Strong valley Zeeman effect of dark excitons in 2D transition metal dichalogenides in a tilted magnetic field

Matthias Van der Donck

Universiteit Antwerpen

Introduction

Introduction

Strong valley Zeeman effect of dark excitons in 2D TMDs in a tilted magnetic field

Introduction

Strong valley Zeeman effect of dark excitons in 2D TMDs in a tilted magnetic field

Introduction

Strong valley Zeeman effect of dark excitons in 2D TMDs in a tilted magnetic field

A bound state of an electron and a hole

Introduction

Strong valley Zeeman effect of dark excitons in 2D TMDs in a tilted magnetic field

Introduction

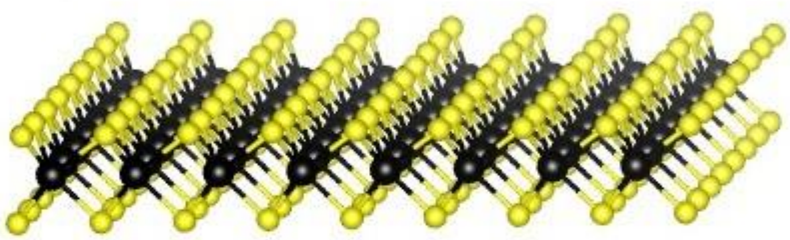
Strong valley Zeeman effect of dark excitons in 2D TMDs in a tilted magnetic field

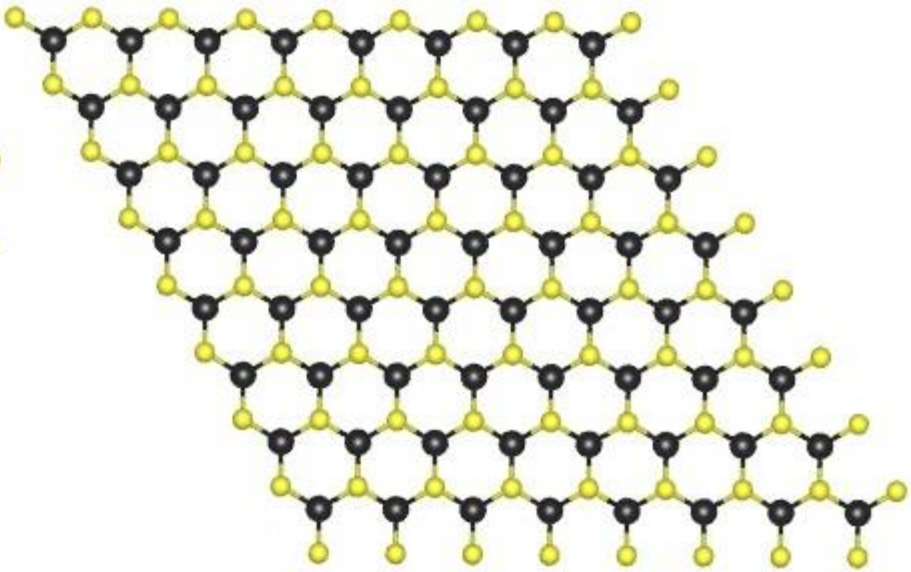
Semiconductors of the type MX_2 with M a transition metal atom (Mo, W, …) and X a chalcogen atom (S, Se, …)

Introduction

Strong valley Zeeman effect of dark excitons in 2D TMDs in a tilted magnetic field

Semiconductors of the type MX_2 with M a transition metal atom (Mo, W, …) and X a chalcogen atom (S, Se, …)

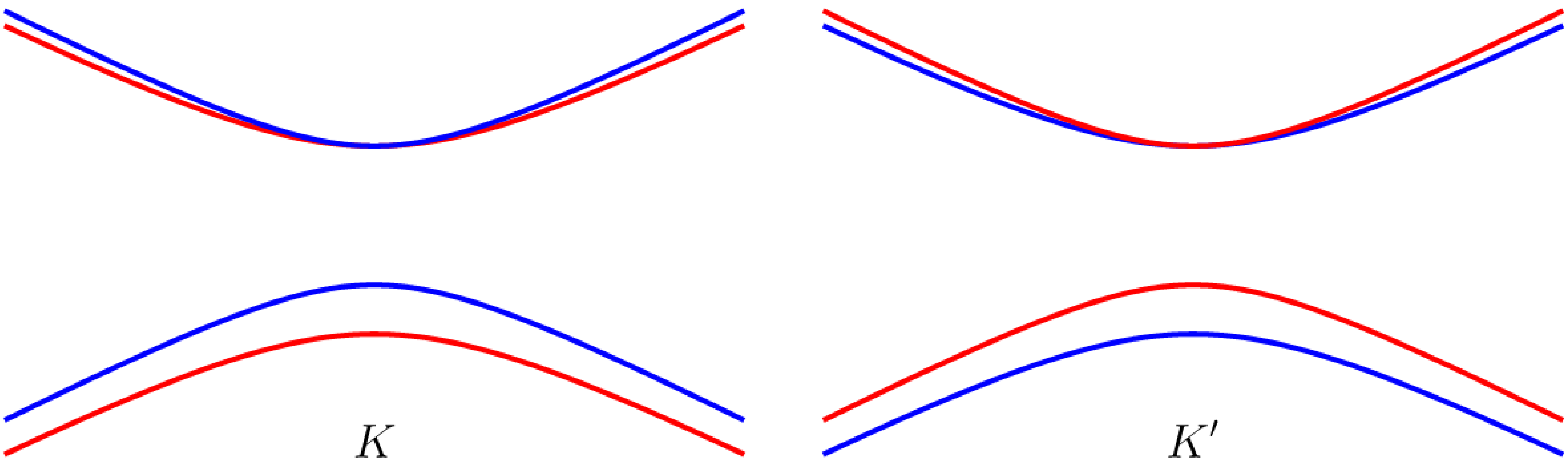




Introduction

Strong valley Zeeman effect of dark excitons in 2D TMDs in a tilted magnetic field

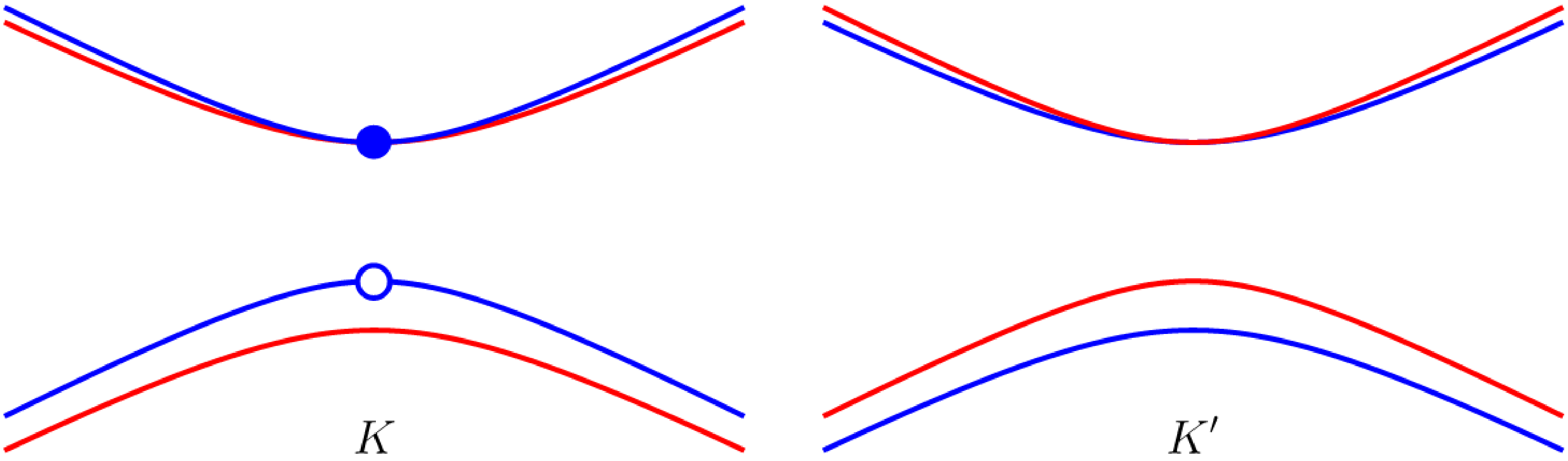
Semiconductors of the type MX_2 with M a transition metal atom (Mo, W, …) and X a chalcogen atom (S, Se, …)



Introduction

Strong valley Zeeman effect of dark excitons in 2D TMDs in a tilted magnetic field

