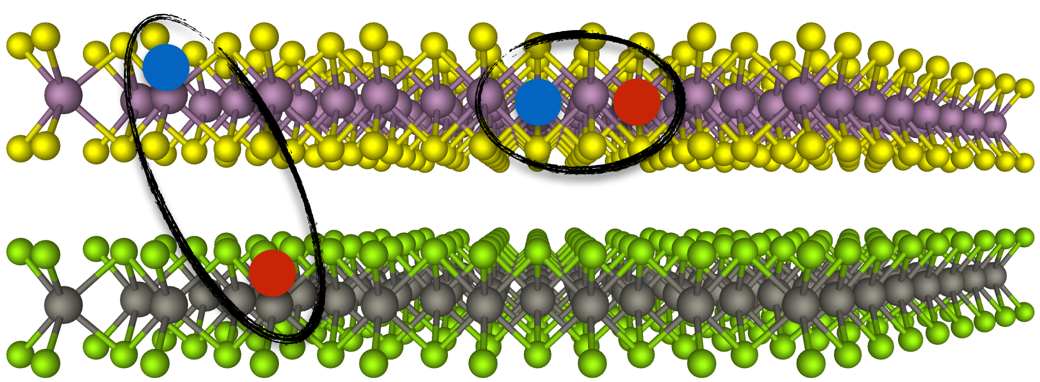
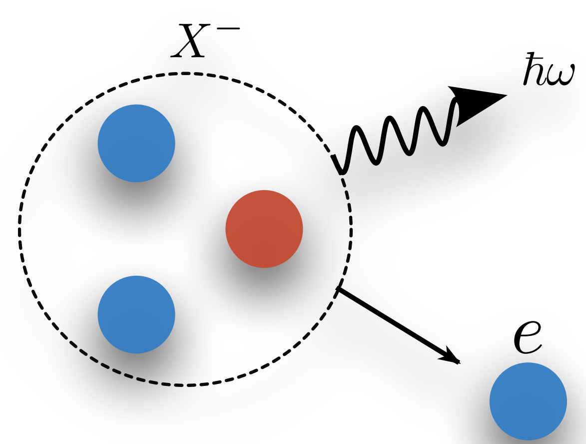
Interlayer excitons in heterobilayer TMDs and recoil in radiative recombination





Mark Danovich

Acknowledgments: David A. Ruiz–Tijerina, Vladimir Fal’ko

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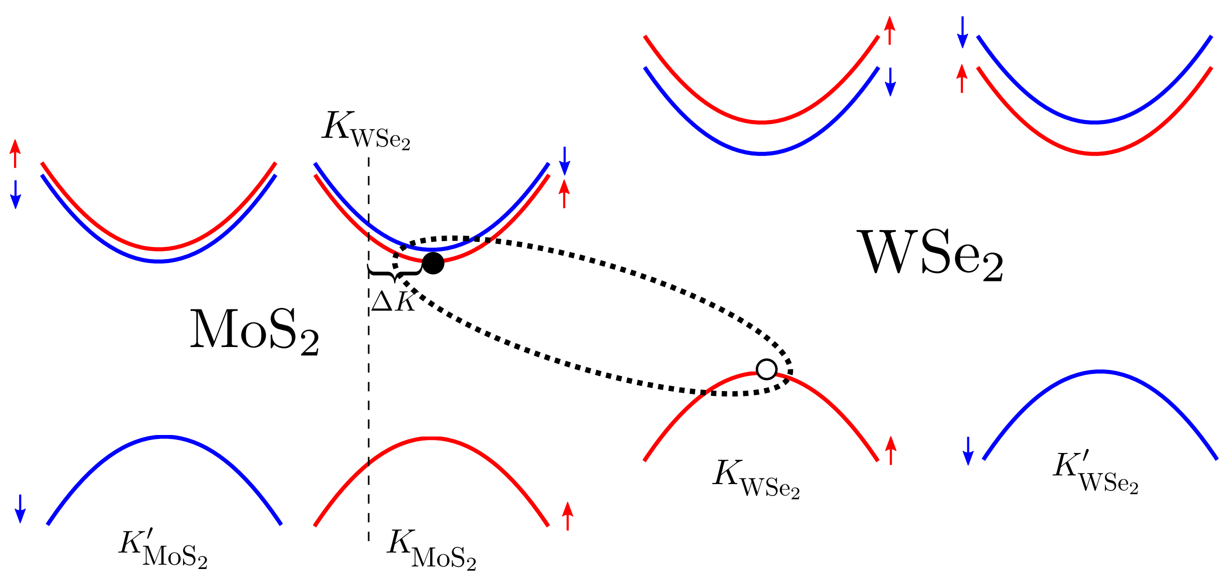
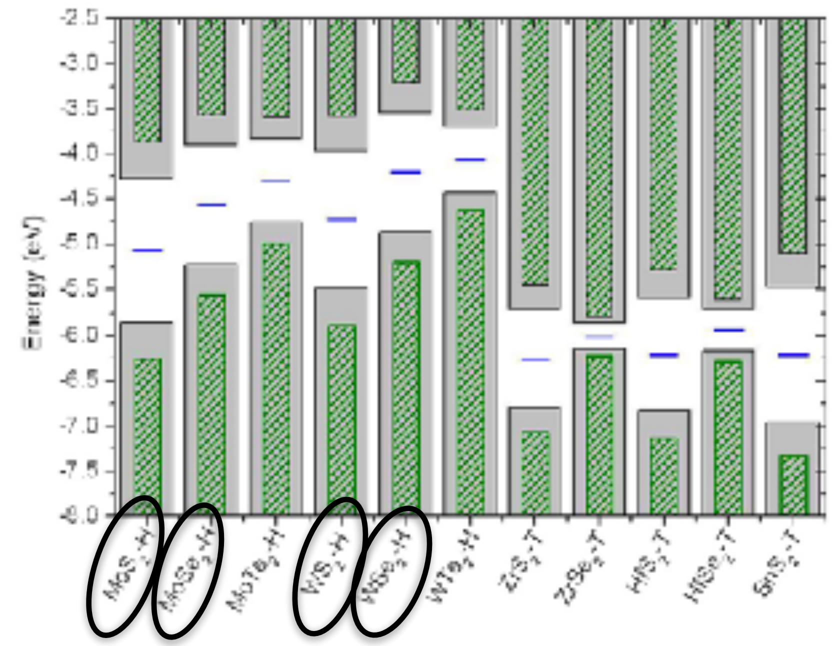
I. Interlayer excitons in heterobilayer TMDs

