Landau levels and SdH oscillations in monolayer transition metal dichalcogenide semiconductors

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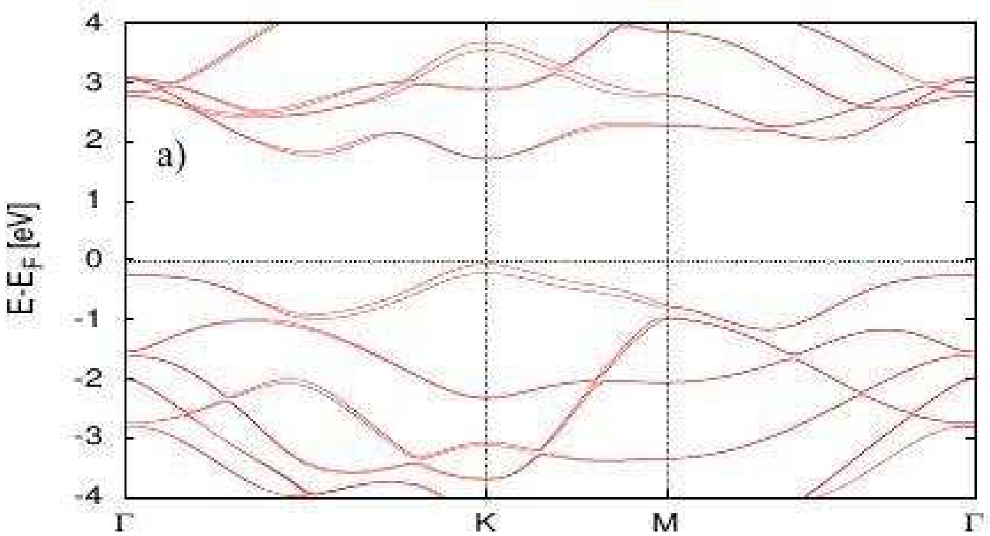
Kormányos et. al., New Journal of Physics **17**, 103006 (2015).

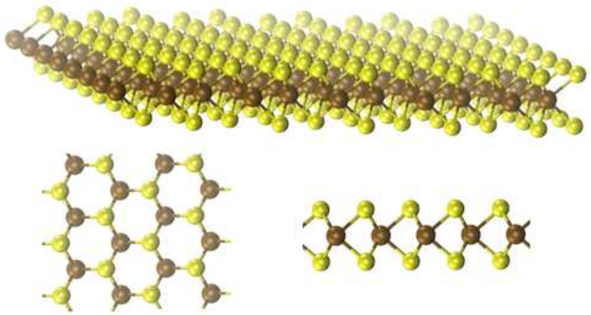
Transition metal dichalcogenides semiconductors

- Top view: three-fold symmetry
- No inversion symmetry.
- Atomically thin material with direct band gap.

$\sim 1 - 2$ eV. DFT, LSDA for MoS_2:



Kormányos et. al, Phys. Rev. B **88**, 045416 (2013).



(Nano-TCAD Group)

Two-band continuum model for valleys $\tau = \pm K$

- seven-band model $\rightarrow \hbar\hat{\boldsymbol{q}} = \boldsymbol{p} + \frac{e}{\hbar}\mathbf{A} \rightarrow$ two-ban model by Löwdin partitioning

$$H^{\tau}_{\text{eff}} = H_0 + H^{\tau}_{\text{so}} + H^{\tau}_{\mathbf{k}\cdot\mathbf{p}}$$

$$H_0 = \frac{\hbar^2}{2m_e}\frac{\hat{q}_+\hat{q}_- + \hat{q}_-\hat{q}_+}{2} + \frac{1}{2}g_e\mu_B B_z s_z \qquad H^{\tau,s}_{\text{so}} = \begin{pmatrix} \tau\Delta_{\text{vb}}s_z & 0 \\ 0 & \tau\Delta_{\text{cb}}s_z \end{pmatrix}$$

$$H^{\tau,s}_{\mathbf{k}\cdot\mathbf{p}} = H^{\tau,s}_{\text{D}} + H^{\tau,s}_{\text{as}} + H^{\tau,s}_{3w} + H^{\tau,s}_{\text{cub}},$$

