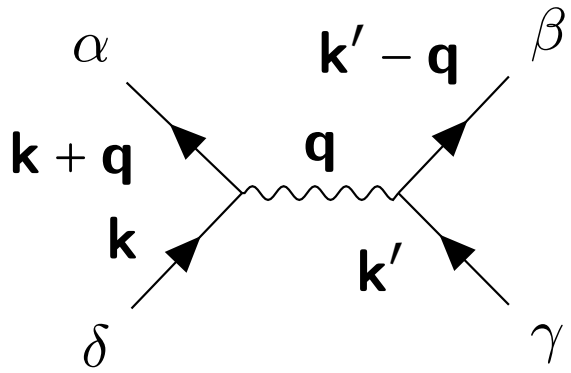
$$\begin{aligned} H =& H_{1e}^{0} + H^{Coul.} + H^{e-L} \\ =& \sum_{\lambda\mathbf{k}} \varepsilon_{\lambda}(\mathbf{k}) c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \sum_{\alpha\beta\gamma\delta} V_{\mathbf{k},\mathbf{k}',\mathbf{q}}^{\alpha\beta\gamma\delta} c_{\alpha\mathbf{k}+\mathbf{q}}^{\dagger} c_{\beta\mathbf{k}'-\mathbf{q}}^{\dagger} c_{\gamma\mathbf{k}} c_{\delta\mathbf{k}'} \\ &+ \sum_{\lambda\lambda'\mathbf{k}\mathbf{k}'} \langle\psi_{\lambda\mathbf{k}}| \frac{e}{m} \mathbf{A}(\mathbf{r},t).\mathbf{p} |\psi_{\lambda'\mathbf{k}'}\rangle c_{\lambda\mathbf{k}}^{\dagger} c_{\lambda'\mathbf{k}'} + \mathrm{O}(\mathbf{A}^2) \end{aligned} \tag{10}$$

in which the creation $c_{\lambda\mathbf{k}}^{\dagger}$ and annihilation $c_{\lambda\mathbf{k}}$ operator satisfied the anti-commutator relation[7]:

$$\{c_{\lambda\mathbf{k}}^{\dagger}, c_{\lambda'\mathbf{k}'}^{\dagger}\} = \{c_{\lambda\mathbf{k}}, c_{\lambda'\mathbf{k}'}\} = 0; \quad \{c_{\lambda\mathbf{k}}, c_{\lambda'\mathbf{k}'}^{\dagger}\} = \delta_{\lambda\lambda'}\delta_{\mathbf{k}\mathbf{k}'}$$

[7] $\{A,B\} = AB + BA$

The coulomb interaction matrix elements:



$$V^{\alpha\beta\gamma\delta}_{\mathbf{k},\mathbf{k'},\mathbf{q}} = \left\langle \psi_{\alpha\mathbf{k}+\mathbf{q}}\psi_{\beta\mathbf{k'}-\mathbf{q}} \right| V_{ee} \left| \psi_{\gamma\mathbf{k}}\psi_{\delta\mathbf{k'}} \right\rangle = \tag{11}$$

$$= \int \frac{d^3r}{V} \int \frac{d^3r'}{V} e^{-i\mathbf{q}(\mathbf{r}-\mathbf{r'})} u^*_{\alpha\mathbf{k}+\mathbf{q}}(\mathbf{r}) u^*_{\beta\mathbf{k}-\mathbf{q}}(\mathbf{r'}) V_{ee} u_{\gamma\mathbf{k'}}(\mathbf{r'}) u_{\delta\mathbf{k}}(\mathbf{r}),$$

With the 3-D Coulomb interaction have the form:

$$V_{ee}(\mathbf{r}) = \frac{e^2}{\varepsilon|\mathbf{r}|} \tag{12}$$

Using Fourier transform for the potential, apply long-wave approximation and take the limit $z \to 0$ to have the 2-D Coulomb matrix elements:

$$V^{\alpha\beta\gamma\delta}_{\mathbf{k},\mathbf{k'},\mathbf{q}} = \frac{e^2}{2\varepsilon L^2} \frac{1}{|\mathbf{q}_\parallel|} \left\langle u_{\alpha\mathbf{k}+\mathbf{q}} \middle| u_{\delta\mathbf{k}} \right\rangle \left\langle u_{\beta\mathbf{k'}-\mathbf{q}} \middle| u_{\gamma\mathbf{k'}} \right\rangle \tag{13}$$