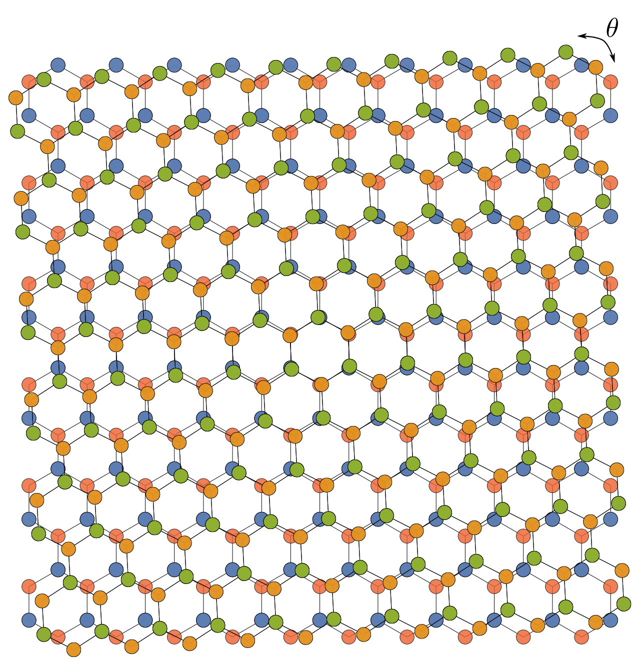


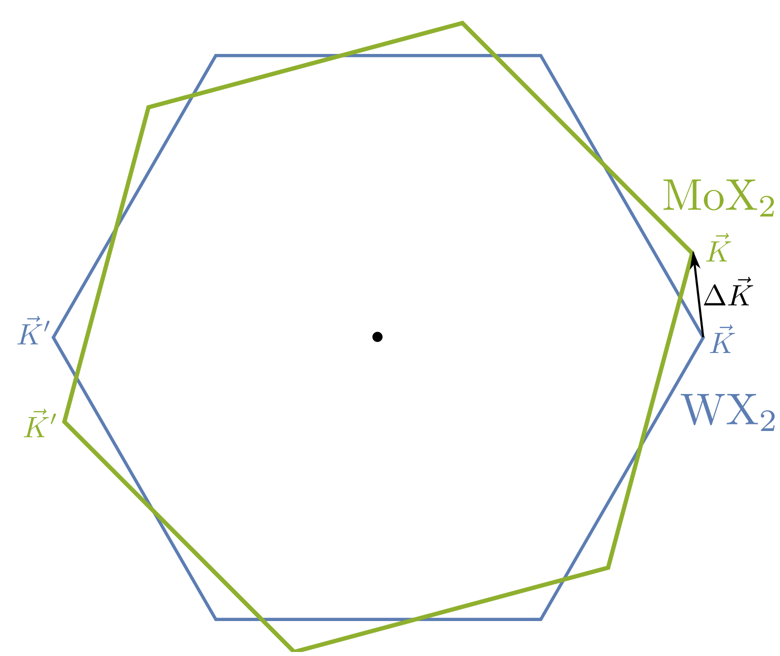
Type II band alignement

TMDs band alignments



Cheng Gong et al. Appl. Phys. Lett. ***103****, 053513 (2013)*





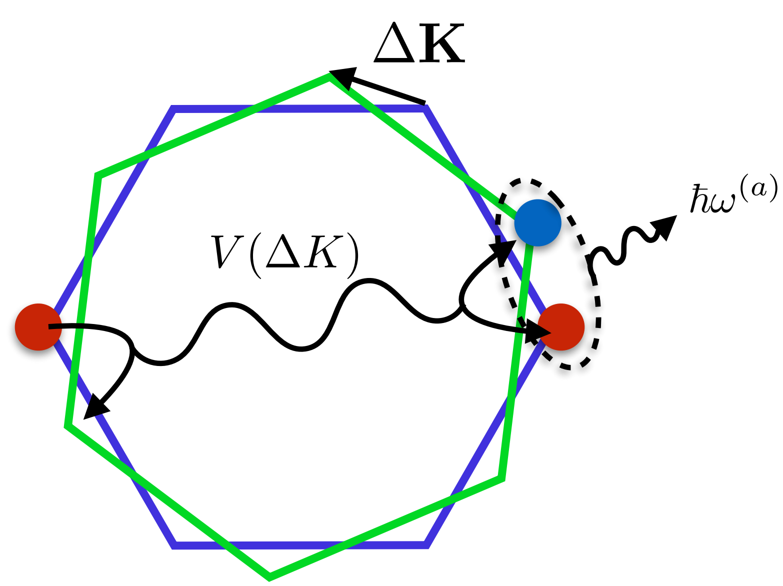
$$\Delta K = K_{\mathrm{MoX_2}}\sqrt{\delta^2+\theta^2}$$

$$\delta = \frac{a_{\mathrm{WX_2}} - a_{\mathrm{MoX_2}}}{a_{\mathrm{WX_2}}}$$

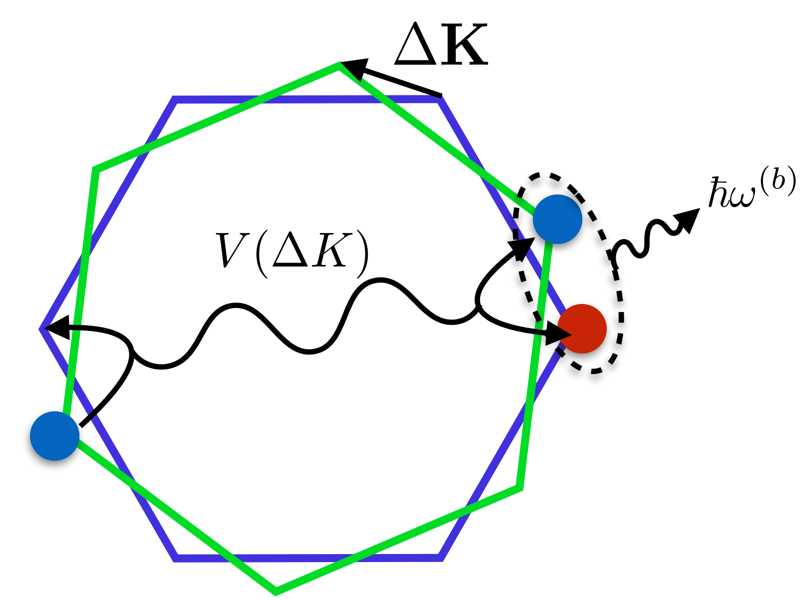
Misaligned heterobilayer

Recombination process

(a) Exciton-hole scattering



(b) Exciton-electron scattering



$$\hbar\omega^{(a)} = \Delta_g - E_b' - \frac{\hbar^2 \Delta K^2}{2m_h}$$

$$\hbar\omega^{(b)} = \Delta_g - E_b' - \frac{\hbar^2 \Delta K^2}{2m_{e'}}$$

Model

$$T_{\nu\nu'} = \sum_{G,G'} \delta_{k-k',\tau K+G-\tau K'+G'}\, t_{\nu\nu'}(\tau K + k + G)$$

$$\mathcal{H}_t = \begin{pmatrix} 0 & 0 & T_{cc'} & T_{vc'} \\ 0 & 0 & T_{cv'} & T_{vv'} \\ T^*_{cc'} & T^*_{cv'} & 0 & 0 \\ T^*_{vc'} & T^*_{vv'} & 0 & 0 \end{pmatrix}$$

$$\mathcal{H}_0(\mathbf{k} \to \mathbf{k} + \frac{e}{\hbar c}\mathbf{A})$$

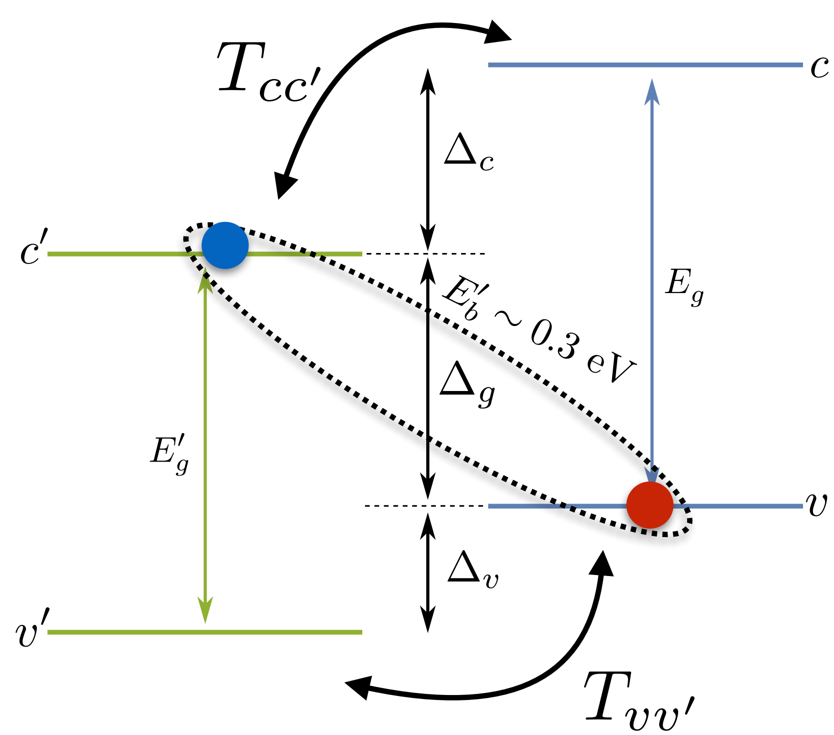
$$\mathcal{H} = \underbrace{\mathcal{H}_0}_{\text{Single layers}} + \underbrace{\overbrace{\mathcal{H}_t}}_{\text{Interlayer Tunneling}} + \underbrace{\mathcal{H}_{ee}}_{\text{e-e scattering}} + \underbrace{\overbrace{\mathcal{H}_r}}_{\text{In-plane polarised light}} + \underbrace{\mathcal{H}_z}_{\text{Out-of-plane polarised light}}$$

