Unusual Landau levels in biased bilayer Bernal graphene

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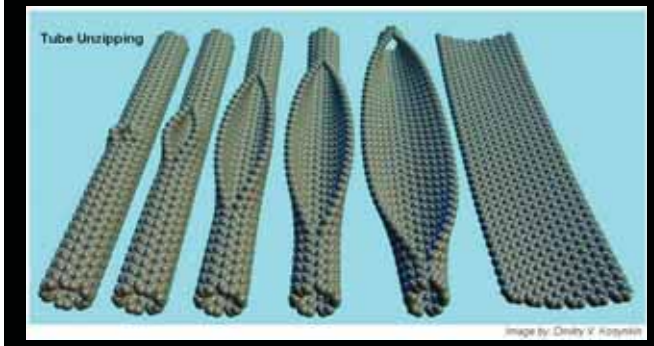
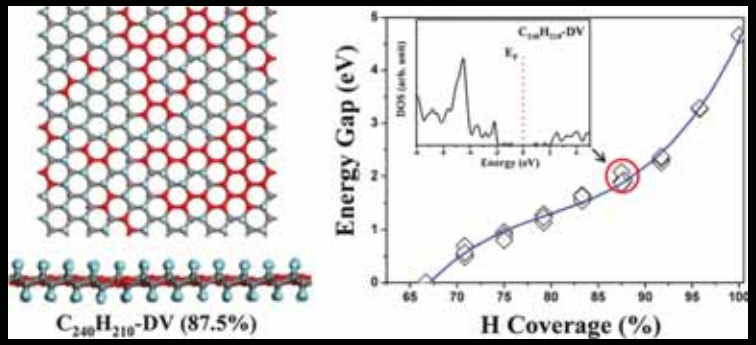
Outline …

- **Motivation**
  Why bilayer graphene?
  Why magneto physical properties?
- **Comprehensive tight-binding method**
- **Landau levels and Landau wave functions**
  Breaking of inter-valley degeneracy
  Coupling of Landau levels
- **Magneto-optical properties**
- **Summary**

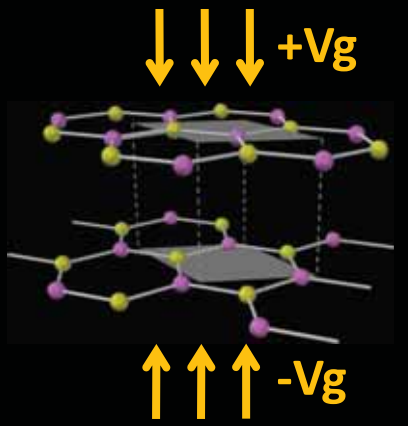
Why bilayer graphene ?

missing of energy gap → Adsorption of H atoms on the C dangling bonds
Cutting G sheet into 1-D ribbons with finite width
Applying a bias E field on top and bottom of G bilayer
(doping level & energy gap)



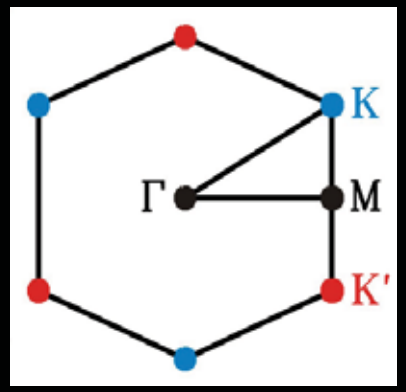


J. Phys. Chem. C, 115, 3236 (2011)



Why magneto physical properties ?

2-D electronic states → discrete LLs:
a better way to study electronic properties



Multiple degeneracy: e-h symmetry
inter-valley symmetry

Atomic structure of bilayer graphene

$$\langle A_{1(2)}|H|B_{1(2)}\rangle \longrightarrow \gamma_0 \ (-3.12 \text{ eV})$$

$$\langle A_{1(2)}|H|A_{2(1)}\rangle \longrightarrow \gamma_1 \ (0.38 \text{ eV})$$