From the equations of motion (in Heisenberg's picture) for $c^\dagger_{\mathbf{k}} c_{\mathbf{k}}$, we have the equations of motion for the expected value $\left\langle c^\dagger_{\mathbf{k}} c_{\mathbf{k}} \right\rangle$:

$$\begin{aligned}
\frac{\mathrm{d}\left\langle c^\dagger_{\mathbf{k}} c_{\mathbf{k}} \right\rangle}{\mathrm{d}t} =& -\frac{i}{\hbar}\left\langle\left[H^0 + H^{Coul.} + H_{e-L}, c^\dagger_{\mathbf{k}} c_{\mathbf{k}} \right]\right\rangle \\
=& \frac{i}{\hbar}\left(\varepsilon_\lambda(\mathbf{k}) - \varepsilon_{\lambda'}(\mathbf{k})\right)\left\langle c^\dagger_{\mathbf{k}} c_{\mathbf{k}} \right\rangle + \left\langle\left[H_{e-L}, c^\dagger_{\mathbf{k}} c_{\mathbf{k}} \right]\right\rangle \\
&+ \frac{i}{\hbar}\sum_{\mathbf{k}'\mathbf{q}}\sum_{\alpha\beta\gamma} V^{\alpha\beta\gamma\lambda}_{\mathbf{k},\mathbf{k}',\mathbf{q}}\left\langle c^\dagger_{\alpha\mathbf{k}+\mathbf{q}} c^\dagger_{\beta\mathbf{k}'-\mathbf{q}} c_{\gamma\mathbf{k}'} c_{\lambda'\mathbf{k}} \right\rangle \\
&+ \frac{i}{\hbar}\sum_{\mathbf{k}'\mathbf{q}}\sum_{\alpha\gamma\delta} V^{\alpha\lambda'\gamma\delta}_{\mathbf{k}',\mathbf{k}+\mathbf{q},\mathbf{q}}\left\langle c^\dagger_{\lambda\mathbf{k}} c^\dagger_{\alpha\mathbf{k}'+\mathbf{q}} c_{\gamma\mathbf{k}+\mathbf{q}} c_{\delta\mathbf{k}'} \right\rangle
\end{aligned} \tag{14}$$

Approximation the expected value of four-operator by multiplication of two expected value (Hatree-Fock Approximation):

$$\begin{aligned}
\left\langle c^\dagger_{\alpha\mathbf{k}+\mathbf{q}} c^\dagger_{\beta\mathbf{k}'-\mathbf{q}} c_{\gamma\mathbf{k}'} c_{\lambda'\mathbf{k}} \right\rangle &\approx -\left\langle c^\dagger_{\alpha\mathbf{k}+\mathbf{q}} c_{\gamma\mathbf{k}'} \right\rangle\left\langle c^\dagger_{\beta\mathbf{k}'-\mathbf{q}} c_{\lambda'\mathbf{k}} \right\rangle \delta_{\mathbf{k}+\mathbf{q}\mathbf{k}'} \\
\left\langle c^\dagger_{\lambda\mathbf{k}} c^\dagger_{\alpha\mathbf{k}'+\mathbf{q}} c_{\gamma\mathbf{k}+\mathbf{q}} c_{\delta\mathbf{k}'} \right\rangle &\approx \left\langle c^\dagger_{\lambda\mathbf{k}+\mathbf{q}} c_{\delta\mathbf{k}'} \right\rangle\left\langle c^\dagger_{\alpha\mathbf{k}'+\mathbf{q}} c_{\gamma\mathbf{k}+\mathbf{q}} \right\rangle \delta_{\mathbf{k}'\mathbf{k}}
\end{aligned} \tag{15}$$

Substituting (15) into (14) and doing some transformations on the light-matter interaction part to have

$$\begin{aligned}\frac{\mathrm{d}\left\langle c^{\dagger}_{\lambda\mathbf{k}}c_{\lambda'\mathbf{k}}\right\rangle}{\mathrm{d}t} =& \frac{i}{\hbar}\left(\varepsilon_{\lambda}(\mathbf{k})-\varepsilon_{\lambda'}(\mathbf{k})\right)\left\langle c^{\dagger}_{\lambda\mathbf{k}}c_{\lambda'\mathbf{k}}\right\rangle \\ &- \frac{i}{\hbar}\sum_{\mu}\left(\Sigma_{\mu\lambda}(\mathbf{k})\left\langle c^{\dagger}_{\mu\mathbf{k}}c_{\lambda'\mathbf{k}}\right\rangle - \left\langle c^{\dagger}_{\lambda\mathbf{k}}c_{\mu\mathbf{k}}\right\rangle\Sigma_{\mu\lambda'}(\mathbf{k})\right) \qquad (16)\end{aligned}$$

in which

$$\Sigma_{\mu\nu} = \frac{e\mathbf{A}(t)}{m}\mathbf{p}_{\mu\nu}(\mathbf{k}) - \sum_{\alpha\beta\mathbf{q}} V^{\alpha\mu\beta\nu}_{\mathbf{k},\mathbf{k}+\mathbf{q},\mathbf{q}}\rho_{\alpha\beta}(\mathbf{k}+\mathbf{q}) \qquad (17)$$

$$\mathbf{p}_{\mu\nu} = \frac{m}{\hbar}\left\langle u_{\lambda\mathbf{k}}\right|\nabla_{\mathbf{k}}H^{0}_{1e}(\mathbf{k})\left|u_{\lambda'\mathbf{k}}\right\rangle \qquad (18)$$

$$H^{0}_{1e}(\mathbf{k}) = e^{-i\mathbf{kr}}H^{0}_{1e}(\mathbf{r})e^{i\mathbf{kr}} = e^{-i\mathbf{kr}}\left(\frac{\mathbf{p}^2}{2m}+V_0(\mathbf{r})\right)e^{i\mathbf{kr}} \qquad (19)$$

Equation (16) can describe the transition between valence bands and conduction bands, but lack of relaxation effect due to scattering.