$$\mathcal{H}_0 = \begin{pmatrix} \frac{E'_g}{2} + \alpha' k'^2 & v'(\tau k'_x - i\epsilon k'_y) & 0 & 0 \\ v'(\tau k'_x + i\epsilon k'_y) & -\frac{E'_g}{2} + \beta' k'^2 & 0 & 0 \\ 0 & 0 & \frac{E_g}{2} + \alpha k^2 + \Delta & v(\tau k_x - i k_y) \\ 0 & 0 & v(\tau k_x + i k_y) & -\frac{E_g}{2} + \beta k^2 + \Delta \end{pmatrix}$$

$$V_k = \pm \frac{2\pi e^2}{k}$$

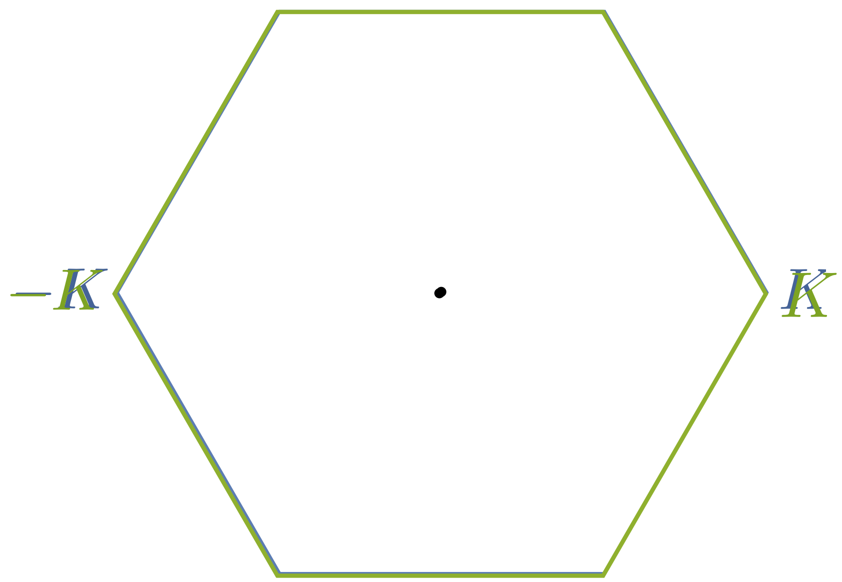
$$d_z = e\langle u_v | \hat{z} | u_{c'} \rangle$$

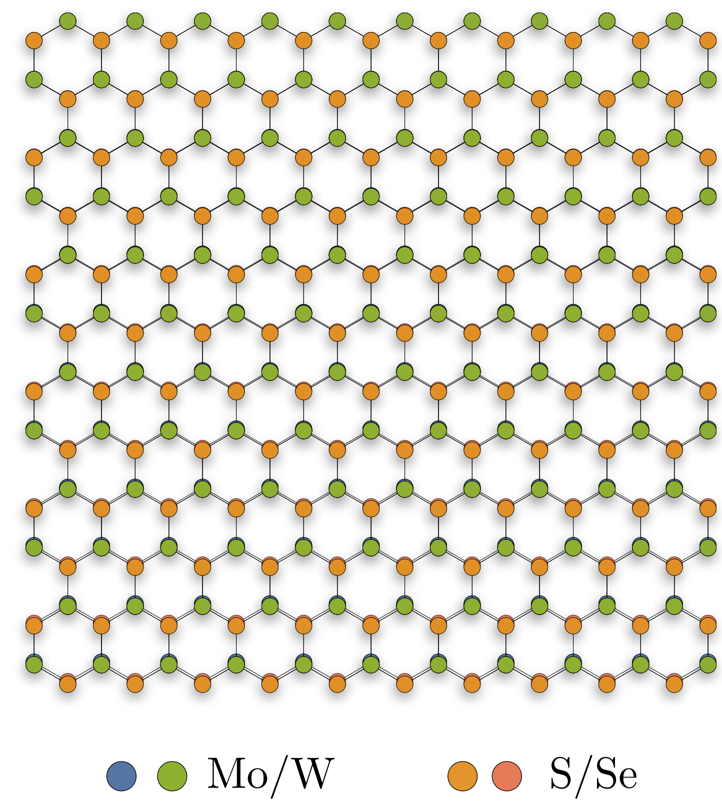
basis: $\{d'_0, d'_{\tau\epsilon 2}, d_0, d_{\tau 2}\}$

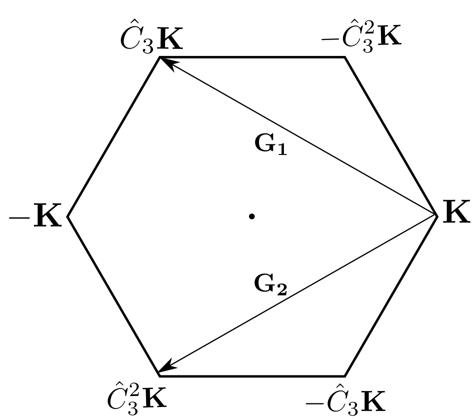


AA stacking

$$\tau = \tau'$$







$$H_t = \left(\begin{array}{cc|cc} 0 & 0 & t_{cc} & 0 \\ 0 & 0 & 0 & t_{vv} \\ \hline t_{cc} & 0 & 0 & 0 \\ 0 & t_{vv} & 0 & 0 \end{array}\right)$$

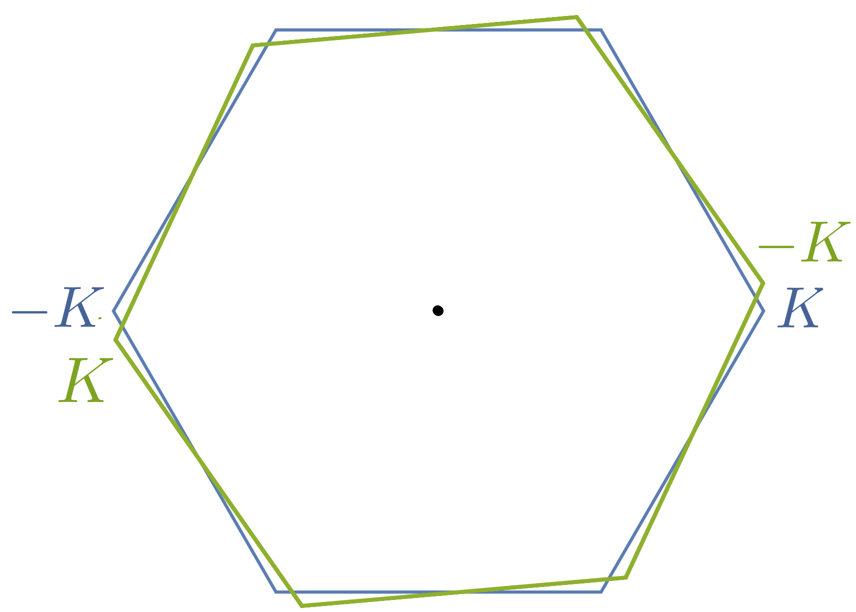
$$t_{cc} \sim 2.5 \text{ meV}^{*}$$
$$t_{vv} \sim 16 \text{ meV}$$

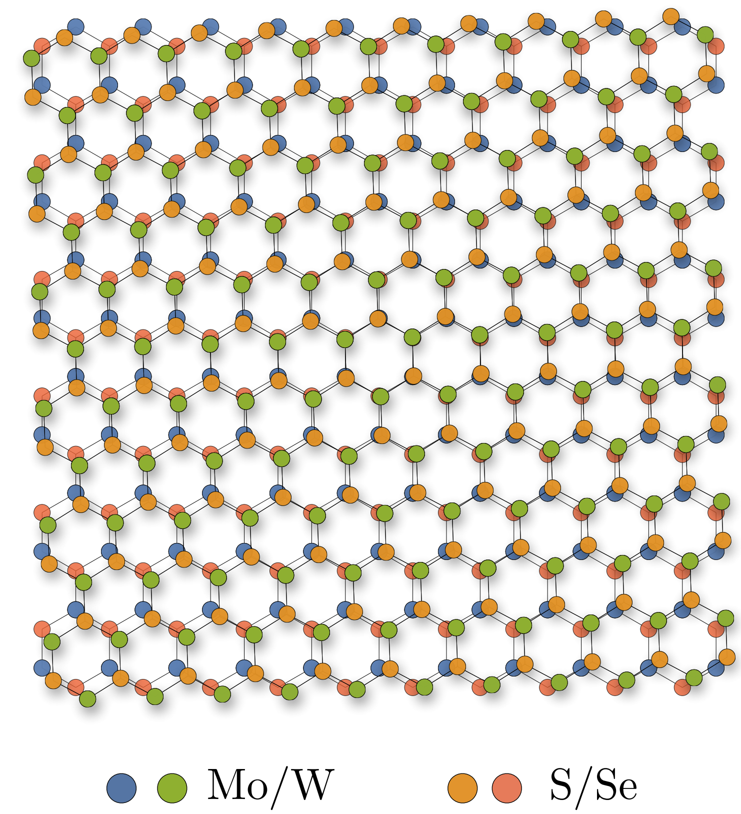
$$T_{\nu\nu'} = \sum_{G,G'} \delta_{k-k',\tau K+G-\tau K'+G'} t_{\nu\nu'}(\tau K + k + G)$$