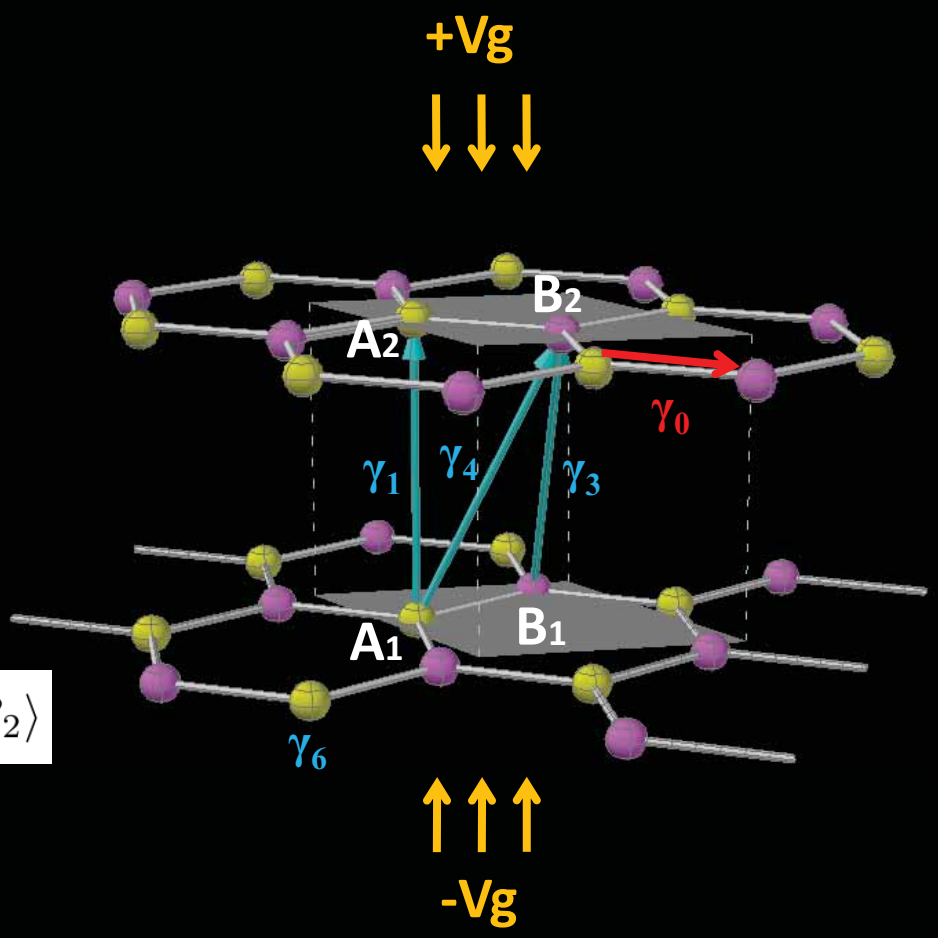
$$\langle B_{1(2)}|H|B_{2(1)}\rangle \longrightarrow \gamma_3 \ (0.28 \text{ eV})$$