Phenomenally characterize the scattering term:

$$\left(\frac{\mathrm{d}\rho(\mathbf{k})}{\mathrm{d}t}\bigg|_{scat.}\right)_{\lambda\lambda'} \to -\frac{\rho_{\lambda\lambda'}(\mathbf{k})}{T_2}(1-\delta_{\lambda\lambda'}) \tag{20}$$

The parameter T_2 can be chosen $\to$ fit with the experiments.

Finally, we have the semiconductor Bloch equations[8]:

$$\begin{aligned}\frac{\mathrm{d}\rho_{\lambda\lambda'}(\mathbf{k})}{\mathrm{d}t} =& \frac{i}{\hbar}(\varepsilon_\lambda(\mathbf{k}) - \varepsilon_{\lambda'}(\mathbf{k}))\rho_{\lambda\lambda'}(\mathbf{k}) \\ &- \frac{i}{\hbar}\sum_\mu \left(\Sigma_{\mu\lambda}(\mathbf{k})\left\langle c^\dagger_{\mu\mathbf{k}} c_{\lambda'\mathbf{k}}\right\rangle - \left\langle c^\dagger_{\lambda\mathbf{k}} c_{\mu\mathbf{k}}\right\rangle \Sigma_{\mu\lambda'}(\mathbf{k})\right) \\ &- \frac{\rho_{\lambda\lambda'}(\mathbf{k})}{T_2}(1-\delta_{\lambda\lambda'}),\end{aligned} \tag{21}$$

where,

$$\Sigma_{\mu\nu} = \frac{e\mathbf{A}(t)}{m}\mathbf{p}_{\mu\nu}(\mathbf{k}) - \sum_{\alpha\beta\mathbf{q}} V^{\alpha\mu\beta\nu}_{\mathbf{k},\mathbf{k+q},\mathbf{q}}\rho_{\alpha\beta}(\mathbf{k+q}) \tag{22}$$

At $0K$, initial conditions at $(t = -\infty)$:

$$\rho_{\lambda\lambda'}(\mathbf{k}) = \delta_{\lambda v}\delta_{\lambda' v} \quad \forall \mathbf{k}$$

[8] Haug and Koch, *Quantum Theory Of The Optical And Electronic Properties Of Semiconductors (fifth Edition)*.

The dipole matrix elements can be obtained through:

$$\vec{\xi}_{\mu\nu}(\mathbf{k}) = \frac{-i\hbar}{m}\frac{\mathbf{p}_{\mu\nu}(\mathbf{k})}{\varepsilon_{\mu}(\mathbf{k}) - \varepsilon_{\nu}(\mathbf{k})}. \quad (23)$$

for $\mu \neq \nu$

For time-dependent interband polarization density:

$$\mathbf{P}(t) = \frac{e}{L^2}\sum_{\mathbf{k}} \mathrm{Tr}\left[\vec{\xi}(\mathbf{k})\rho(\mathbf{k},t)\right] \quad (24)$$

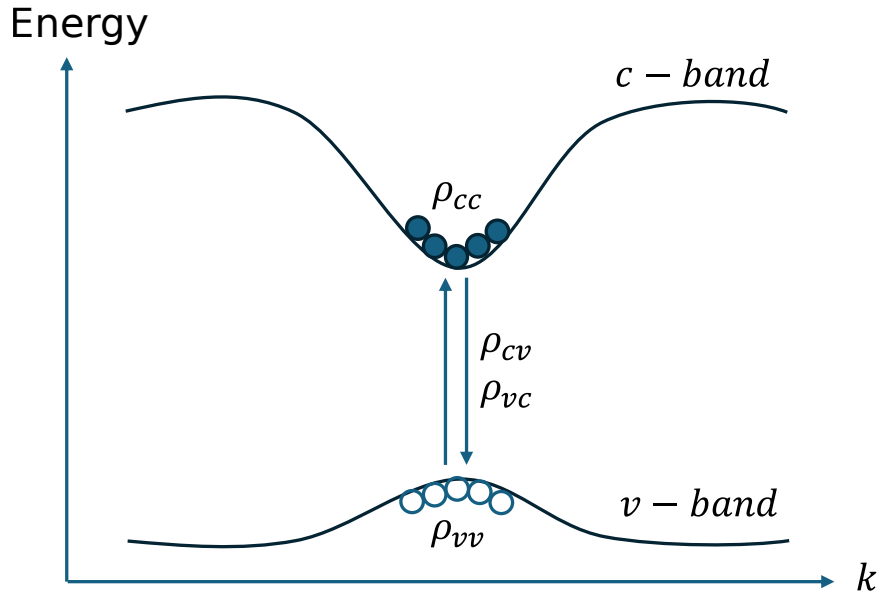


Figure: Density matrix element illustration

Three-band Tightbinding model

Using basic functions of d-type orbitals:

$$|\phi_1\rangle = d_{z^2}, |\phi_2\rangle = d_{xy}, |\phi_3\rangle = d_{x^2-y^2} \Rightarrow H^{TB}_{3\times3}(\mathbf{k})$$