$$H^{\tau,s}_{D} = \begin{pmatrix} \varepsilon_{\text{vb}} & \tau\,\gamma_{\tau,s}\hat{q}^{\tau}_{-} \\ \tau\,\gamma^{*}_{\tau,s}\hat{q}^{\tau}_{+} & \varepsilon_{\text{cb}} \end{pmatrix} \qquad H^{\tau,s}_{\text{as}} = \begin{pmatrix} \alpha_{\tau,s}\hat{q}^{\tau}_{+}\hat{q}^{\tau}_{-} & 0 \\ 0 & \beta_{\tau,s}\hat{q}^{\tau}_{-}\hat{q}^{\tau}_{+} \end{pmatrix}$$

$$H^{\tau,s}_{3w} = \begin{pmatrix} 0 & \kappa_{\tau,s}(\hat{q}^{\tau}_{+})^2 \\ \kappa^{*}_{\tau,s}(\hat{q}^{\tau}_{-})^2 & 0 \end{pmatrix}, \qquad H^{\tau,s}_{cub,1} = \dots$$

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Landau Levels (LLs)

- harmonic oscillator eigenfunctions as basis states: $\pi_- = \frac{2}{l_B}a, \pi_+ = \frac{2}{l_B}a^\dagger, l_B\sqrt{\hbar/eB}$.
- matrix representation of H^{τ}_{eff} on a finite subspace spanned by the basis functions.
- Landau Levels: eigenvalues of H^{τ}_{eff}.

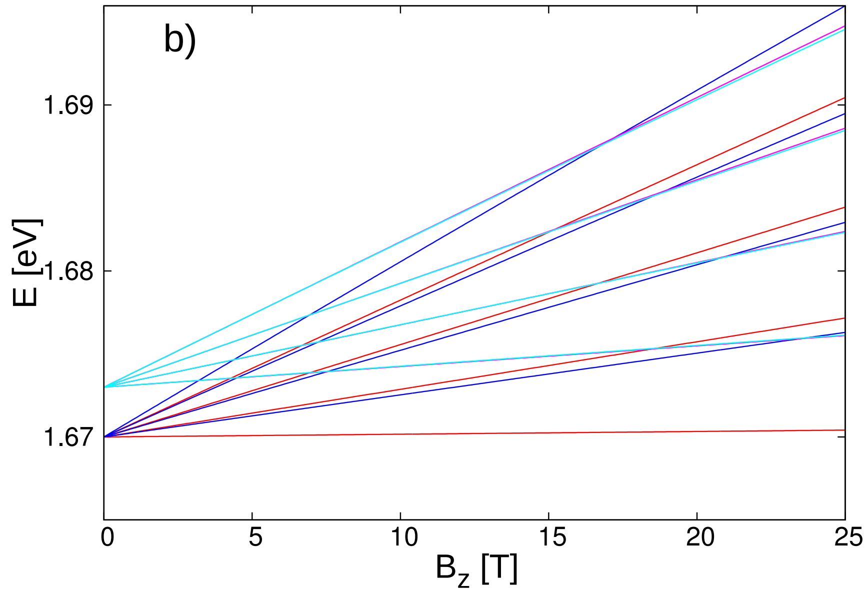
LLs in the conductance band:

spin $\uparrow$, K-valley

spin $\uparrow$, K'-valley

spin $\downarrow$, K-valley

spin $\downarrow$, K'-valley



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Approximation of the LLs

- Neglecting the trigonal warping and cubic terms ($H_{3w}^{\tau,s}$, $H_{cub,1}^{\tau,s}$).
- Another Löwdin-partitioning to obtain effective single-band Hamiltonian separately for conduction and valence bands.
- Leading to a harmonic oscillator-like Hamiltonians:

$$E_{n,\mathrm{vb}}^{\tau,s} = \varepsilon_{\mathrm{vb}}^{\tau\cdot s} + \hbar\omega_{\mathrm{vb}}^{(\tau\cdot s)}\left(n+\frac{1}{2}\right) + \frac{1}{2}g_e\mu_B B_z s + \frac{1}{2}g_{vl,\mathrm{vb}}^{(s)}\mu_B B_z\,\tau,$$

$$E_{n,\mathrm{cb}}^{\tau,s} = \varepsilon_{\mathrm{cb}}^{\tau\cdot s} + \hbar\omega_{\mathrm{cb}}^{(\tau\cdot s)}\left(n+\frac{1}{2}\right) + \frac{1}{2}g_e\mu_B B_z s + \frac{1}{2}g_{vl,\mathrm{cb}}^{(s)}\mu_B B_z\,\tau.$$

- valley splitting linearly depends on B_z.