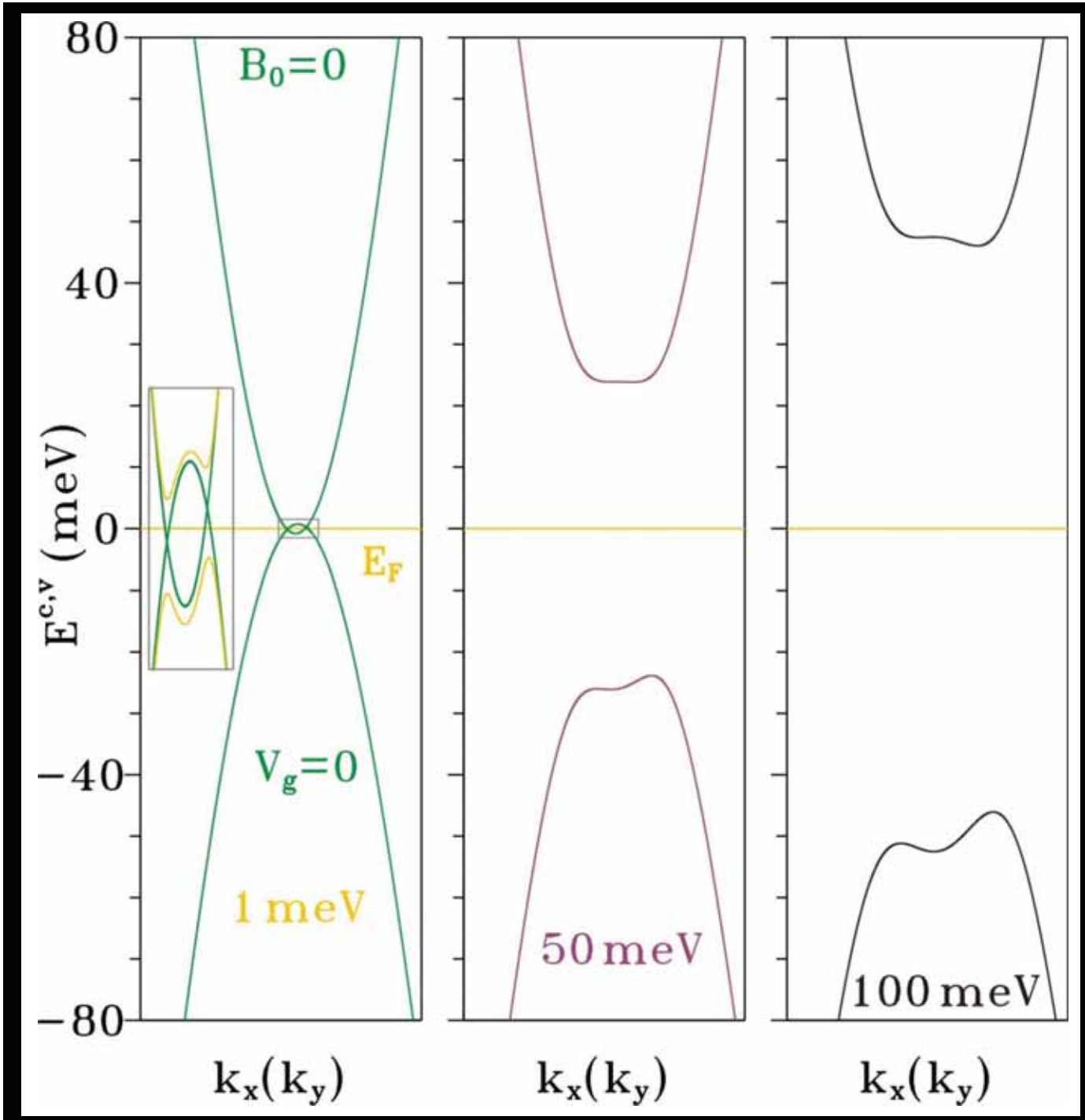
$$\langle A_{1(2)}|H|B_{2(1)}\rangle \longrightarrow \gamma_4 \ (0.12 \text{ eV})$$

$$\langle A_{1(2)}|H|A_{1(2)}\rangle \longrightarrow \gamma_6 \ (0.016 \text{ eV})$$

$$\Psi = c_a|A_1\rangle + c_{a'}|A_2\rangle + c_b|B_1\rangle + c_{b'}|B_2\rangle$$

$$H = \begin{pmatrix} H_{B_2B_2} & H_{B_2A_2} & H_{B_2A_1} & H_{B_2B_1} \\ H_{A_2B_2} & H_{A_2A_2} & H_{A_2A_1} & H_{A_2B_1} \\ H_{A_1B_2} & H_{A_1A_2} & H_{A_1A_1} & H_{A_1B_1} \\ H_{B_1B_2} & H_{B_1A_2} & H_{B_1A_1} & H_{B_1B_1} \end{pmatrix}$$