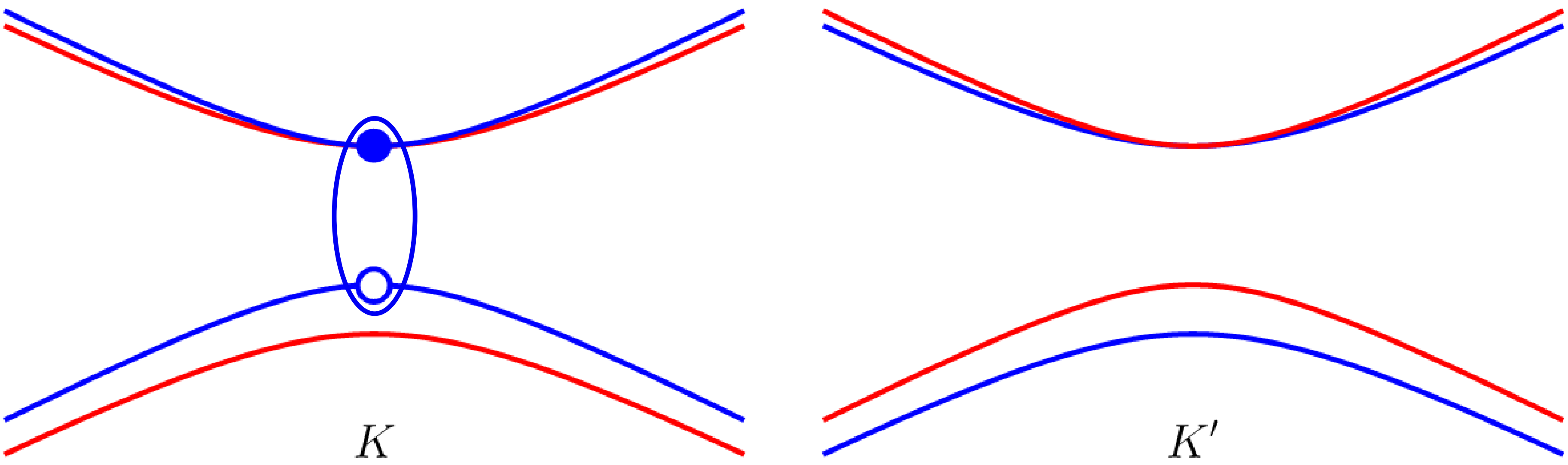
Semiconductors of the type MX_2 with M a transition metal atom (Mo, W, …) and X a chalcogen atom (S, Se, …)



Introduction

Strong valley Zeeman effect of dark excitons in 2D TMDs in a tilted magnetic field

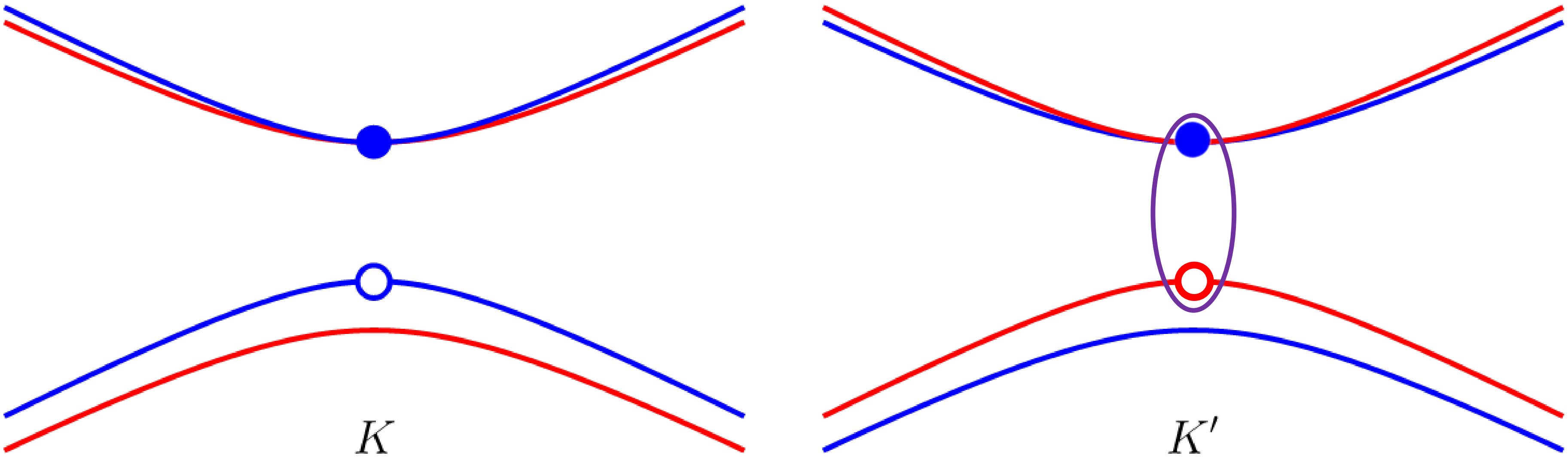
Semiconductors of the type MX_2 with M a transition metal atom (Mo, W, …) and X a chalcogen atom (S, Se, …)



Introduction

Strong valley Zeeman effect of dark excitons in 2D TMDs in a tilted magnetic field

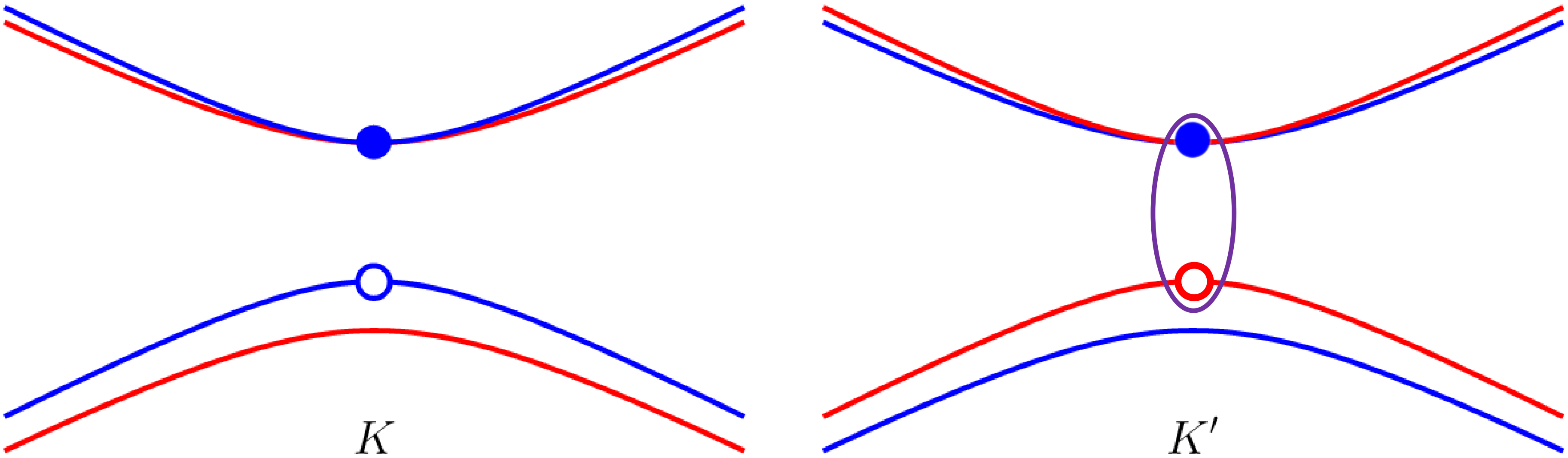
Semiconductors of the type MX_2 with M a transition metal atom (Mo, W, …) and X a chalcogen atom (S, Se, …)



Introduction

Strong valley Zeeman effect of dark excitons in 2D TMDs in a tilted magnetic field

Semiconductors of the type MX_2 with M a transition metal atom (Mo, W, …) and X a chalcogen atom (S, Se, …)



Introduction

Introduction

- Monolayer system ➡ strong interactions ➡ binding energies are one to two orders of magnitude larger than in typical (3D) semiconductors

Introduction

- Monolayer system ➡ strong interactions ➡ binding energies are one to two orders of magnitude larger than in typical (3D) semiconductors
- 2D confinement of the electric field lines leads to screening

Introduction

- Monolayer system ➡ strong interactions ➡ binding energies are one to two orders of magnitude larger than in typical (3D) semiconductors
- 2D confinement of the electric field lines leads to screening

$$V(r_{ij}) = \frac{e^2}{4\pi\kappa\varepsilon_0}\frac{\pi}{2r_0}\left[H_0\left(\frac{r_{ij}}{r_0}\right) - Y_0\left(\frac{r_{ij}}{r_0}\right)\right]$$

Introduction

- Monolayer system ➡ strong interactions ➡ binding energies are one to two orders of magnitude larger than in typical (3D) semiconductors
- 2D confinement of the electric field lines leads to screening

$$V(r_{ij}) = \frac{e^2}{4\pi\kappa\varepsilon_0}\frac{\pi}{2r_0}\left[H_0\left(\frac{r_{ij}}{r_0}\right) - Y_0\left(\frac{r_{ij}}{r_0}\right)\right]$$

$$= \begin{cases} \frac{e^2}{4\pi\kappa\varepsilon_0 r_{ij}} & \lim r_0 \to 0 \\ & \end{cases}$$