Three-band TB Hamiltonian with SOC has the form[9]:

$$H^{TB}_{6\times6}(\mathbf{k}) = \begin{bmatrix} H^{TB}_{3\times3}(\mathbf{k}) + \gamma L_z & 0 \\ 0 & H^{TB}_{3\times3}(\mathbf{k}) - \gamma L_z \end{bmatrix}, \quad L_z = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & i \\ 0 & -i & 0 \end{bmatrix}.$$

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

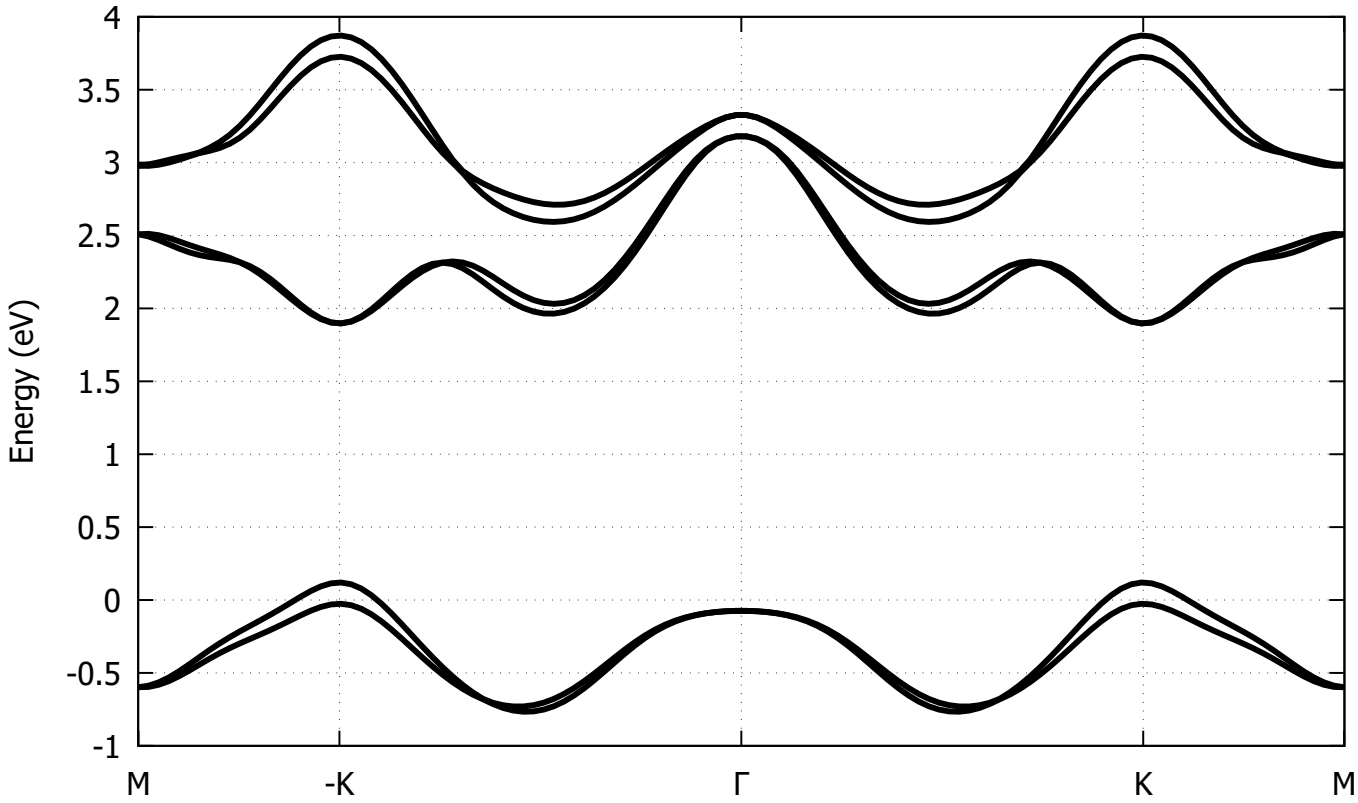


Figure: Band structure of MoS_2 monolayer

Numerical Evaluation of The Sum Over k-space