* *Yong Wang et al. Appl. Phys. Rev. B* ***95****, 115429 (2017)*

AB stacking

$$\tau = -\tau'$$

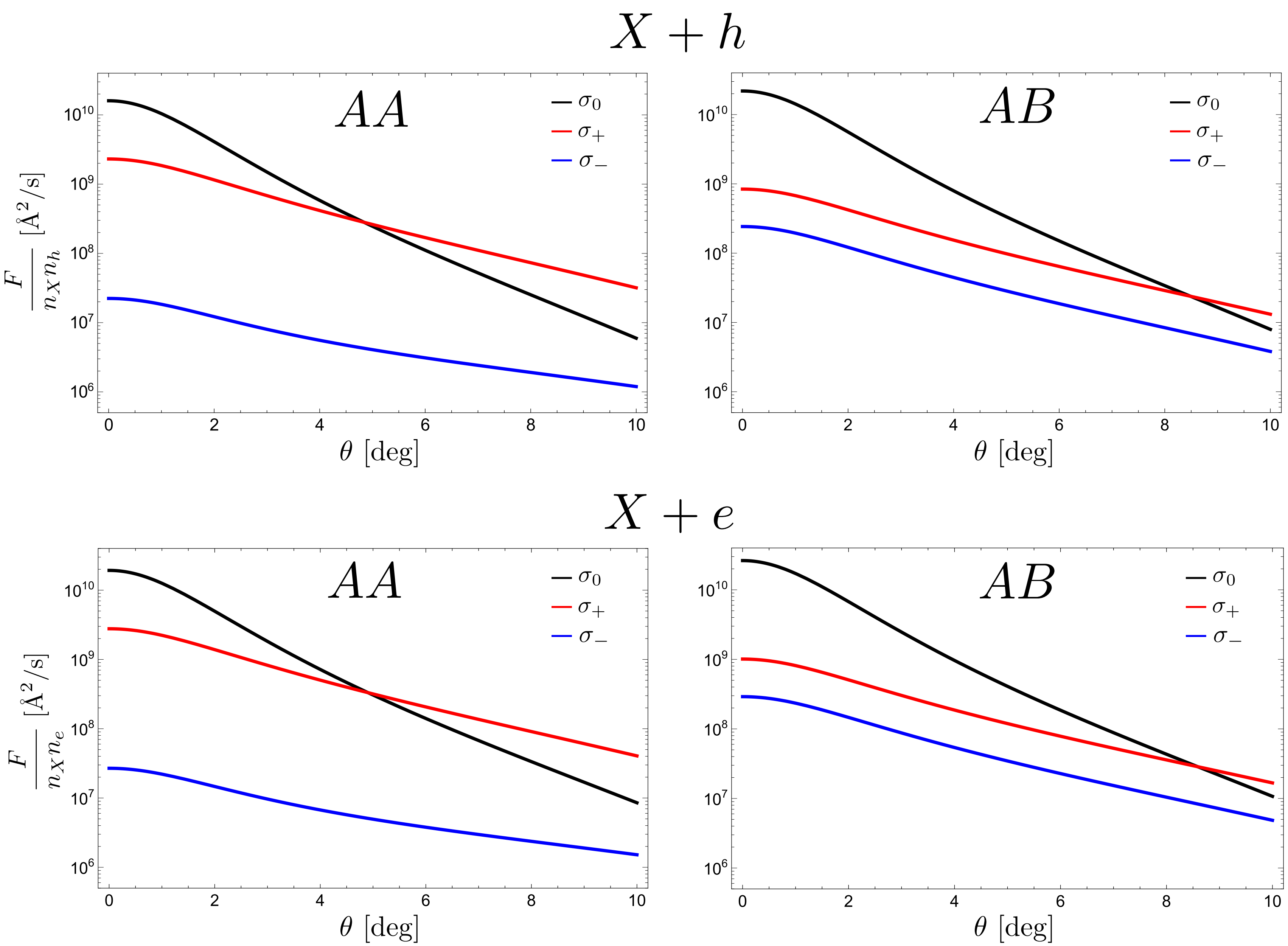




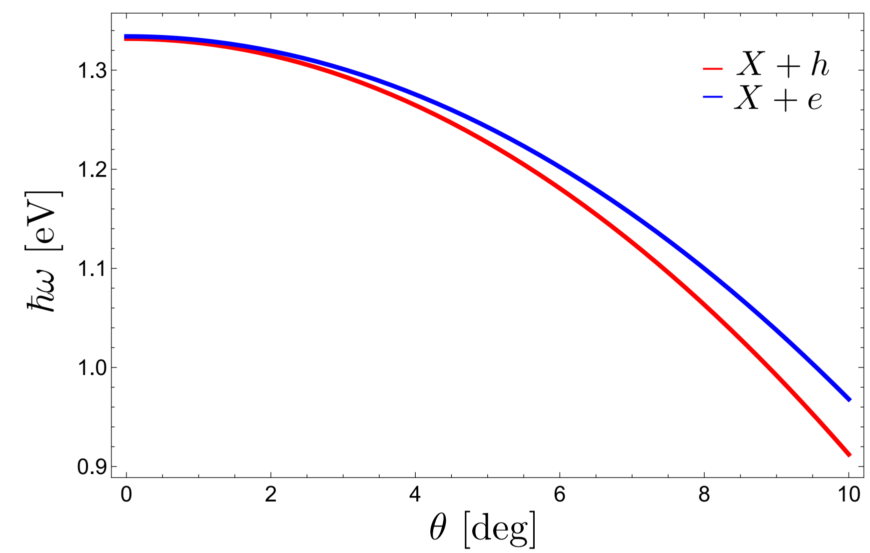
$$H_t = \left(\begin{array}{cc|cc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & t_{vv} \\ \hline 0 & 0 & 0 & 0 \\ 0 & t_{vv} & 0 & 0 \end{array}\right)$$

Results

Photon flux



Photon energy

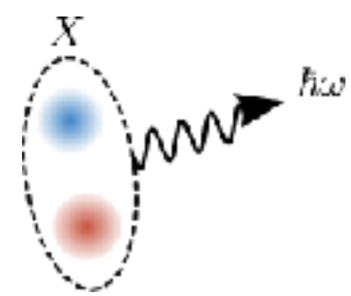


II. Recoil energy in radiative recombination

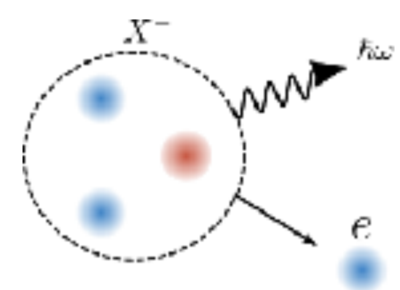
$$\boxed{\Delta E = E_K \left(1 - \frac{m_i}{m_f}\right)}$$