Introduction

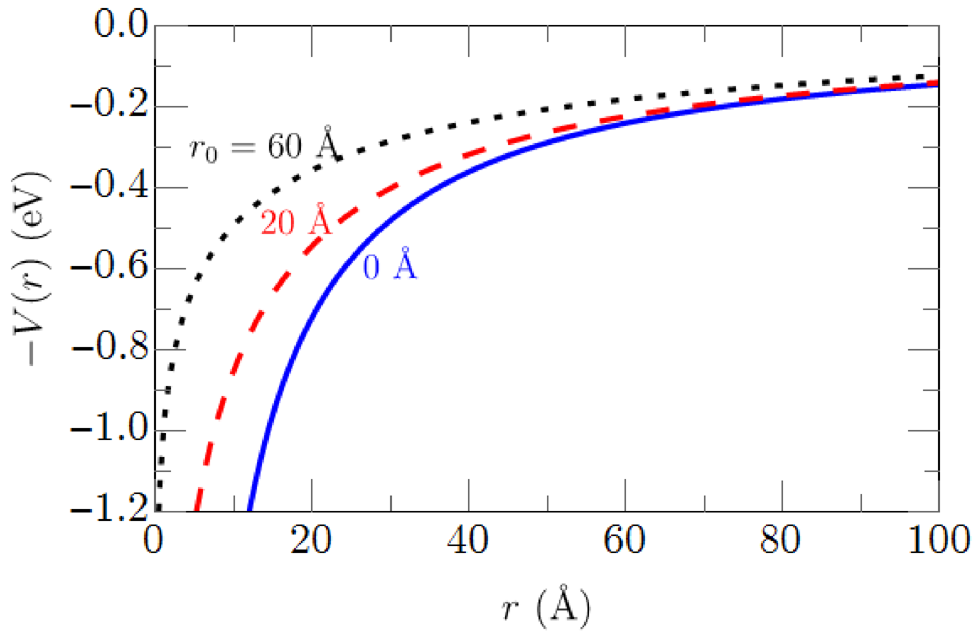
- Monolayer system ➡ strong interactions ➡ binding energies are one to two orders of magnitude larger than in typical (3D) semiconductors
- 2D confinement of the electric field lines leads to screening

$$V(r_{ij}) = \frac{e^2}{4\pi\kappa\varepsilon_0}\frac{\pi}{2r_0}\left[H_0\left(\frac{r_{ij}}{r_0}\right) - Y_0\left(\frac{r_{ij}}{r_0}\right)\right]$$

$$= \begin{cases} \frac{e^2}{4\pi\kappa\varepsilon_0 r_{ij}} & \lim r_0 \to 0 \\ \frac{e^2}{4\pi\kappa\varepsilon_0 r_0}\ln\left(\frac{r_0}{r_{ij}}\right) & \lim r_0 \to \infty \end{cases}$$

Introduction

- Monolayer system ➡ strong interactions ➡ binding energies are one to two orders of magnitude larger than in typical (3D) semiconductors
- 2D confinement of the electric field lines leads to screening



Model

Model

- Single-electron Hamiltonian

Model

- Single-electron Hamiltonian

$$\mathcal{B}_{\tau}^{e} = \{\left|\phi_{c,\uparrow,\tau}^{e}\right\rangle, \left|\phi_{v,\uparrow,\tau}^{e}\right\rangle, \left|\phi_{c,\downarrow,\tau}^{e}\right\rangle, \left|\phi_{v,\downarrow,\tau}^{e}\right\rangle\}$$

Model

- Single-electron Hamiltonian

$$H^q_\tau(\vec{\Pi}) = I^s_2 \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I^p_2 - \sigma_z}{2}\right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s}\right) \otimes I^p_2 + \tau s_z \otimes \left(\lambda_c \frac{I^p_2 + \sigma_z}{2} + \lambda_v \frac{I^p_2 - \sigma_z}{2}\right)$$

$$\mathcal{B}^e_\tau = \left\{ \left|\phi^e_{c,\uparrow,\tau}\right\rangle, \left|\phi^e_{v,\uparrow,\tau}\right\rangle, \left|\phi^e_{c,\downarrow,\tau}\right\rangle, \left|\phi^e_{v,\downarrow,\tau}\right\rangle \right\}$$

Model

- Single-electron Hamiltonian

$$H_\tau^q(\vec{\Pi}) = I_2^s \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I_2^p - \sigma_z}{2} \right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s} \right) \otimes I_2^p + \tau s_z \otimes \left(\lambda_c \frac{I_2^p + \sigma_z}{2} + \lambda_v \frac{I_2^p - \sigma_z}{2} \right)$$

$$\mathcal{B}_\tau^e = \left\{ \left|\phi_{c,\uparrow,\tau}^e\right\rangle, \left|\phi_{v,\uparrow,\tau}^e\right\rangle, \left|\phi_{c,\downarrow,\tau}^e\right\rangle, \left|\phi_{v,\downarrow,\tau}^e\right\rangle \right\}$$

Model

- Single-electron Hamiltonian

$$H_\tau^q(\vec{\Pi}) = I_2^s \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I_2^p - \sigma_z}{2} \right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s} \right) \otimes I_2^p + \tau s_z \otimes \left(\lambda_c \frac{I_2^p + \sigma_z}{2} + \lambda_v \frac{I_2^p - \sigma_z}{2} \right)$$

$$\mathcal{B}_\tau^e = \left\{ \left|\phi_{c,\uparrow,\tau}^e\right\rangle, \left|\phi_{v,\uparrow,\tau}^e\right\rangle, \left|\phi_{c,\downarrow,\tau}^e\right\rangle, \left|\phi_{v,\downarrow,\tau}^e\right\rangle \right\}$$

Model

- Single-electron Hamiltonian

$$H^q_\tau(\vec{\Pi}) = I^s_2 \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I^p_2 - \sigma_z}{2}\right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s}\right) \otimes I^p_2 + \tau s_z \otimes \left(\lambda_c \frac{I^p_2 + \sigma_z}{2} + \lambda_v \frac{I^p_2 - \sigma_z}{2}\right)$$

$$\mathcal{B}^e_\tau = \left\{\left|\phi^e_{c,\uparrow,\tau}\right\rangle, \left|\phi^e_{v,\uparrow,\tau}\right\rangle, \left|\phi^e_{c,\downarrow,\tau}\right\rangle, \left|\phi^e_{v,\downarrow,\tau}\right\rangle\right\}$$

Model

- Single-electron Hamiltonian

$$H_\tau^q(\vec{\Pi}) = I_2^s \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I_2^p - \sigma_z}{2} \right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s} \right) \otimes I_2^p + \tau s_z \otimes \left(\lambda_c \frac{I_2^p + \sigma_z}{2} + \lambda_v \frac{I_2^p - \sigma_z}{2} \right)$$

$$\mathcal{B}_\tau^e = \left\{ \left|\phi_{c,\uparrow,\tau}^e\right\rangle, \left|\phi_{v,\uparrow,\tau}^e\right\rangle, \left|\phi_{c,\downarrow,\tau}^e\right\rangle, \left|\phi_{v,\downarrow,\tau}^e\right\rangle \right\}$$

Model

- Single-electron Hamiltonian

$$H^q_\tau(\vec{\Pi}) = I^s_2 \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I^p_2 - \sigma_z}{2}\right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s}\right) \otimes I^p_2 + \tau s_z \otimes \left(\lambda_c \frac{I^p_2 + \sigma_z}{2} + \lambda_v \frac{I^p_2 - \sigma_z}{2}\right)$$

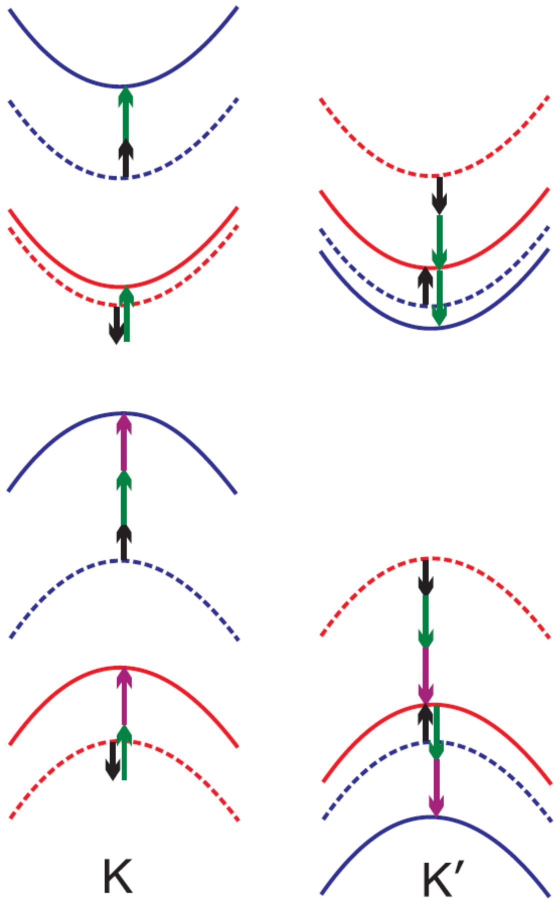
$$\mathcal{B}^e_\tau = \left\{ \left|\phi^e_{c,\uparrow,\tau}\right\rangle, \left|\phi^e_{v,\uparrow,\tau}\right\rangle, \left|\phi^e_{c,\downarrow,\tau}\right\rangle, \left|\phi^e_{v,\downarrow,\tau}\right\rangle \right\}$$