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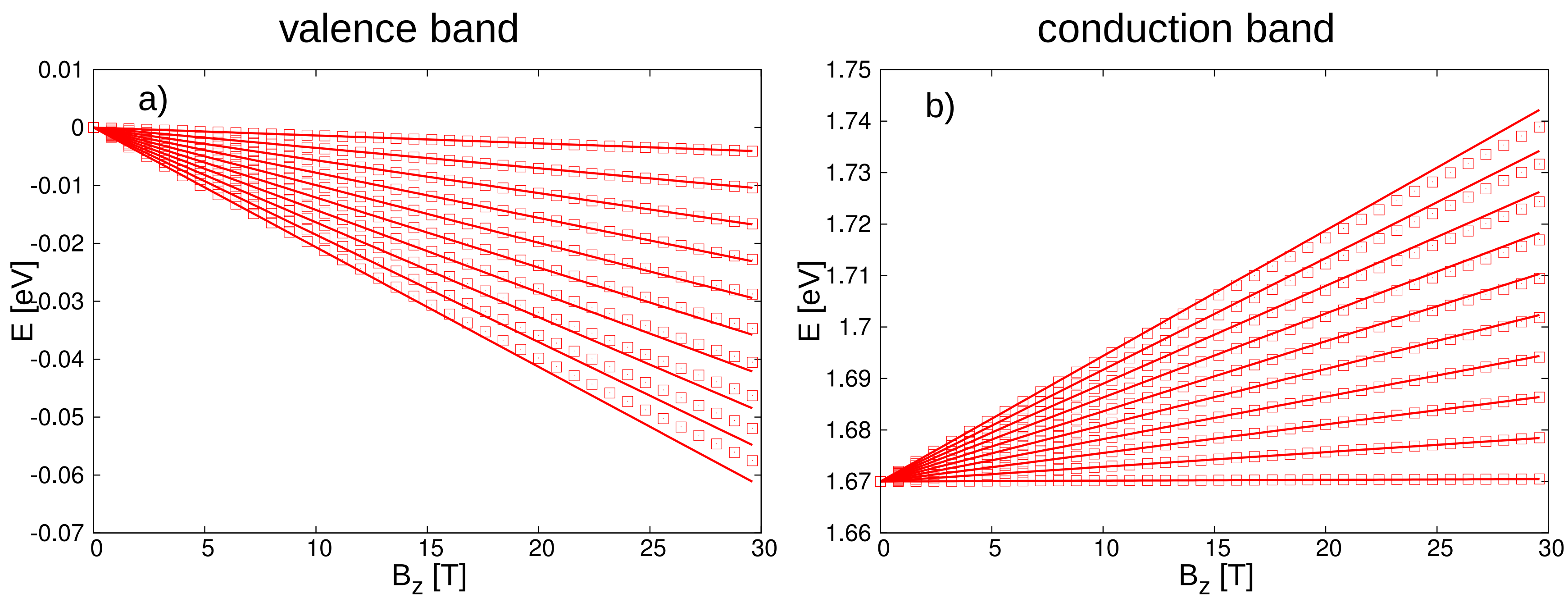
Approximation vs full quantum □

valley K, spin ↓



➠ The trigonal warping is relevant for higher magnetic fields.

➠ At higher magnetic fields the valley splitting is not linear in B.

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Calculation of the SdH oscillations

Calculation of the conductivity σ_{xx}:

- neglecting the intra-valley scattering between the spin-split bands: due to the specific form of the intrinsic SOC
- neglecting the inter-valley scattering in the absence of magnetic impurity: large momentum change, requires simultaneous spin-flip
- Considering the intra-valley, intra-band scatterings and short range scatterers.

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Self-consistent Born approximation

- random disorder potential $V(\mathbf{r})$ with short range correlations
  $\langle V(\mathbf{r})V(\mathbf{r}')\rangle = \lambda_{sc}\delta(\mathbf{r}-\mathbf{r}')$
- self-energy $\Sigma_R^{\tau,s} = \Sigma_r^{\tau,s} + i\Sigma_i^{\tau,s}$

$$\Sigma_r^{\tau,s} + i\Sigma_i^{\tau,s} = \frac{\lambda_{sc}}{2\pi l_B^2}\sum_{n=0}^{\infty}\frac{1}{E - E_n^{\tau,s} - (\Sigma_r^{\tau,s} + i\Sigma_i^{\tau,s})}$$

- $E_n^{\tau,s}$ are the approximated or exact LL energies.
- $\lambda_{sc} \sim$ scattering rate calculated by the Born-approximation in zero magnetic field.

Ando T, J. Phys. Soc. Jpn. **37**, 1233 (1974).