$$E_k \sim k_B T$$

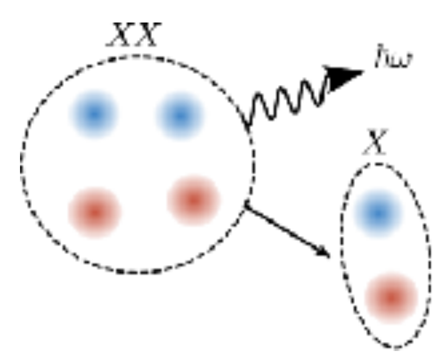
Excitons: No recoil



Trions: $\Delta E = -E_K \frac{m_X}{m_e}$



Biexcitons: $\Delta E = -E_K$

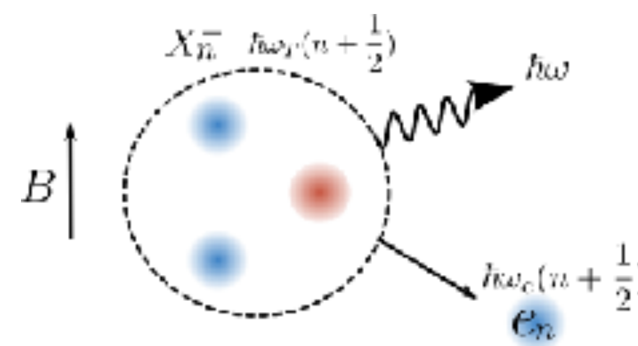


Recoil energy in recombination - with magnetic field

weak field approximation: $l_B \gg a_T$

Selection rule: $F_{nm} = \langle e_m | \hat{H}_r | T_n \rangle \propto \delta_{n,m}$

The Landau level index is conserved

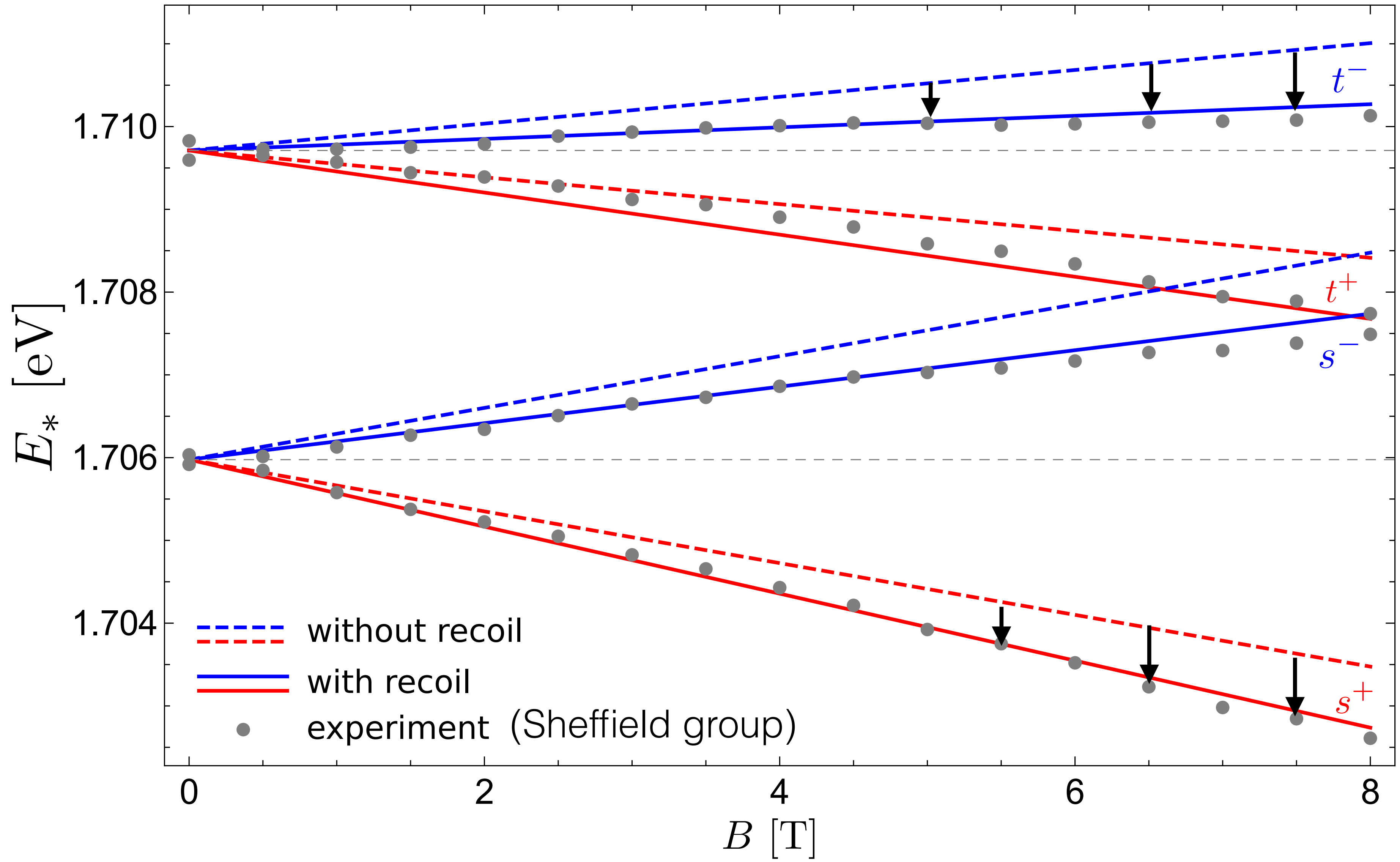


Recoil due to difference in cyclotron frequencies for trion and electron.

$$\boxed{\Delta E_n = (\hbar\omega_T - \hbar\omega_e)(n + \frac{1}{2})}$$

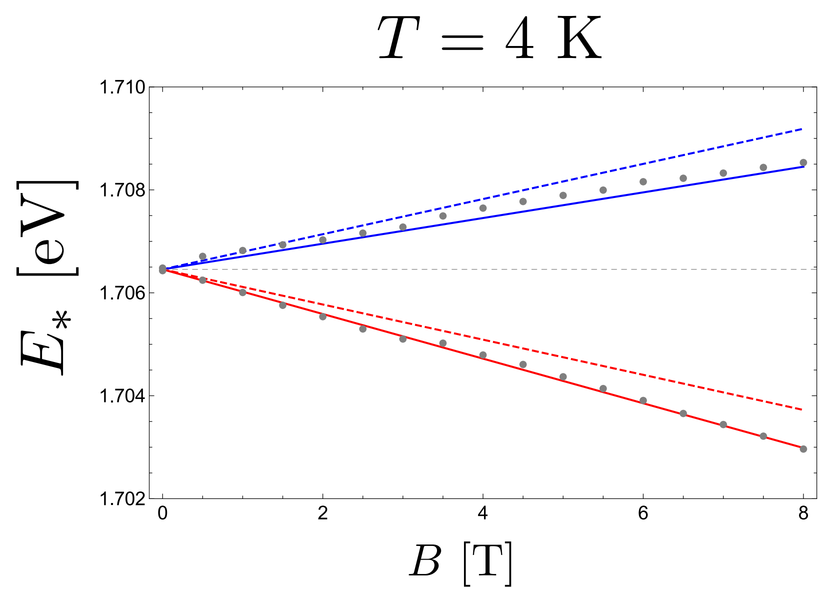
$$\hbar\omega_{T/e} = \frac{\hbar e B}{m_{T/e}}$$

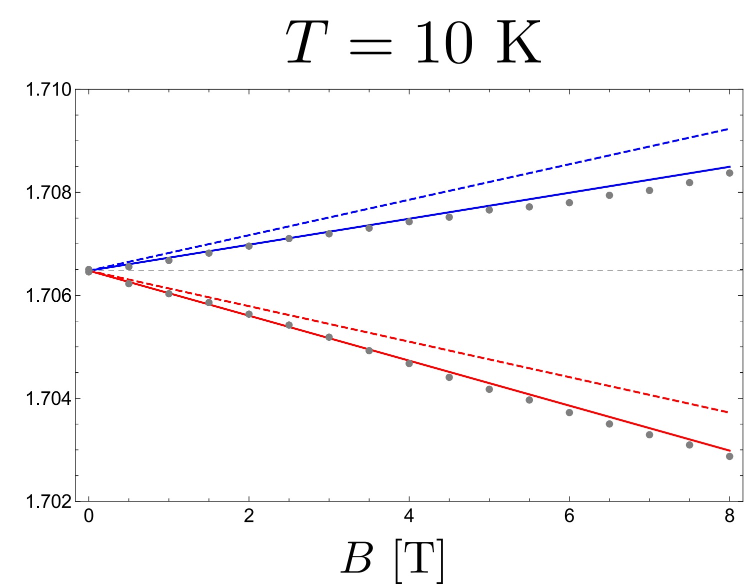
Comparison with experiment (WSe2, T= 30 K) using the recoil from n=0 Landau level only