Model

- Single-electron Hamiltonian

$$H^q_\tau(\vec{\Pi}) = I^s_2 \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z\frac{I^p_2-\sigma_z}{2}\right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s}\right)\otimes I^p_2 + \tau s_z \otimes\left(\lambda_c\frac{I^p_2+\sigma_z}{2} + \lambda_v\frac{I^p_2-\sigma_z}{2}\right)$$

$$\mathcal{B}^e_\tau = \{|\phi^e_{c,\uparrow,\tau}\rangle, |\phi^e_{v,\uparrow,\tau}\rangle, |\phi^e_{c,\downarrow,\tau}\rangle, |\phi^e_{v,\downarrow,\tau}\rangle\}$$

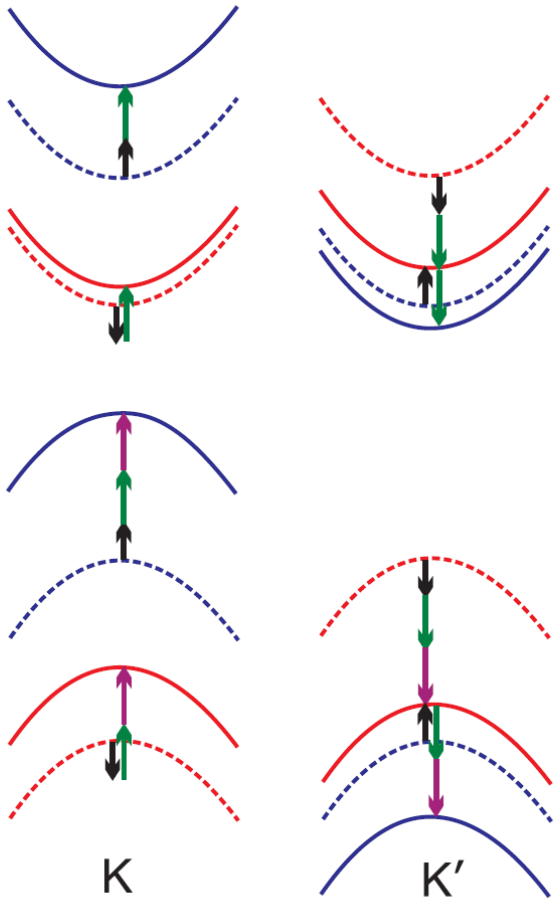


Model

- Single-electron Hamiltonian

$$H^q_\tau(\vec{\Pi}) = I^s_2 \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I^p_2 - \sigma_z}{2} \right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s} \right) \otimes I^p_2 + \tau s_z \otimes \left(\lambda_c \frac{I^p_2 + \sigma_z}{2} + \lambda_v \frac{I^p_2 - \sigma_z}{2} \right)$$

$$\mathcal{B}^e_\tau = \{ |\phi^e_{c,\uparrow,\tau}\rangle, |\phi^e_{v,\uparrow,\tau}\rangle, |\phi^e_{c,\downarrow,\tau}\rangle, |\phi^e_{v,\downarrow,\tau}\rangle \}$$



$$\vec{m}(\vec{k}) = i\frac{q}{2\hbar} \langle \vec{\nabla}_{\vec{k}} u | \times \left(H^q_{s,\tau}(\vec{k}) - E_{s,\tau}(\vec{k}) \right) | \vec{\nabla}_{\vec{k}} u \rangle$$

$$= \tau \frac{qa^2t^2\Delta_{s,\tau}}{4\hbar a^2 t^2 k^2 + \hbar \Delta^2_{s,\tau}} \vec{e}_z$$

Model

- Single-electron Hamiltonian

$$H_\tau^q(\vec{\Pi}) = I_2^s \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I_2^p - \sigma_z}{2}\right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s}\right) \otimes I_2^p + \tau s_z \otimes \left(\lambda_c \frac{I_2^p + \sigma_z}{2} + \lambda_v \frac{I_2^p - \sigma_z}{2}\right)$$

- Treat in-plane magnetic field in first-order perturbation

Model

- Single-electron Hamiltonian

$$H_{\tau}^{q}(\vec{\Pi}) = I_2^s \otimes \left(at\vec{\Pi}^{\tau}.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I_2^p - \sigma_z}{2} \right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s} \right) \otimes I_2^p + \tau s_z \otimes \left(\lambda_c \frac{I_2^p + \sigma_z}{2} + \lambda_v \frac{I_2^p - \sigma_z}{2} \right)$$

- Treat in-plane magnetic field in first-order perturbation

$$\mathcal{B}_{s,\tau}^{e} = \left\{ \left|\phi_{c,s,\tau}^{e}\right\rangle, \left|\phi_{v,s,\tau}^{e}\right\rangle \right\}$$

Model

- Single-electron Hamiltonian

$$H_\tau^q(\vec{\Pi}) = I_2^s \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I_2^p - \sigma_z}{2}\right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s}\right) \otimes I_2^p + \tau s_z \otimes \left(\lambda_c \frac{I_2^p + \sigma_z}{2} + \lambda_v \frac{I_2^p - \sigma_z}{2}\right)$$

- Treat in-plane magnetic field in first-order perturbation

$$H_{s,\tau}^q(\vec{\Pi}) = at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I_2^p - \sigma_z}{2} - s\frac{q}{e}\mu_B B_z I_2 + s\tau\left(\tilde{\lambda}_c \frac{I_2^p + \sigma_z}{2} + \tilde{\lambda}_v \frac{I_2^p - \sigma_z}{2}\right)$$

$$\mathcal{B}_{s,\tau}^e = \left\{\left|\phi_{c,s,\tau}^e\right\rangle, \left|\phi_{v,s,\tau}^e\right\rangle\right\}$$

Model

- Single-electron Hamiltonian

$$H^q_\tau(\vec{\Pi}) = I^s_2 \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I^p_2 - \sigma_z}{2} \right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s} \right) \otimes I^p_2 + \tau s_z \otimes \left(\lambda_c \frac{I^p_2 + \sigma_z}{2} + \lambda_v \frac{I^p_2 - \sigma_z}{2} \right)$$

- Treat in-plane magnetic field in first-order perturbation

$$H^q_{s,\tau}(\vec{\Pi}) = at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I^p_2 - \sigma_z}{2} - s\frac{q}{e}\mu_B B_z I_2 + s\tau \left(\tilde{\lambda}_c \frac{I^p_2 + \sigma_z}{2} + \tilde{\lambda}_v \frac{I^p_2 - \sigma_z}{2} \right)$$

$$\tilde{\lambda}_{c(v)} = \lambda_{c(v)} + \frac{\mu_B^2 B_x^2}{2\lambda_{c(v)}}$$

$$\mathcal{B}^e_{s,\tau} = \left\{ \left|\phi^e_{c,s,\tau}\right\rangle, \left|\phi^e_{v,s,\tau}\right\rangle \right\}$$

Model

- Single-electron Hamiltonian

$$H_\tau^q(\vec{\Pi}) = I_2^s \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I_2^p - \sigma_z}{2}\right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s}\right) \otimes I_2^p + \tau s_z \otimes \left(\lambda_c \frac{I_2^p + \sigma_z}{2} + \lambda_v \frac{I_2^p - \sigma_z}{2}\right)$$

- Treat in-plane magnetic field in first-order perturbation

$$H_{s,\tau}^q(\vec{\Pi}) = at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I_2^p - \sigma_z}{2} - s\frac{q}{e}\mu_B B_z I_2 + s\tau\left(\tilde{\lambda}_c \frac{I_2^p + \sigma_z}{2} + \tilde{\lambda}_v \frac{I_2^p - \sigma_z}{2}\right)$$

$$\tilde{\lambda}_{c(v)} = \lambda_{c(v)} + \frac{\mu_B^2 B_x^2}{2\lambda_{c(v)}}$$

$$\mathcal{B}_{s,\tau}^e = \left\{\left|\phi_{c,s,\tau}^e\right\rangle, \left|\phi_{v,s,\tau}^e\right\rangle\right\}$$

$$\left|\Psi_{n,i}^{s,\tau}\right\rangle = \frac{1}{\sqrt{1+\delta_i^2}}\left(\left|\Psi_{n,i}^{s,\tau}\right\rangle_0 + s\tau\delta_i\left|\Psi_{n,i}^{-s,\tau}\right\rangle_0\right) \qquad \delta_i = \frac{\mu_B B_x}{2\lambda_i}$$