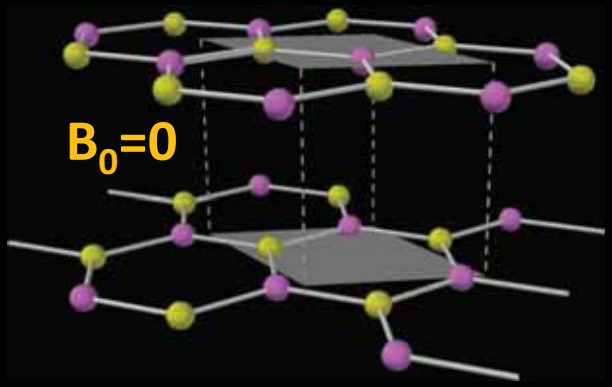
Energy bands:
$B_0=0$
$Vg\neq0$

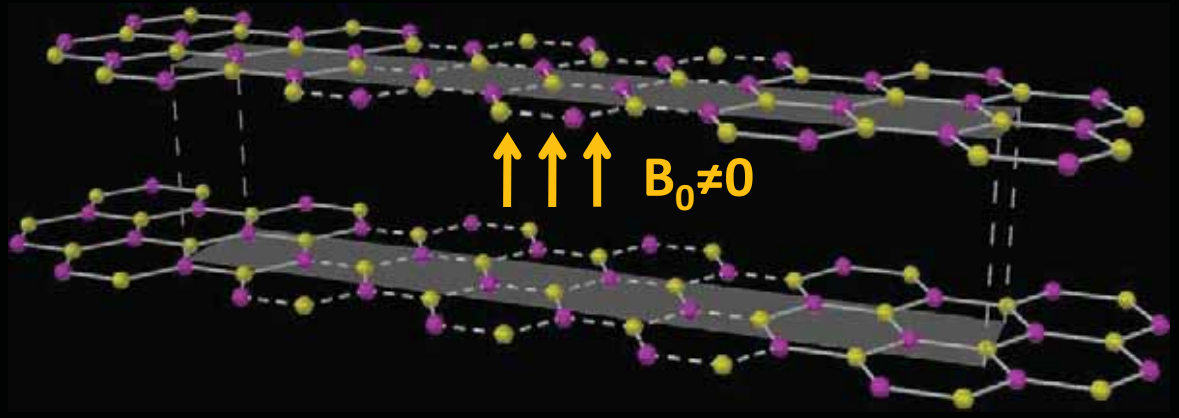
Mexican-hat shape

Apply a magnetic field perpendicular to the plane…

Peierls phase $\Delta G(\vec{R}_{j_l}, \vec{R}_{k_{l'}}) = \int_0^1 (\vec{R}_{k_{l'}} - \vec{R}_{j_l}) \cdot \vec{A}[\vec{R}_{j_l} + \lambda(\vec{R}_{k_{l'}} - \vec{R}_{j_l})] d\lambda$

$$\langle k_{l'}|H|j_l\rangle = \gamma_s(\vec{R}_{j_l}, \vec{R}_{k_{l'}}) \sum \exp\left[i\vec{k} \cdot (\vec{R}_{j_l} - \vec{R}_{k_{l'}}) + i\frac{e}{\hbar}\Delta G(\vec{R}_{j_l}, \vec{R}_{k_{l'}})\right]$$