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conductivity σ_{xx}

- Kubo-formalism:

$$\sigma_{xx}^{\tau,s} = \frac{e^2}{\pi^2\hbar}\int dE \left(-\frac{\partial f(E)}{\partial E}\right)\sigma_{xx}^{\tau,s}(E)$$

$$\frac{\sigma_{xx}^{\tau,s}(E)}{(\hbar\omega_c^{(i)})^2} = \sum_{n=0}^{\infty}(n+1)\mathrm{Re}[G_A^{\tau,s}(n,E)G_R^{\tau,s}(n+1,E) - G_A^{\tau,s}(n,E)G_A^{\tau,s}(n,E)]$$

- $G_R^{\tau,s}(n,E)$ and $G_A^{\tau,s}(n,E)$ are the retarded and advanced Greens-functions:

$$G_{R,A}^{\tau,s}(n,E) = [E - E_n^{\tau,s} - \Sigma_{R,A}^{\tau,s}]^{-1}$$

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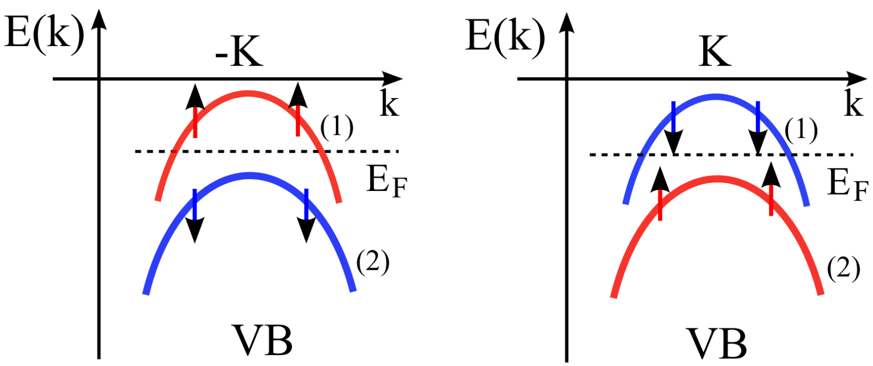
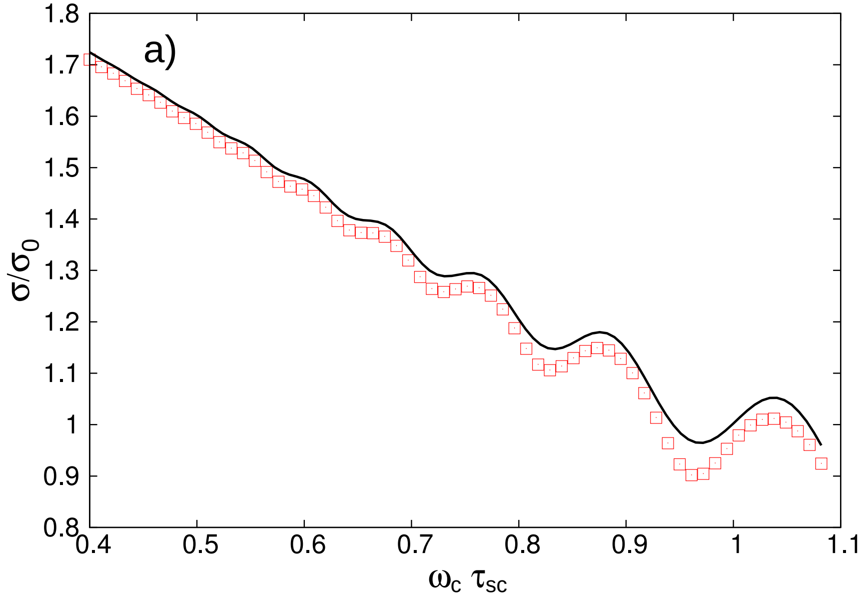
Calculated SdH oscillations for p-doped WSe_2

- The amplitudes of the oscillations are not captured well by the approximated LLs.
- Reason: few LLs under the Fermi level.