Model

- Single-electron Hamiltonian

$$H^q_\tau(\vec{\Pi}) = I^s_2 \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I^p_2 - \sigma_z}{2}\right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s}\right) \otimes I^p_2 + \tau s_z \otimes \left(\lambda_c \frac{I^p_2 + \sigma_z}{2} + \lambda_v \frac{I^p_2 - \sigma_z}{2}\right)$$

- Treat in-plane magnetic field in first-order perturbation

$$H^q_{s,\tau}(\vec{\Pi}) = at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I^p_2 - \sigma_z}{2} - s\frac{q}{e}\mu_B B_z I_2 + s\tau\left(\tilde{\lambda}_c \frac{I^p_2 + \sigma_z}{2} + \tilde{\lambda}_v \frac{I^p_2 - \sigma_z}{2}\right)$$

- Single-hole Hamiltonian

Model

- Single-electron Hamiltonian

$$H^q_\tau(\vec{\Pi}) = I^s_2 \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I^p_2 - \sigma_z}{2}\right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s}\right) \otimes I^p_2 + \tau s_z \otimes \left(\lambda_c \frac{I^p_2 + \sigma_z}{2} + \lambda_v \frac{I^p_2 - \sigma_z}{2}\right)$$

- Treat in-plane magnetic field in first-order perturbation

$$H^q_{s,\tau}(\vec{\Pi}) = at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I^p_2 - \sigma_z}{2} - s\frac{q}{e}\mu_B B_z I_2 + s\tau\left(\tilde{\lambda}_c \frac{I^p_2 + \sigma_z}{2} + \tilde{\lambda}_v \frac{I^p_2 - \sigma_z}{2}\right)$$

- Single-hole Hamiltonian $H^{q,h}_{s,\tau}(\vec{\Pi}) = -H^{-q,e}_{-s,-\tau}(-\vec{\Pi})$

Model

- Single-electron Hamiltonian

$$H^q_\tau(\vec{\Pi}) = I^s_2 \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I^p_2 - \sigma_z}{2}\right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s}\right) \otimes I^p_2 + \tau s_z \otimes \left(\lambda_c \frac{I^p_2 + \sigma_z}{2} + \lambda_v \frac{I^p_2 - \sigma_z}{2}\right)$$

- Treat in-plane magnetic field in first-order perturbation

$$H^q_{s,\tau}(\vec{\Pi}) = at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I^p_2 - \sigma_z}{2} - s\frac{q}{e}\mu_B B_z I_2 + s\tau\left(\tilde{\lambda}_c \frac{I^p_2 + \sigma_z}{2} + \tilde{\lambda}_v \frac{I^p_2 - \sigma_z}{2}\right)$$

- Single-hole Hamiltonian $H^{q,h}_{s,\tau}(\vec{\Pi}) = -H^{-q,e}_{-s,-\tau}(-\vec{\Pi})$
- Total exciton Hamiltonian in the basis $\mathcal{B}_\alpha = \mathcal{B}^e_{s^e,\tau^e} \otimes \mathcal{B}^h_{s^h,\tau^h}$

Model

- Single-electron Hamiltonian

$$H^q_\tau(\vec{\Pi}) = I^s_2 \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I^p_2 - \sigma_z}{2} \right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s} \right) \otimes I^p_2 + \tau s_z \otimes \left(\lambda_c \frac{I^p_2 + \sigma_z}{2} + \lambda_v \frac{I^p_2 - \sigma_z}{2} \right)$$

- Treat in-plane magnetic field in first-order perturbation

$$H^q_{s,\tau}(\vec{\Pi}) = at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I^p_2 - \sigma_z}{2} - s\frac{q}{e}\mu_B B_z I_2 + s\tau \left(\tilde{\lambda}_c \frac{I^p_2 + \sigma_z}{2} + \tilde{\lambda}_v \frac{I^p_2 - \sigma_z}{2} \right)$$

- Single-hole Hamiltonian $H^{q,h}_{s,\tau}(\vec{\Pi}) = -H^{-q,e}_{-s,-\tau}(-\vec{\Pi})$
- Total exciton Hamiltonian in the basis $\mathcal{B}_\alpha = \mathcal{B}^e_{s^e,\tau^e} \otimes \mathcal{B}^h_{s^h,\tau^h}$

$$H^{\text{exc}}_\alpha(\vec{\Pi}^e, \vec{\Pi}^h, r_{eh}) = H^{q^e}_{s^e,\tau^e}(\vec{\Pi}^e) \otimes I_2 - I_2 \otimes H^{-q^h}_{-s^h,-\tau^h}(-\vec{\Pi}^h) - V(r_{eh}) I_4$$

Model

- Single-electron Hamiltonian

$$H_\tau^q(\vec{\Pi}) = I_2^s \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I_2^p - \sigma_z}{2}\right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s}\right) \otimes I_2^p + \tau s_z \otimes \left(\lambda_c \frac{I_2^p + \sigma_z}{2} + \lambda_v \frac{I_2^p - \sigma_z}{2}\right)$$

- Treat in-plane magnetic field in first-order perturbation

$$H_{s,\tau}^q(\vec{\Pi}) = at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I_2^p - \sigma_z}{2} - s\frac{q}{e}\mu_B B_z I_2 + s\tau\left(\tilde{\lambda}_c \frac{I_2^p + \sigma_z}{2} + \tilde{\lambda}_v \frac{I_2^p - \sigma_z}{2}\right)$$

- Single-hole Hamiltonian $H_{s,\tau}^{q,h}(\vec{\Pi}) = -H_{-s,-\tau}^{-q,e}(-\vec{\Pi})$
- Total exciton Hamiltonian in the basis $\mathcal{B}_\alpha = \mathcal{B}_{s^e,\tau^e}^e \otimes \mathcal{B}_{s^h,\tau^h}^h$

$$H_\alpha^{\rm exc}(\vec{\Pi}^e, \vec{\Pi}^h, r_{eh}) = H_{s^e,\tau^e}^{q^e}(\vec{\Pi}^e) \otimes I_2 - I_2 \otimes H_{-s^h,-\tau^h}^{-q^h}(-\vec{\Pi}^h) - V(r_{eh}) I_4$$

- Exciton eigenvalue equation

Model

- Single-electron Hamiltonian

$$H^q_\tau(\vec{\Pi}) = I^s_2 \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I^p_2 - \sigma_z}{2} \right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s} \right) \otimes I^p_2 + \tau s_z \otimes \left(\lambda_c \frac{I^p_2 + \sigma_z}{2} + \lambda_v \frac{I^p_2 - \sigma_z}{2} \right)$$

- Treat in-plane magnetic field in first-order perturbation

$$H^q_{s,\tau}(\vec{\Pi}) = at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I^p_2 - \sigma_z}{2} - s\frac{q}{e}\mu_B B_z I_2 + s\tau \left(\tilde{\lambda}_c \frac{I^p_2 + \sigma_z}{2} + \tilde{\lambda}_v \frac{I^p_2 - \sigma_z}{2} \right)$$

- Single-hole Hamiltonian $H^{q,h}_{s,\tau}(\vec{\Pi}) = -H^{-q,e}_{-s,-\tau}(-\vec{\Pi})$
- Total exciton Hamiltonian in the basis $\mathcal{B}_\alpha = \mathcal{B}^e_{s^e,\tau^e} \otimes \mathcal{B}^h_{s^h,\tau^h}$

$$H^{\text{exc}}_\alpha(\vec{\Pi}^e, \vec{\Pi}^h, r_{eh}) = H^{q^e}_{s^e,\tau^e}(\vec{\Pi}^e) \otimes I_2 - I_2 \otimes H^{-q^h}_{-s^h,-\tau^h}(-\vec{\Pi}^h) - V(r_{eh}) I_4$$

- Exciton eigenvalue equation

$$H^{exc}_\alpha(\vec{k}^e, \vec{k}^h, r_{eh}) \left|\Psi^{exc}_\alpha\right\rangle = E^{exc}_\alpha(\vec{k}^e, \vec{k}^h) \left|\Psi^{exc}_\alpha\right\rangle$$

Model

- Single-electron Hamiltonian

$$H^q_\tau(\vec{\Pi}) = I^s_2 \otimes \left(at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I^p_2-\sigma_z}{2}\right) - \left(\frac{q}{e}\mu_B \vec{B}.\vec{s}\right) \otimes I^p_2 + \tau s_z \otimes \left(\lambda_c \frac{I^p_2+\sigma_z}{2} + \lambda_v \frac{I^p_2-\sigma_z}{2}\right)$$

- Treat in-plane magnetic field in first-order perturbation

$$H^q_{s,\tau}(\vec{\Pi}) = at\vec{\Pi}^\tau.\vec{\sigma} + \frac{\Delta}{2}\sigma_z - 2\tau\frac{q}{e}\mu_B B_z \frac{I^p_2-\sigma_z}{2} - s\frac{q}{e}\mu_B B_z I_2 + s\tau\left(\tilde{\lambda}_c \frac{I^p_2+\sigma_z}{2} + \tilde{\lambda}_v \frac{I^p_2-\sigma_z}{2}\right)$$