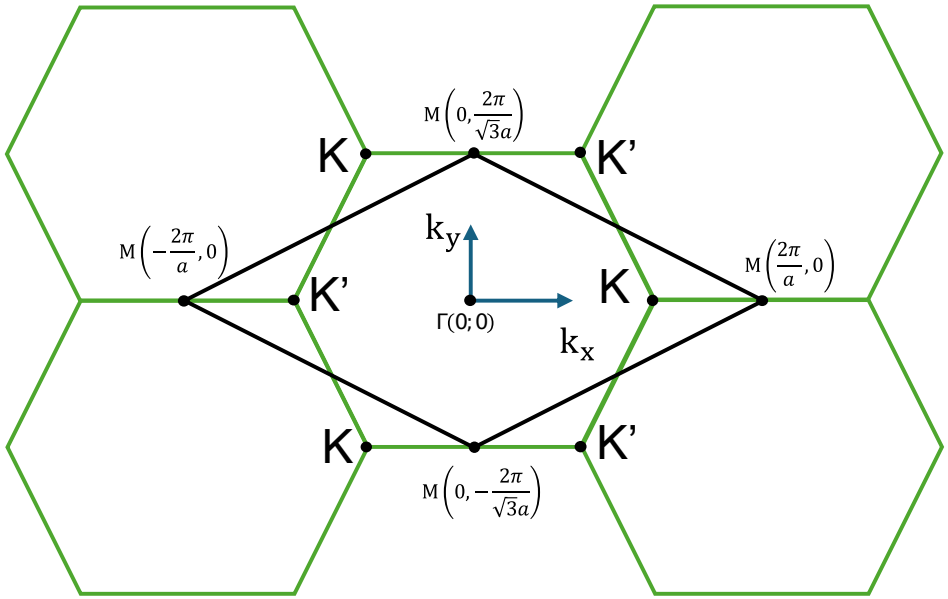
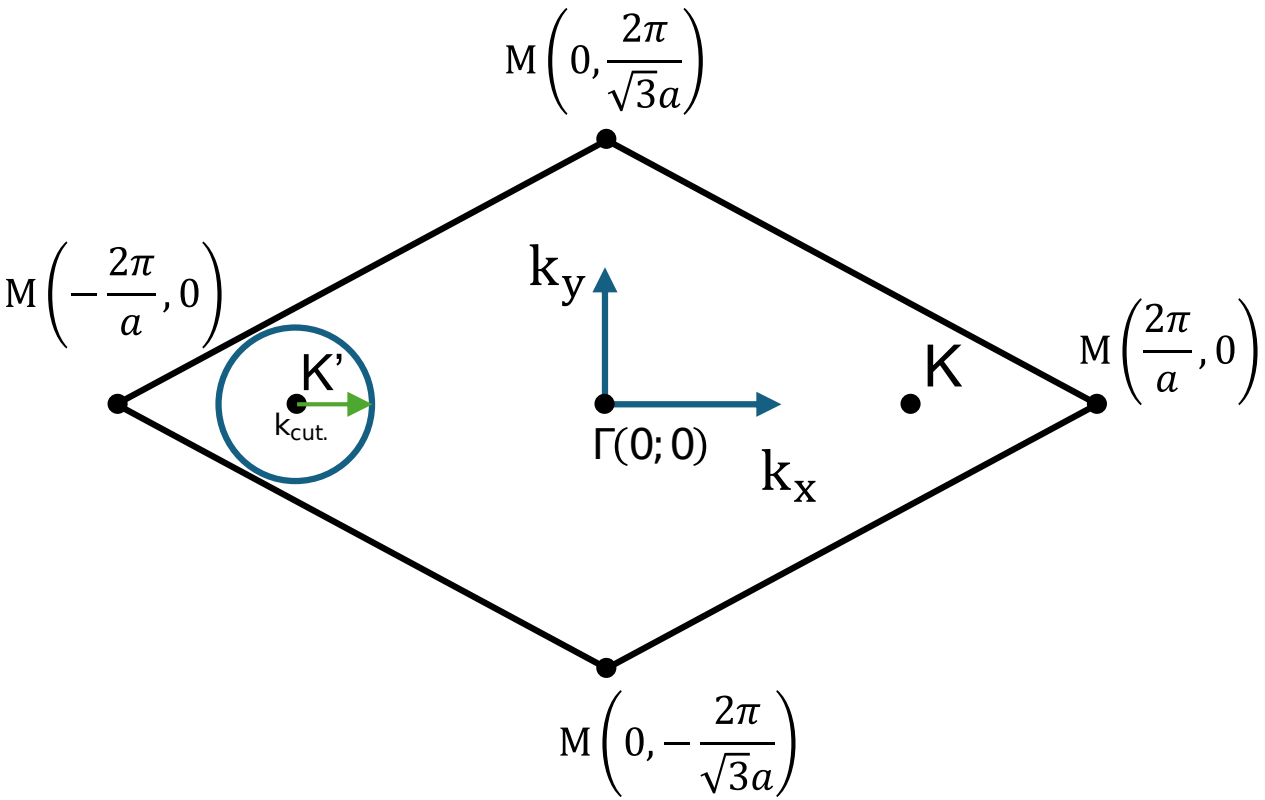


Figure: Rhombus primitive cell

$$\sum_{\mathbf{k}} ... \rightarrow \frac{L^2}{4\pi^2} \int \int_{BZ} dk_x dk_y ... \tag{25}$$

k-cutoff approximation method



For k-points around **K'** point

$$W^{\alpha\mu\beta\nu}_{\mathbf{k},\mathbf{k}',\mathbf{q}} \approx W^{\alpha\mu\beta\nu}_{\mathbf{k},\mathbf{k}',\mathbf{q}} \theta(k_{cut.} - |\mathbf{k} - \mathbf{k}_{K'}|)\theta(k_{cut.} - |\mathbf{k}' - \mathbf{k}_{K'}|). \tag{26}$$