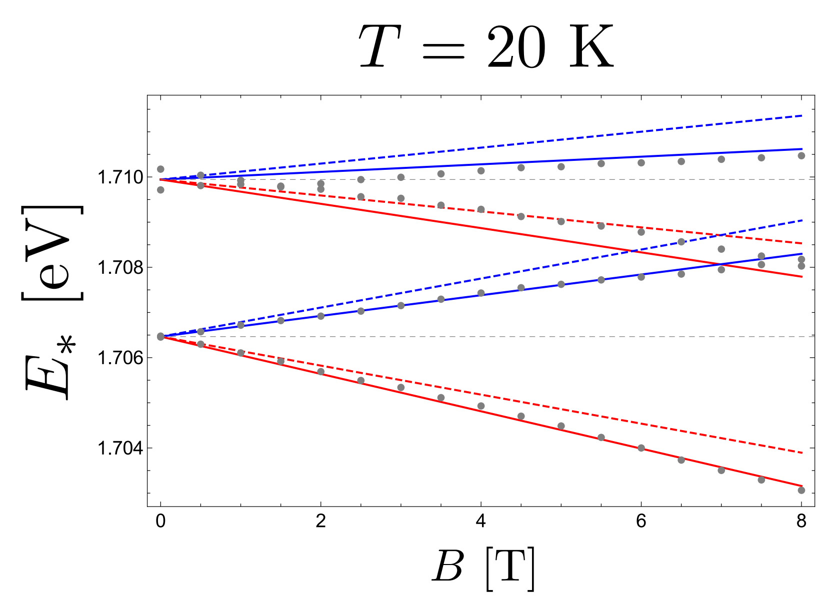


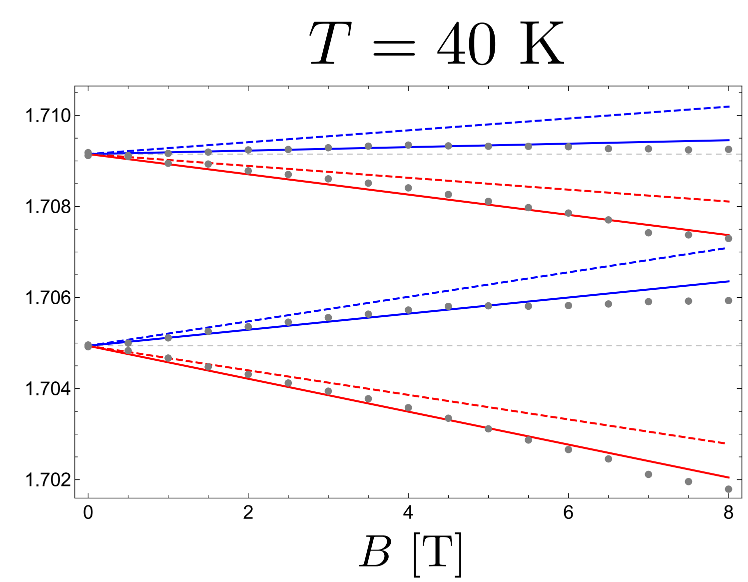
Experimental data courtesy of Tom Lyons

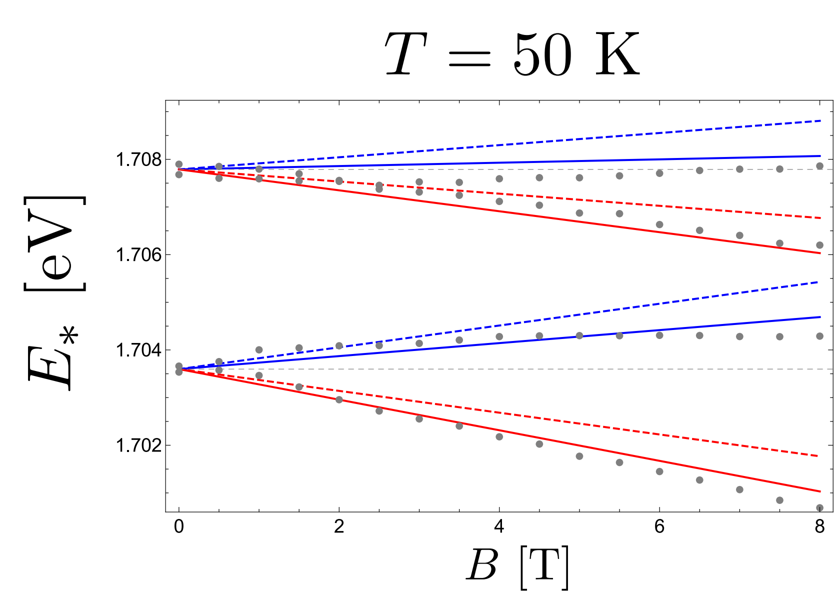
Different temperatures, 0th Landau level recoil







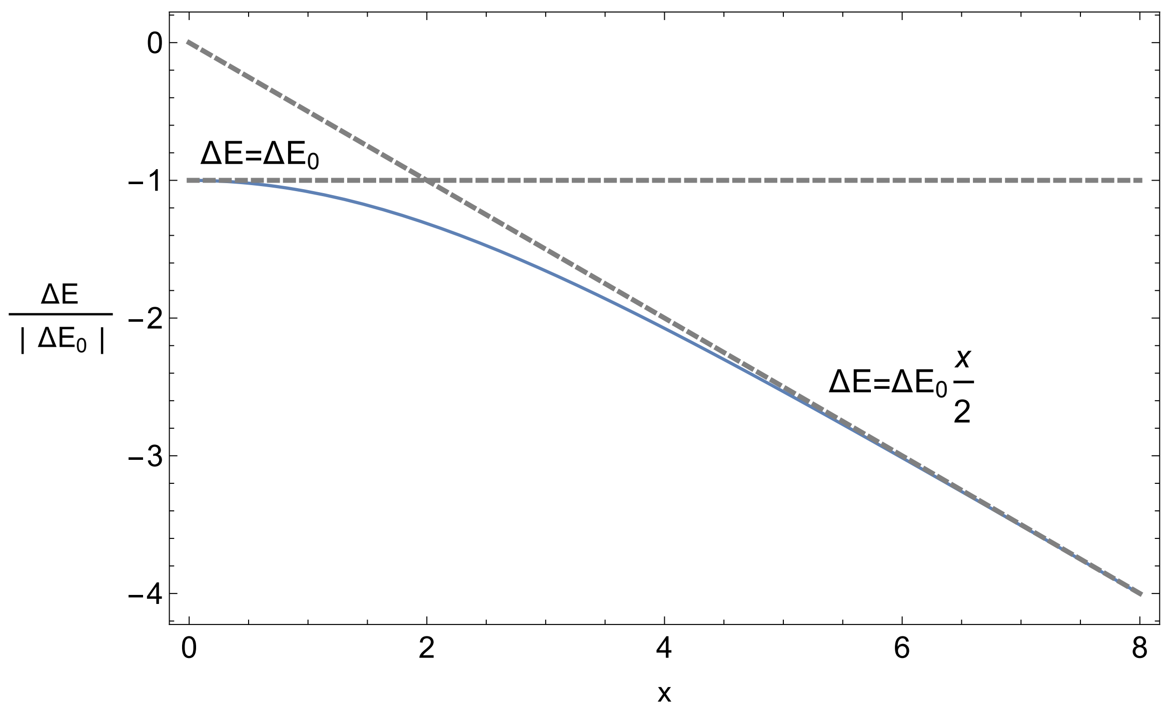




Experimental data courtesy of Tom Lyons

Temperature dependent recoil:

$$\Delta E = \mathcal{N}\sum_n \Delta E_n e^{-\frac{\hbar\omega_T(n+1/2)}{k_B T}} = \frac{1}{2}(\hbar\omega_T - \hbar\omega_e)\coth\left(\frac{\hbar\omega_T}{2k_B T}\right)$$