- Single-hole Hamiltonian $H^{q,h}_{s,\tau}(\vec{\Pi}) = -H^{-q,e}_{-s,-\tau}(-\vec{\Pi})$
- Total exciton Hamiltonian in the basis $\mathcal{B}_\alpha = \mathcal{B}^e_{s^e,\tau^e} \otimes \mathcal{B}^h_{s^h,\tau^h}$

$$H^{\rm exc}_\alpha(\vec{\Pi}^e, \vec{\Pi}^h, r_{eh}) = H^{q^e}_{s^e,\tau^e}(\vec{\Pi}^e) \otimes I_2 - I_2 \otimes H^{-q^h}_{-s^h,-\tau^h}(-\vec{\Pi}^h) - V(r_{eh}) I_4$$

- Exciton eigenvalue equation

$$H^{exc}_\alpha(\vec{k}^e, \vec{k}^h, r_{eh}) \left|\Psi^{exc}_\alpha\right\rangle = E^{exc}_\alpha(\vec{k}^e, \vec{k}^h) \left|\Psi^{exc}_\alpha\right\rangle$$

- Decouple to 1 equation, solve self-consistently

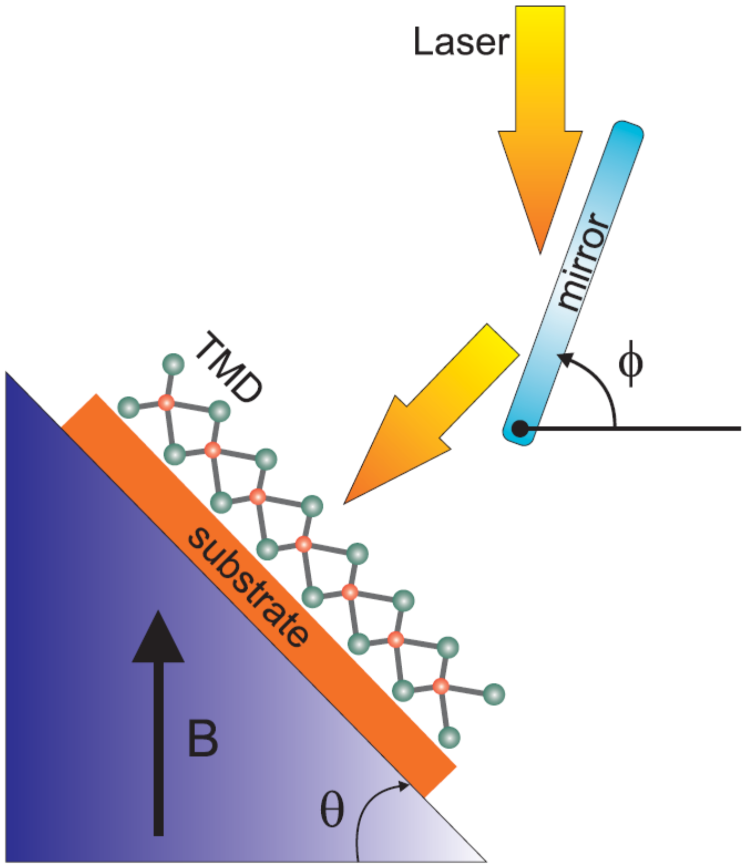
Results

Results

$$\alpha_{\pm}(\omega) \propto \frac{1}{\omega}\mathrm{Im}\left(\sum_{s^e,\tau^e,s^h,n} \frac{|\mathcal{P}_{\pm}^{s^e\tau^e}|^2|\phi_{c,v,\alpha,n}^{e,h}(0,0)|^2}{E_{\alpha,n}-\hbar\omega-i\gamma}\right)$$

Results

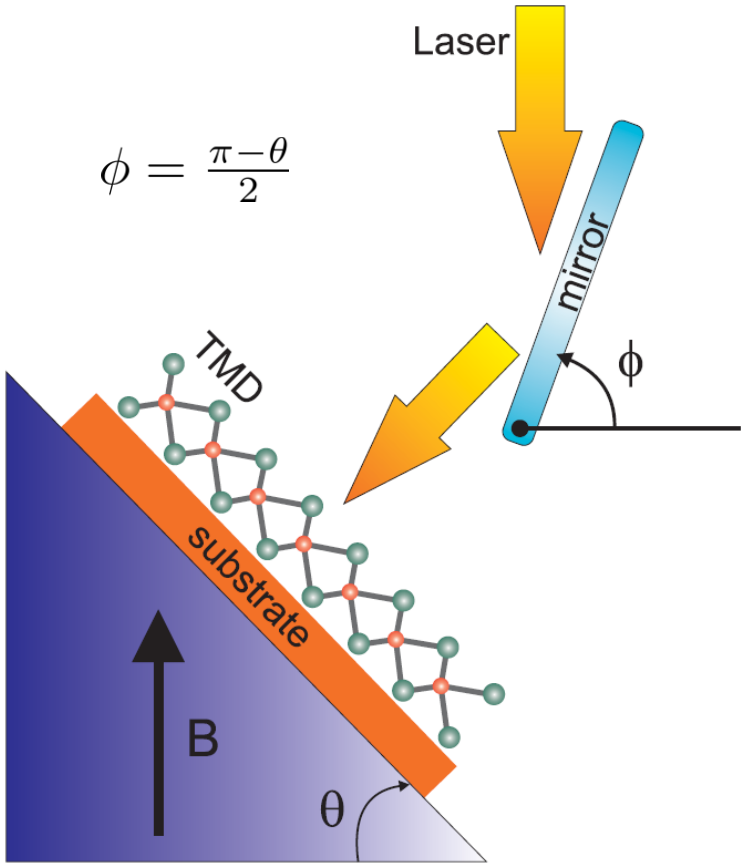
$$\alpha_{\pm}(\omega) \propto \frac{1}{\omega}\mathrm{Im}\left(\sum_{s^e,\tau^e,s^h,n} \frac{|\mathcal{P}_{\pm}^{s^e\tau^e}|^2 |\phi_{c,v,\alpha,n}^{e,h}(0,0)|^2}{E_{\alpha,n}-\hbar\omega-i\gamma}\right)$$



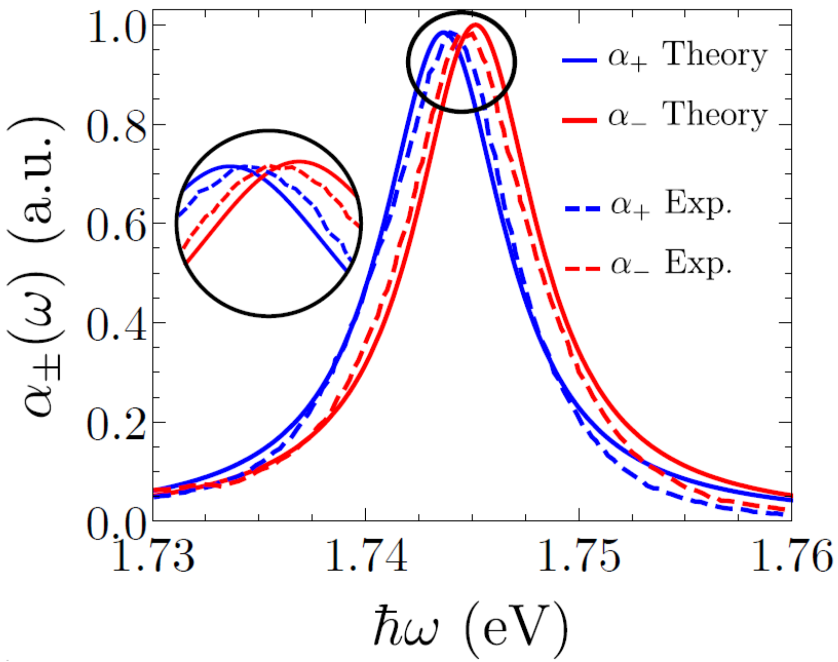
Results

$$\alpha_{\pm}(\omega) \propto \frac{1}{\omega}\mathrm{Im}\left(\sum_{s^e,\tau^e,s^h,n} \frac{|\mathcal{P}_{\pm}^{s^e\tau^e}|^2|\phi_{c,v,\alpha,n}^{e,h}(0,0)|^2}{E_{\alpha,n}-\hbar\omega-i\gamma}\right)$$