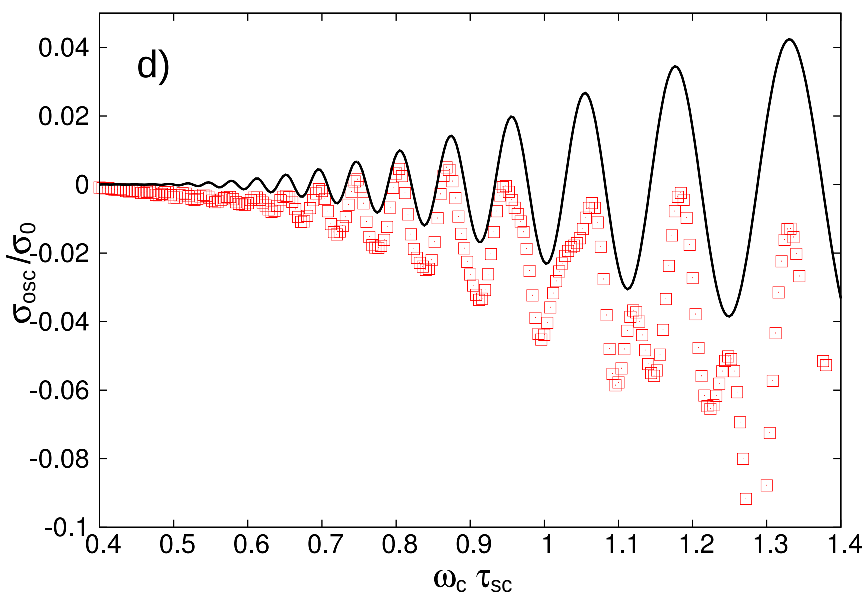
numerical SdH, and approximated SdH

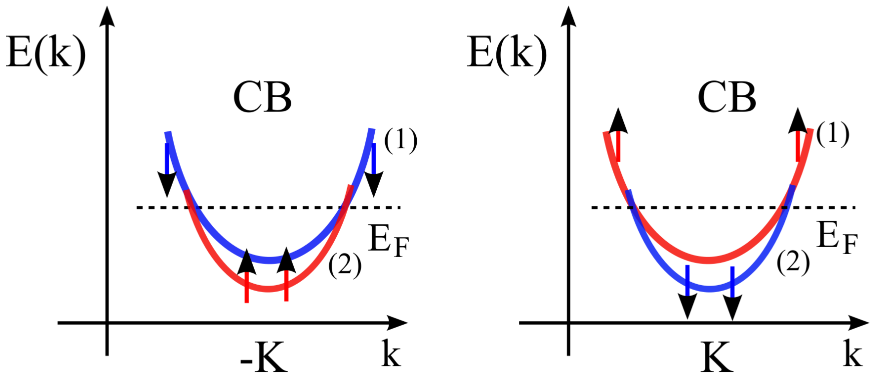


Calculated SdH oscillations for n-doped MoS_2

- two bands contribute to $\sigma_{xx} = \sigma_{xx}^{(1)} + \sigma_{xx}^{(2)}$
- parameters from GW calculations
- complex oscillation pattern due to valley splitting (different oscillation periods in the two valleys)

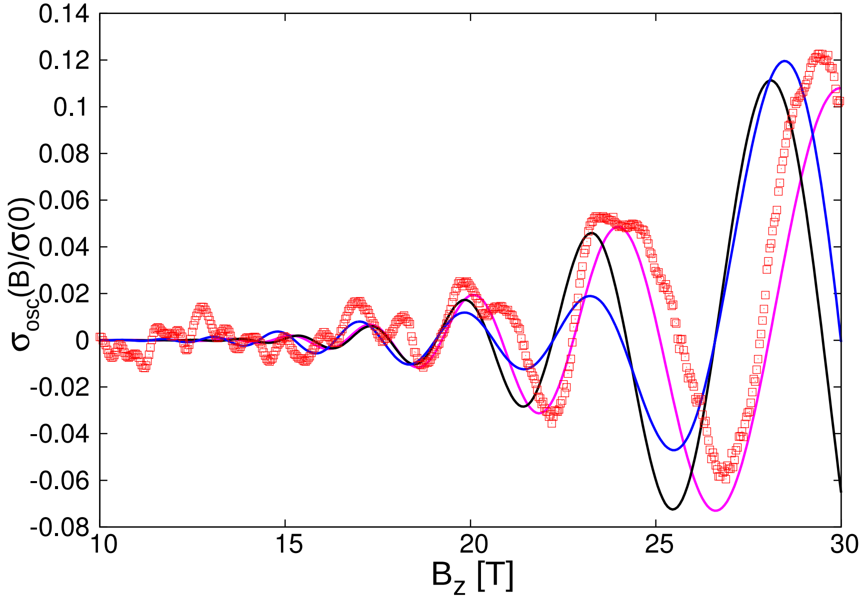
numerical SdH, and approximated SdH





Comparing to experiments on MoS_2

experimental SdH, and approximated SdH



- Fitting the **analytical expression** to the experimental data of X. Cui et. al., 2015 advance online publication in Nature Nanotechnology (arXiv:1412.5977)