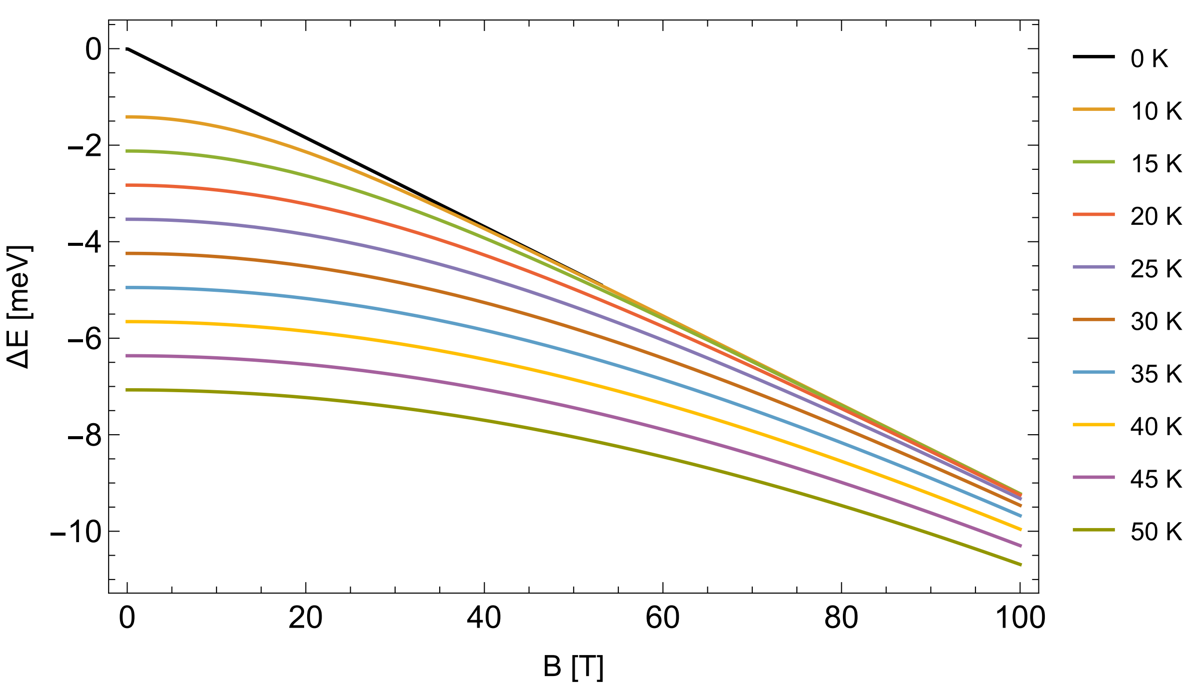


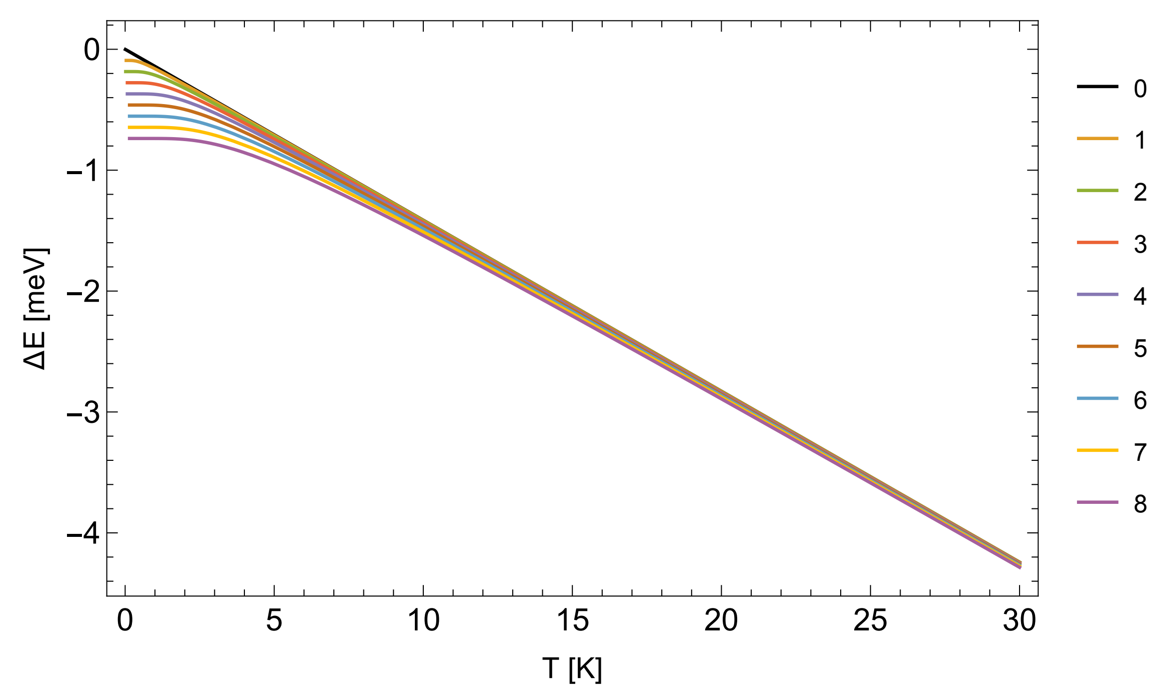
$$x = \frac{\hbar\omega_T}{k_B T}$$

For WSe_2 at B=4T, T=30K: $x \sim 0.2$

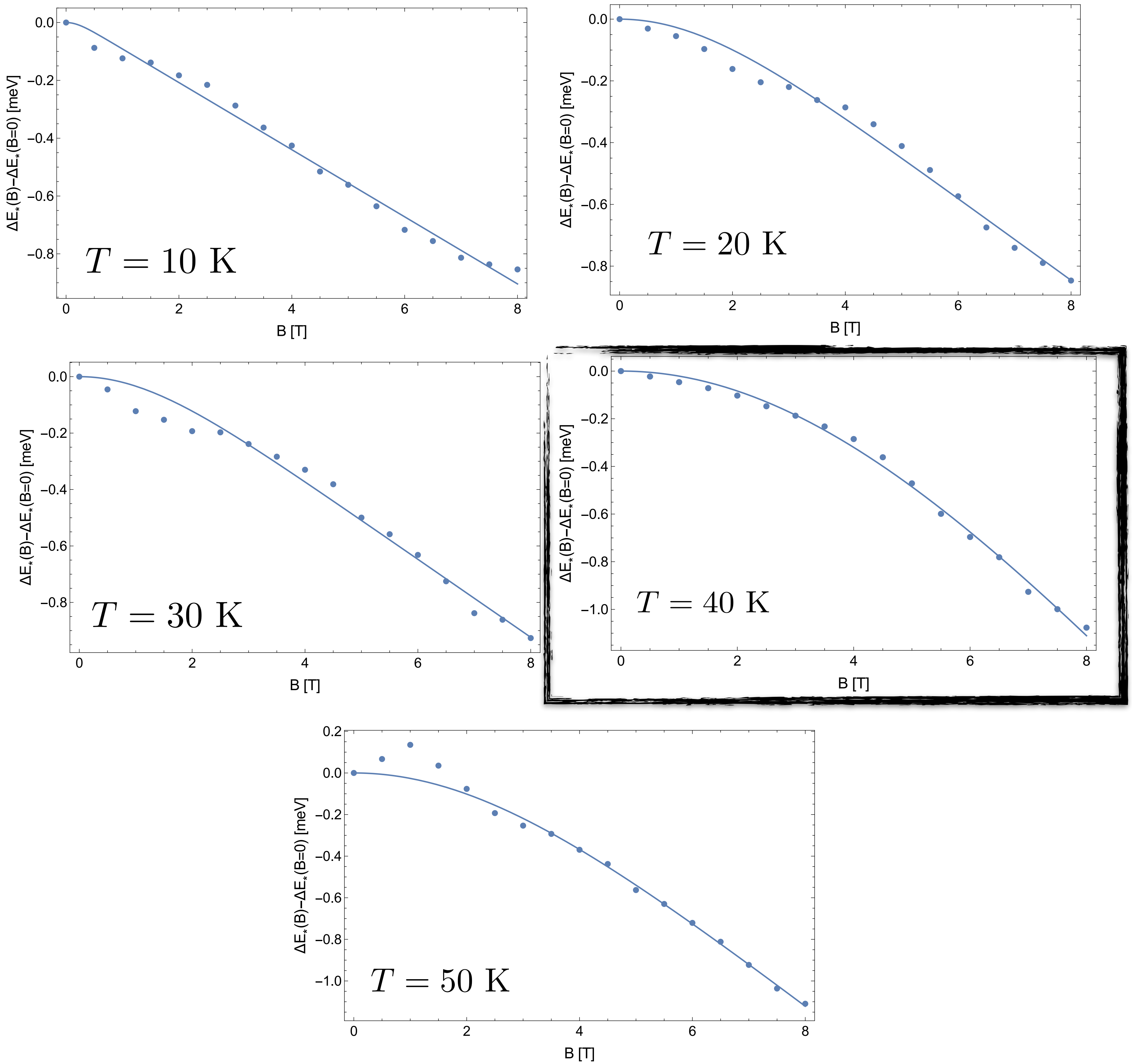
$$\Delta E_0 = k_B T\left(1 - \frac{m_T}{m_e}\right)$$