$$\phi = \frac{\pi-\theta}{2}$$

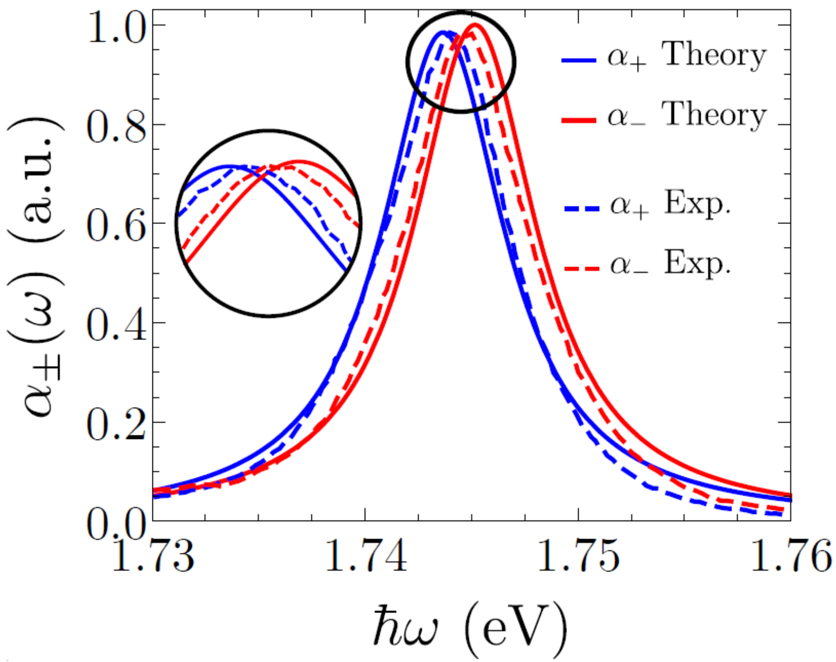


Results

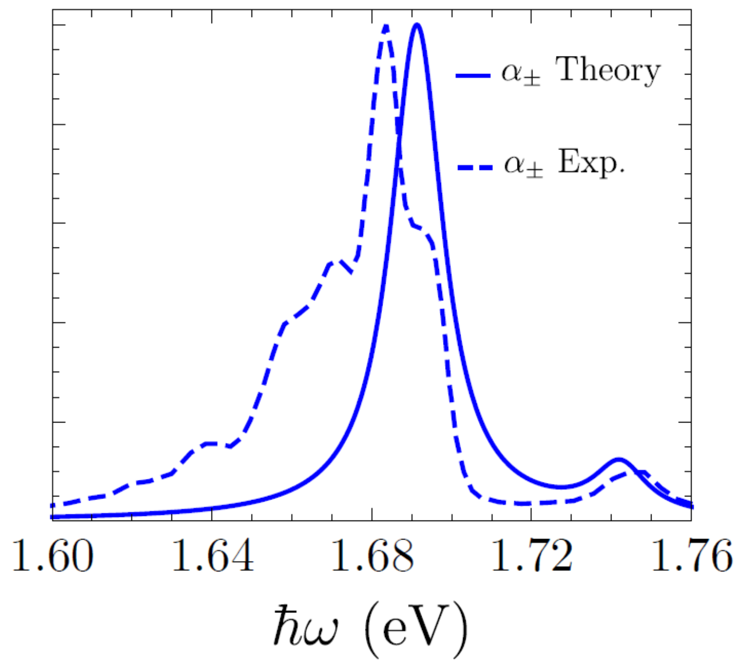


$\theta = 0°$

Results

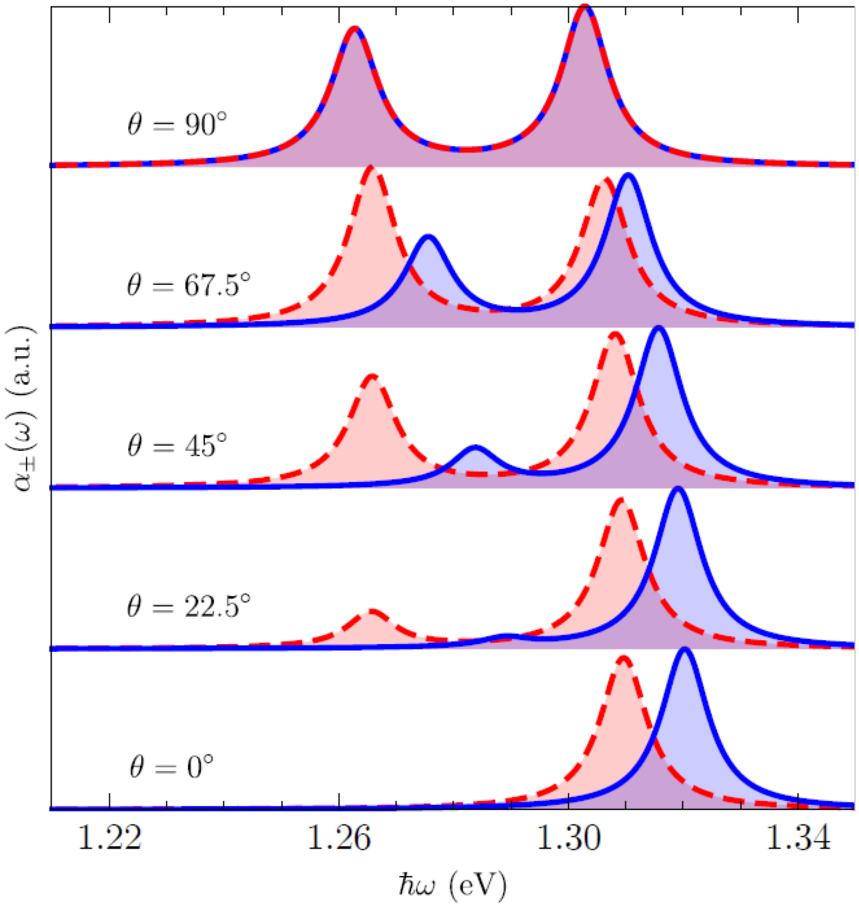


$\theta = 0°$



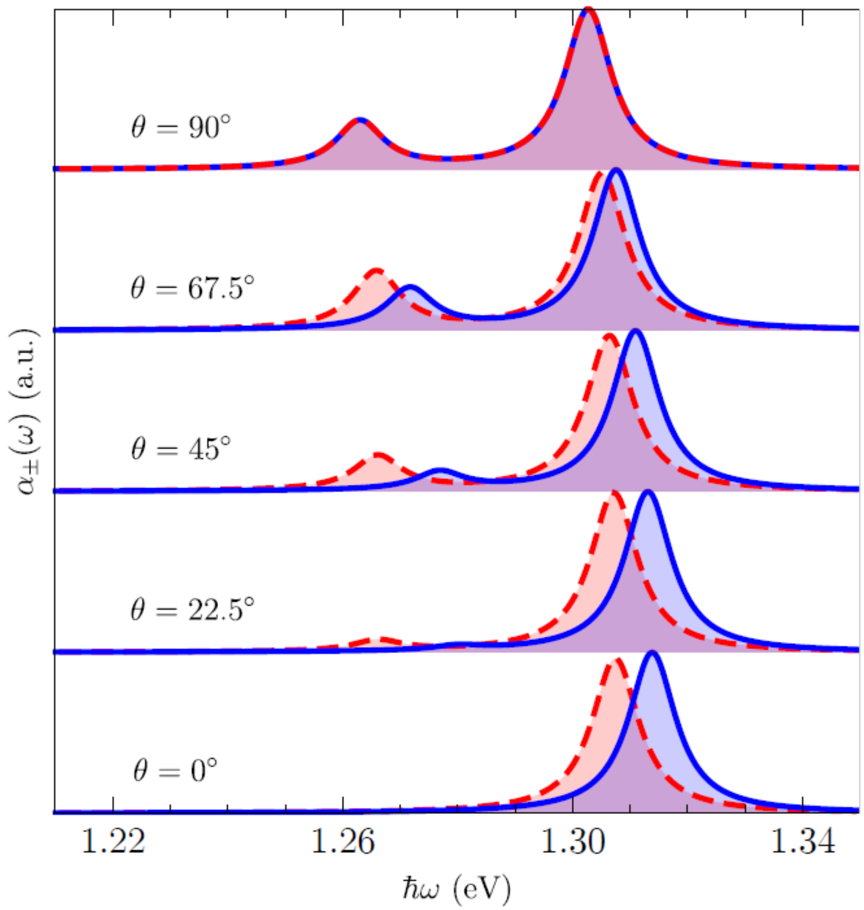
$\theta = 90°$

Results



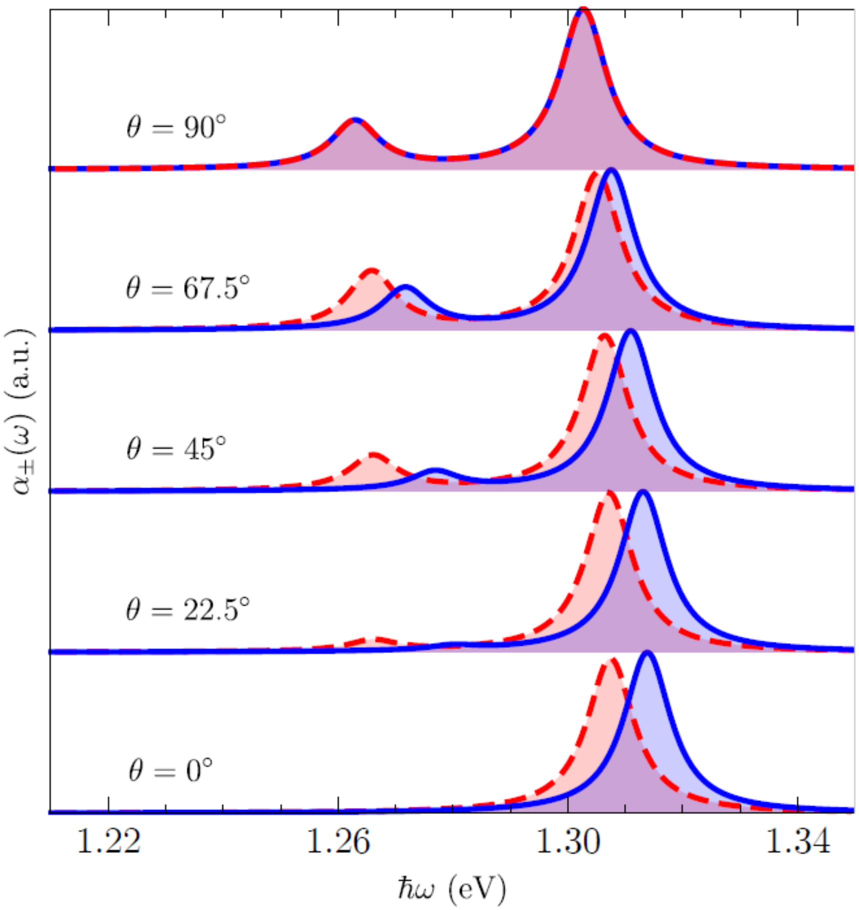
$\theta = 90°$
$\theta = 67.5°$
$\theta = 45°$
$\theta = 22.5°$
$\theta = 0°$
$\alpha_\pm(\omega)$ (a.u.)
1.22
1.26
1.30
1.34
$\hbar\omega$ (eV)

Results

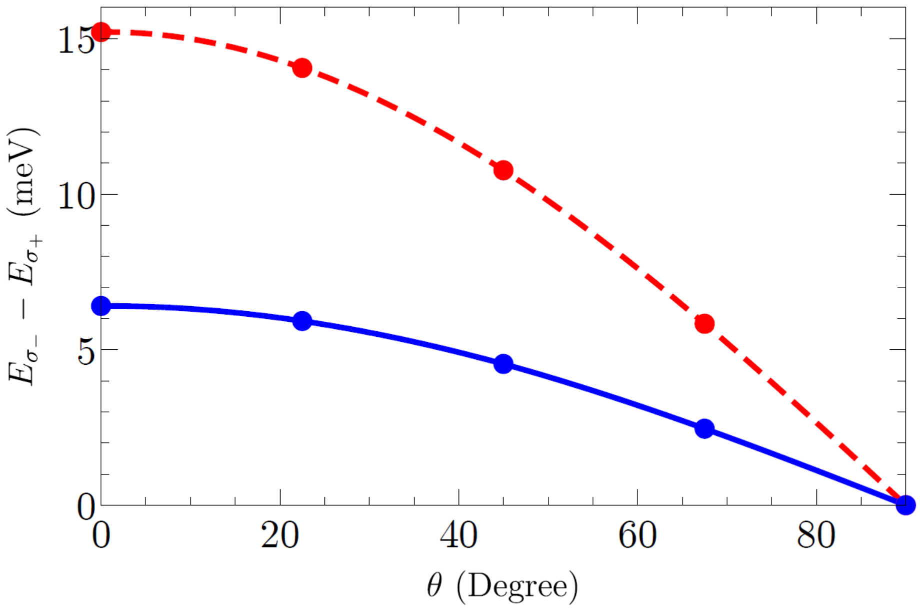


$\theta = 90°$
$\theta = 67.5°$
$\theta = 45°$
$\theta = 22.5°$
$\theta = 0°$
$\alpha_{\pm}(\omega)$ (a.u.)
1.22
1.26
1.30
1.34
$\hbar\omega$ (eV)

Results

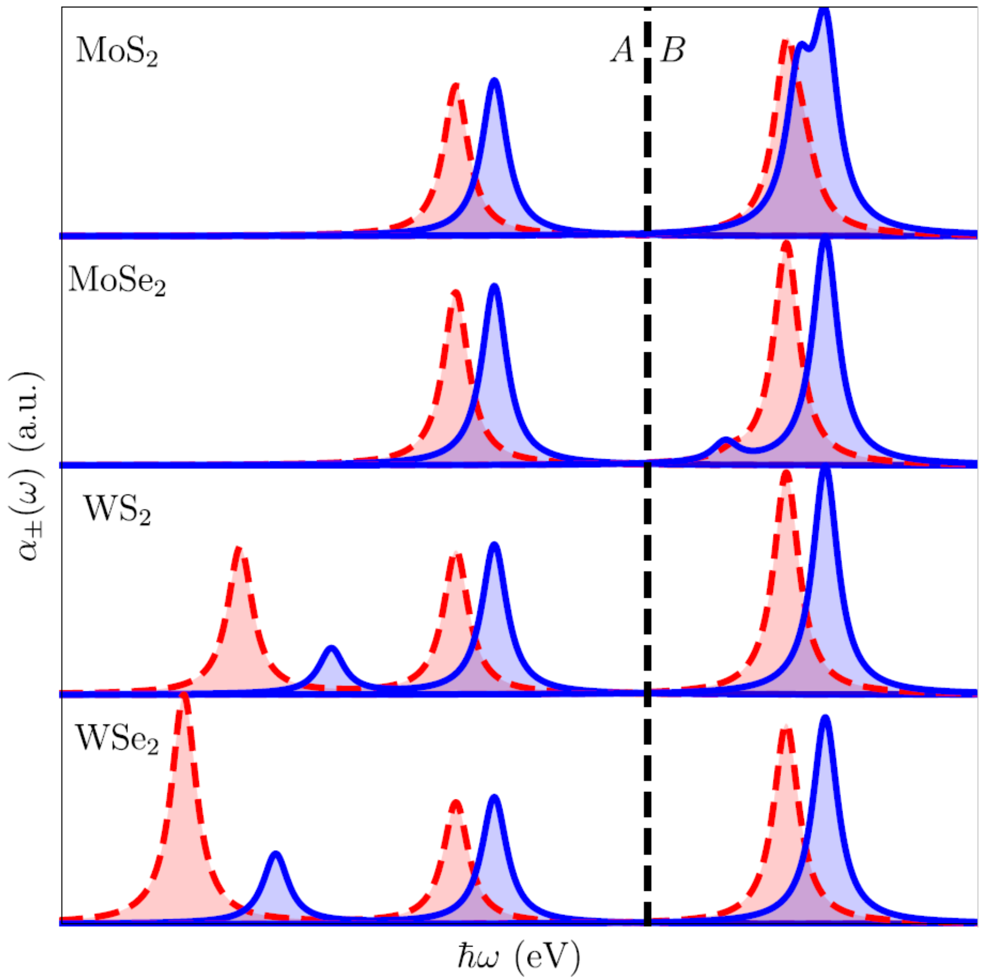


$\theta = 90°$
$\theta = 67.5°$
$\theta = 45°$
$\theta = 22.5°$
$\theta = 0°$
$\alpha_{\pm}(\omega)$ (a.u.)
1.22
1.26
1.30
1.34
$\hbar\omega$ (eV)



$E_{\sigma_-} - E_{\sigma_+}$ (meV)
0
5
10
15
0
20
40
60
80
θ (Degree)

Results



$\theta = 45°$

Summary and conclusions

Summary and conclusions

- Perpendicular magnetic field

Summary and conclusions

- Perpendicular magnetic field
  ➡ Valley Zeeman effect

Summary and conclusions

- Perpendicular magnetic field
  ➡ Valley Zeeman effect
- Parallel magnetic field

Summary and conclusions

- Perpendicular magnetic field
  ➡ Valley Zeeman effect
- Parallel magnetic field
  ➡ Brightening of dark excitons

Summary and conclusions

- Perpendicular magnetic field
  ➡ Valley Zeeman effect
- Parallel magnetic field
  ➡ Brightening of dark excitons
- Tilted magnetic field

Summary and conclusions

- Perpendicular magnetic field
  ➡ Valley Zeeman effect
- Parallel magnetic field
  ➡ Brightening of dark excitons
- Tilted magnetic field
  ➡ Valley Zeeman effect of brightened dark excitons

Summary and conclusions

- Perpendicular magnetic field
  ➡ Valley Zeeman effect
- Parallel magnetic field
  ➡ Brightening of dark excitons
- Tilted magnetic field
  ➡ Valley Zeeman effect of brightened dark excitons
  ➡ Twice as large as valley Zeeman effect of bright excitons in the case of A excitons in tungsten-based TMDs