The same for k-points around **K** point

Electromagnetic Field

The electric field has a Gaussian envelope form:

$$\mathbf{E}(t) = \mathbf{E}_0 \cos(\omega_0 t) e^{-\frac{t^2}{\tau_L^2}} \qquad (27)$$

- small $E_0 : \rho_{cc}(\mathbf{k}) \to 0$
- $\hbar\omega_0 = E_{gap.}$
- small $\tau_L \to$ rounder Fourier transform's peak around ω_0

In numerical solving, choose time step Δt

$$\Delta t \ll \tau_L$$

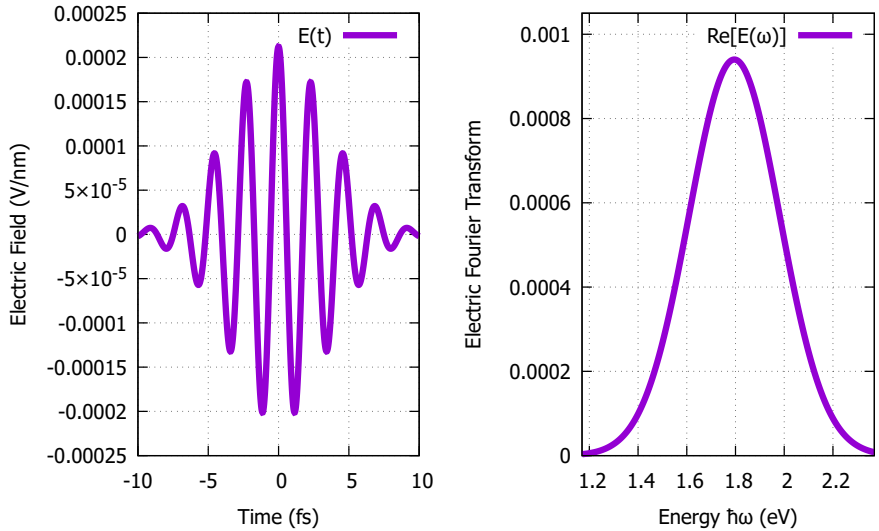


Figure: Electric field and it fourier transform

Absorption coefficient[10]:

$$\alpha(\omega) \propto \frac{P(\omega)}{E(\omega)}. \qquad (28)$$

[10] Haug and Koch, *Quantum Theory Of The Optical And Electronic Properties Of Semiconductors (fifth Edition)*.

Experiment measure:

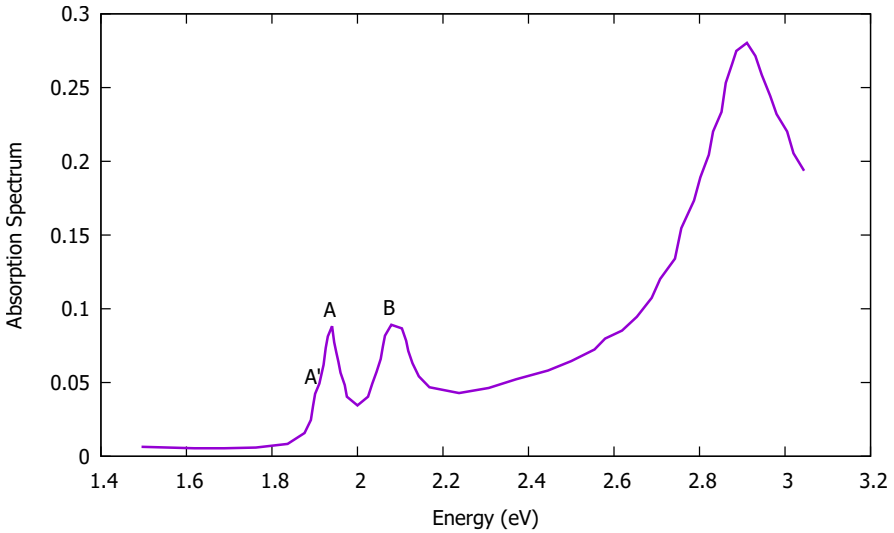


Figure: Measured Absorption Spectrum of MoS_2 at $T = 5K$ extracted from Ref.[11]

$$E_{gap} = 2.15 \pm 0.06\ eV$$

Binding energy:

$E_{bind.} = E_{gap} - E_A = 0.22\ eV$

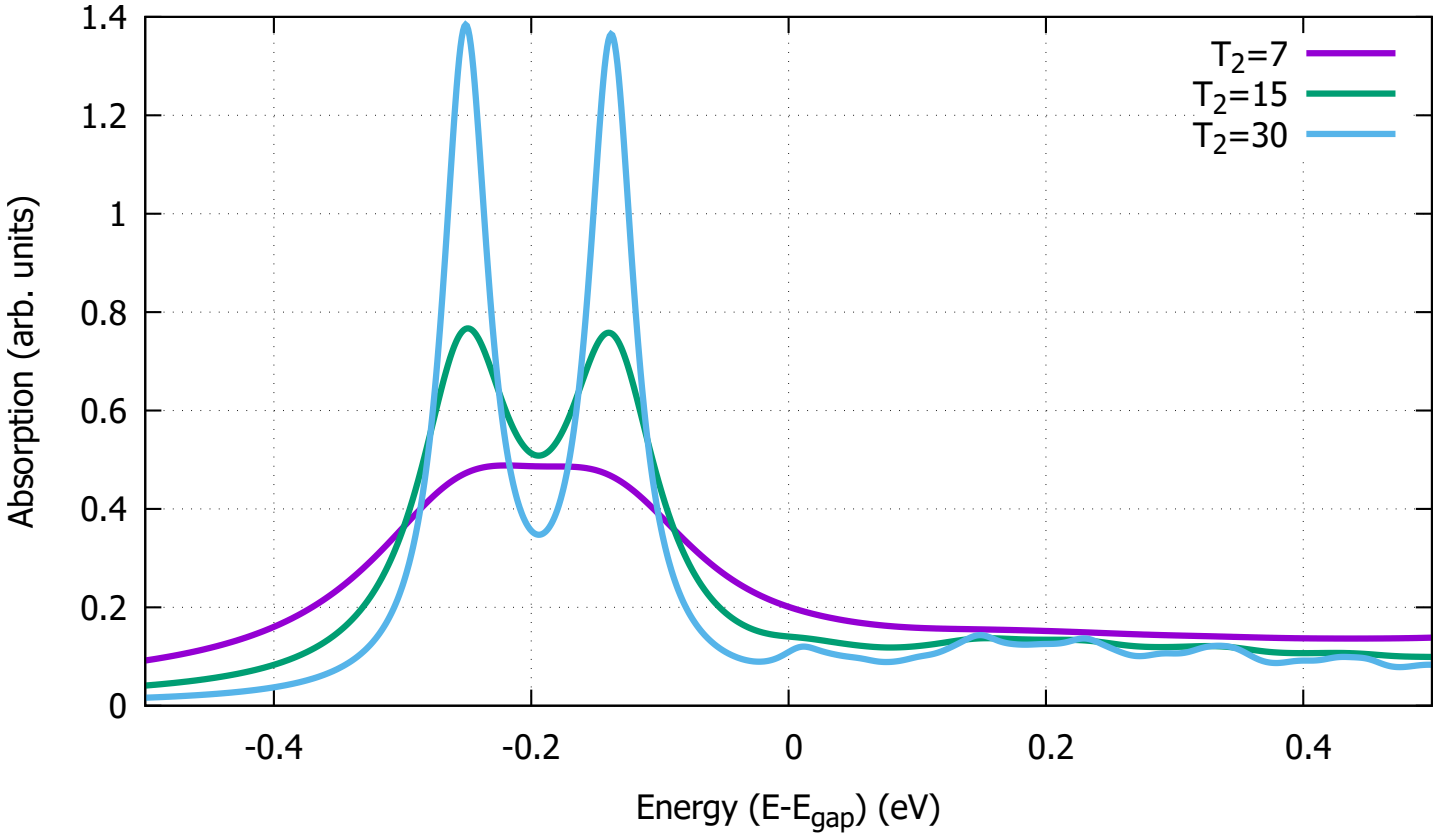
From this figure, we see

- Two resonance labeled by A $(1.93\ eV)$ and B $(2.1\ eV)$ are exciton peaks (band split due to SOC)
- Weak trion peak near A labeled by A' $(18\ meV)$

To fit with experiment, we can change:

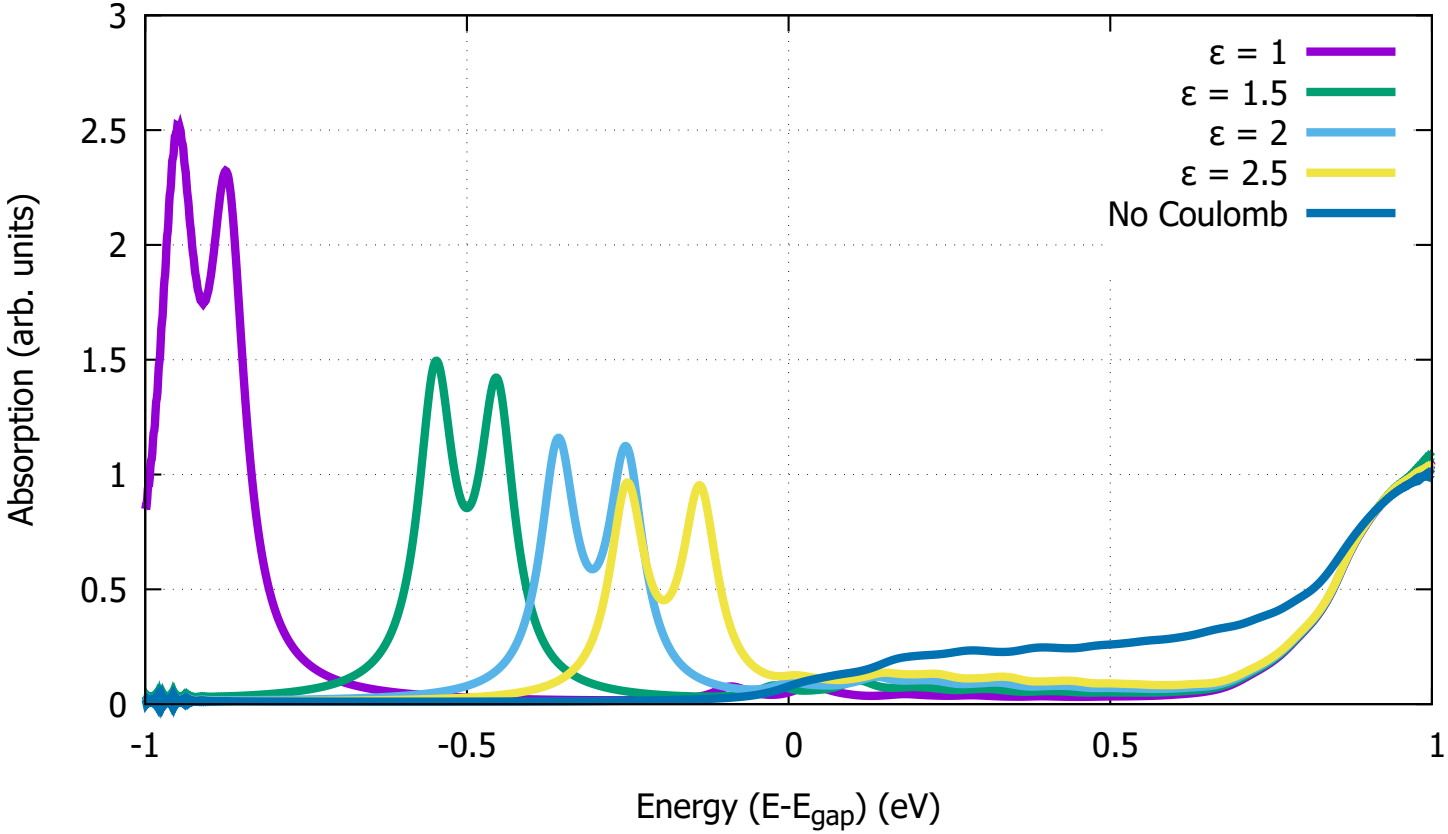
- Relative permittivity ε
- Dephasing time T_2

[11] Zhang et al., "Absorption of light by excitons and trions in monolayers of metal dichalcogenide MoS_2".



Choosing the T_2 for clearer Exciton peak:

- The bigger T_2, the clearer main Exciton peaks → confirm two peak.
- At $T_2 = 30\ fs$ show other smaller peaks → predict other peaks.



- Choosing the ε for fitting with the experiment.
- For 3-band TB model: $\varepsilon \in (1.5, 2.5)$ is in good agreement with measurement binding energy of $E_{bind.} = 0.2 - 0.5eV$[12]

[12] Zhang et al., "Absorption of light by excitons and trions in monolayers of metal dichalcogenide MoS_2".

Summary:

- From three-band TB + SBE → Linear Absorption Spectrum.
- We confirm the Exciton binding energy in this model is in agreement with experimental data, and predict smaller exciton peaks.

Further research:

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

Thank you for your listening.

For deeper calculation, source code, beamer e-pdf,... scan this.

- Ataca, C., H. Şahin, and S. Ciraci. "Stable, Single-Layer MX2 Transition-Metal Oxides and Dichalcogenides in a Honeycomb-Like Structure". In: (2012).
- Cheiwchanchamnangij, Tawinan and Walter R. L. Lambrecht. "Quasiparticle band structure calculation of monolayer, bilayer, and bulk MoS_2". In: *Phys. Rev. B* 85.20 (May 2012). Publisher: American Physical Society, p. 205302.
- Diakite, Yacouba Issa et al. *Accurate Electronic, Transport, and Bulk Properties of Gallium Arsenide (GaAs)*. 2016.
- Haug, Hartmut and Stephan W. Koch. *Quantum Theory Of The Optical And Electronic Properties Of Semiconductors (fifth Edition)*. en. Google-Books-ID: 1J1IDQAAQBAJ. Jan. 2009.
- Liu, Gui-Bin et al. "Electronic structures and theoretical modelling of two-dimensional group-VIB transition metal dichalcogenides". In: (2015).
- Liu, Gui-Bin et al. "Three-band tight-binding model for monolayers of group-VIB transition metal dichalcogenides". In: (2013).
- Qiu, Diana Y., Felipe H. da Jornada, and Steven G. Louie. "Optical Spectrum of MoS_2: Many-Body Effects and Diversity of Exciton