$\mathrm{WSe_2}$





Recoil - temperature dependent fits

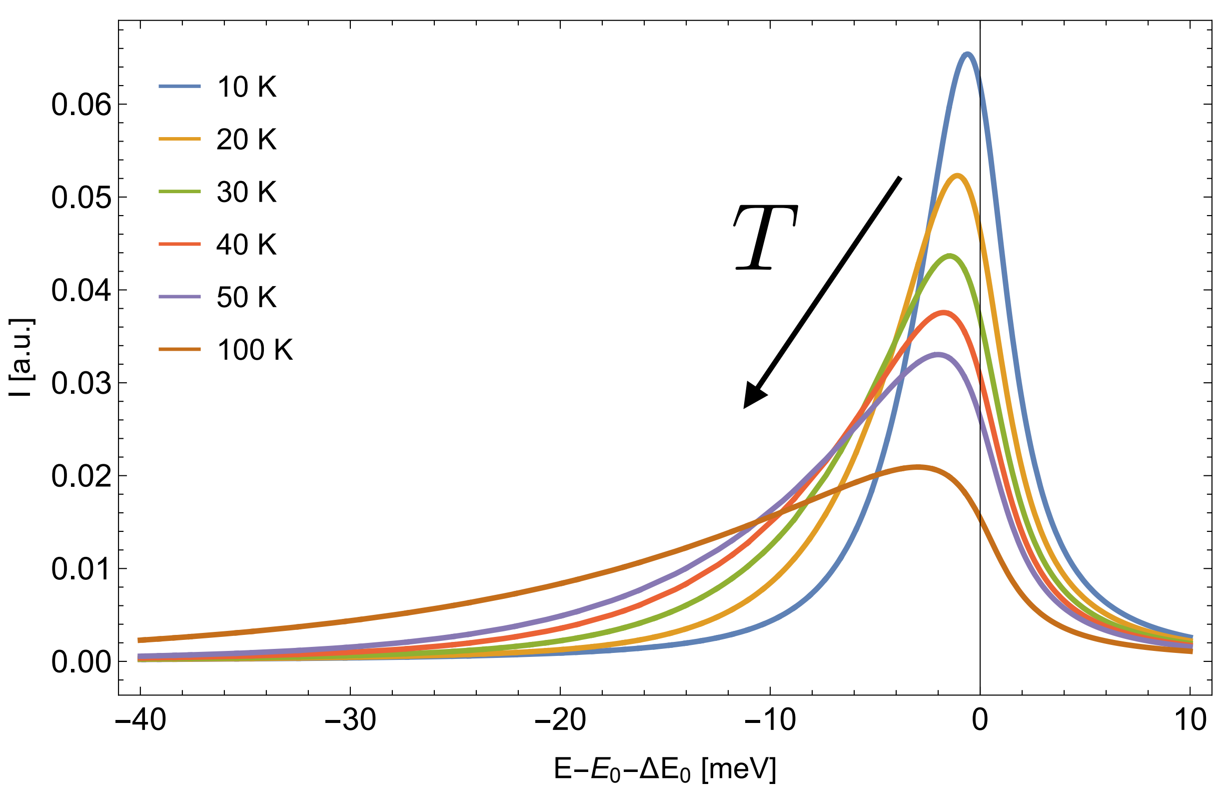


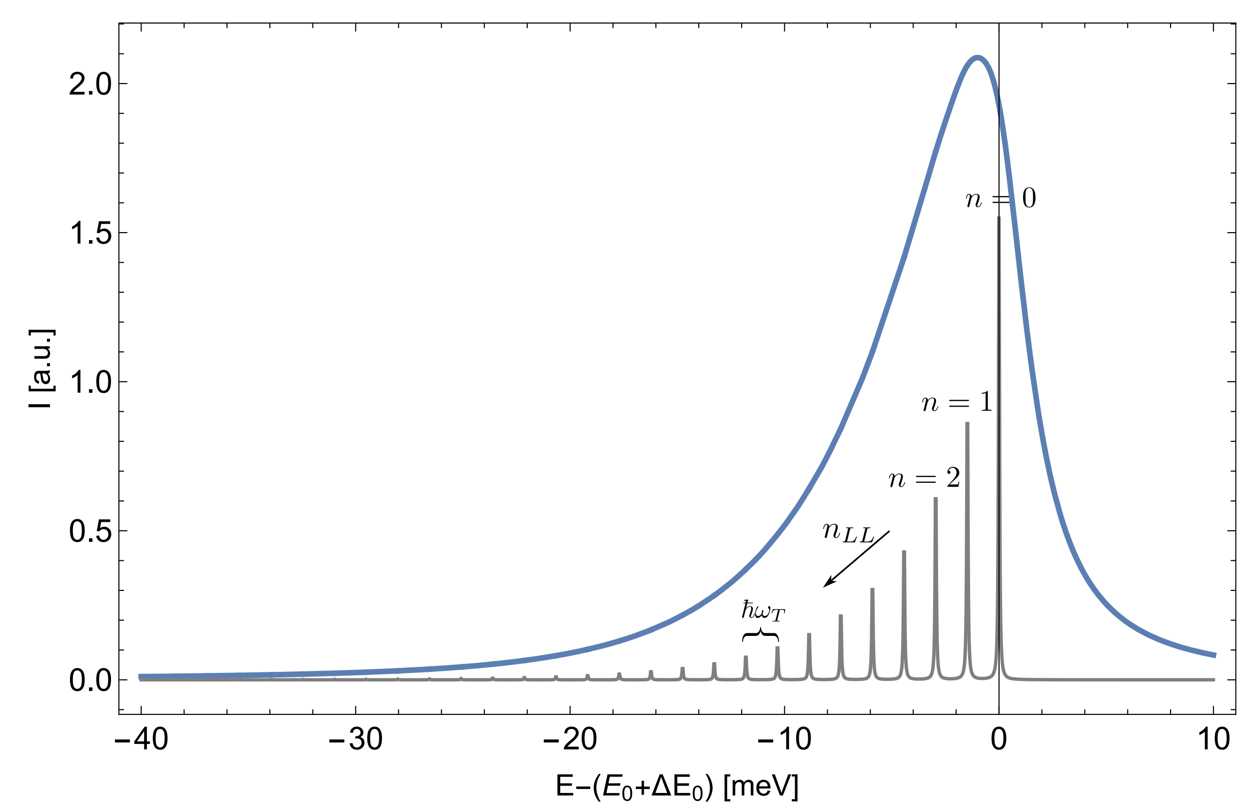
Experimental data courtesy of Tom Lyons

Trion line shape in magnetic field

$$I(E) = \mathcal{N} \sum_n f(E - (E_0 + \Delta E_n)) e^{-\frac{\hbar\omega_T (n+1/2)}{k_B T}(n+1/2)}$$

$\mathrm{WSe}_2, B = 4\mathrm{T}$





Summary

Interlayer excitons in TMDs

- Interlayer excitons in misaligned TMDs, can recombine with the aid of e/h scattering.
- Dominant z-polarised light emission, and stacking dependent right/left handed polarised light
- Redshifted photon energy as a function of misalignment.

Recoil in PL

- Recoil in PL allows to distinguish trions and biexcitons from excitons.
- In a magnetic field, Landau level quantisation results in asymmetric trion peak splitting allowing to distinguish trions from excitons.