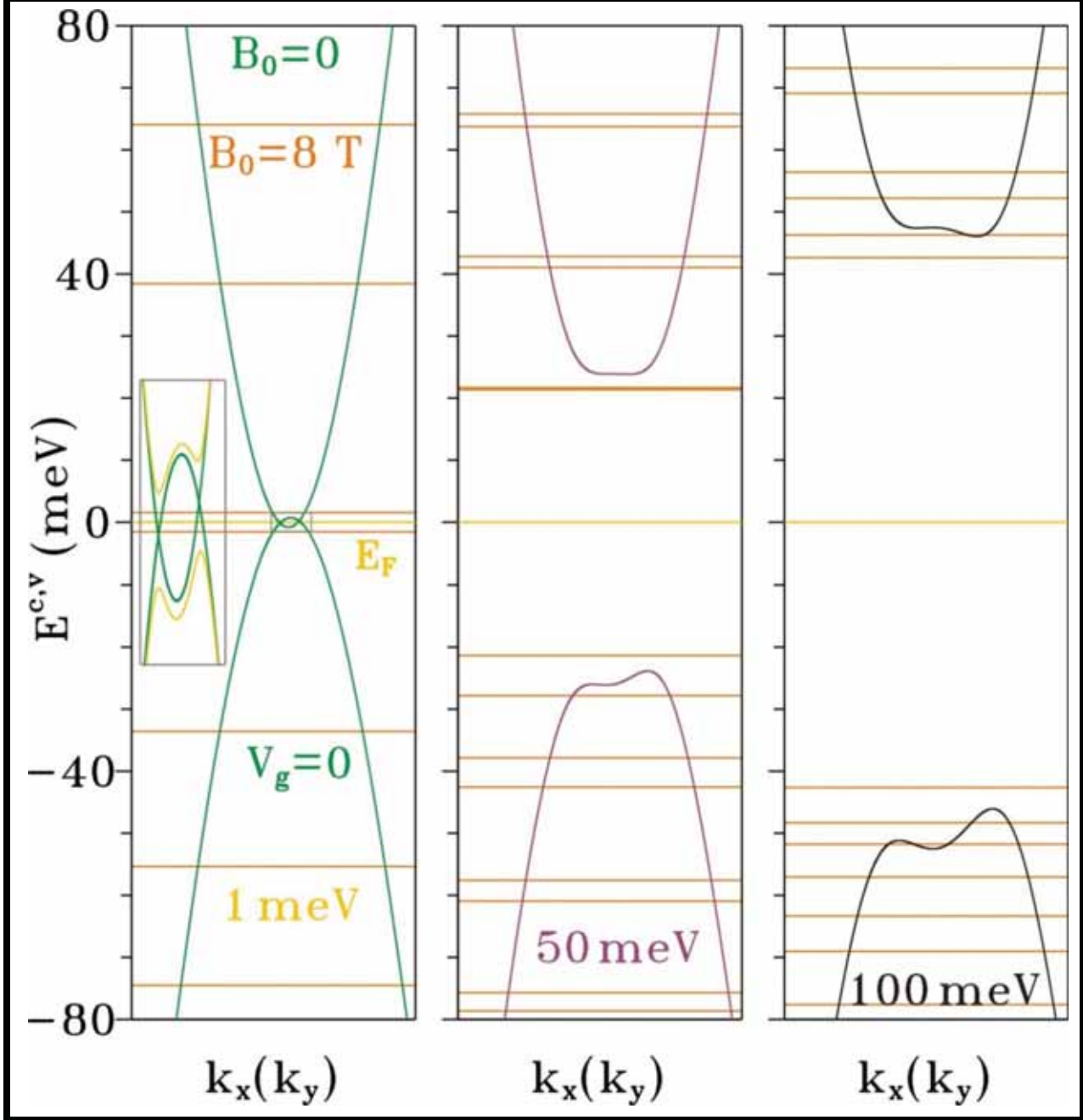


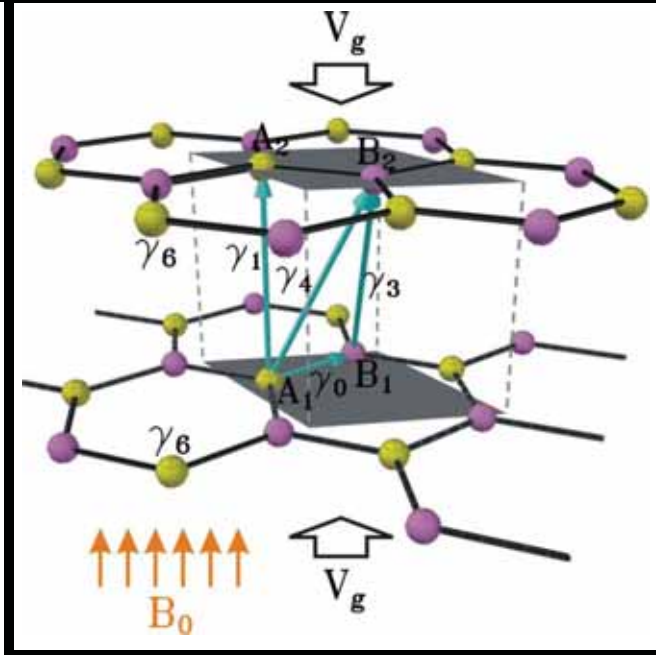
0 T: 4 atoms

8 T: 80,000 atoms

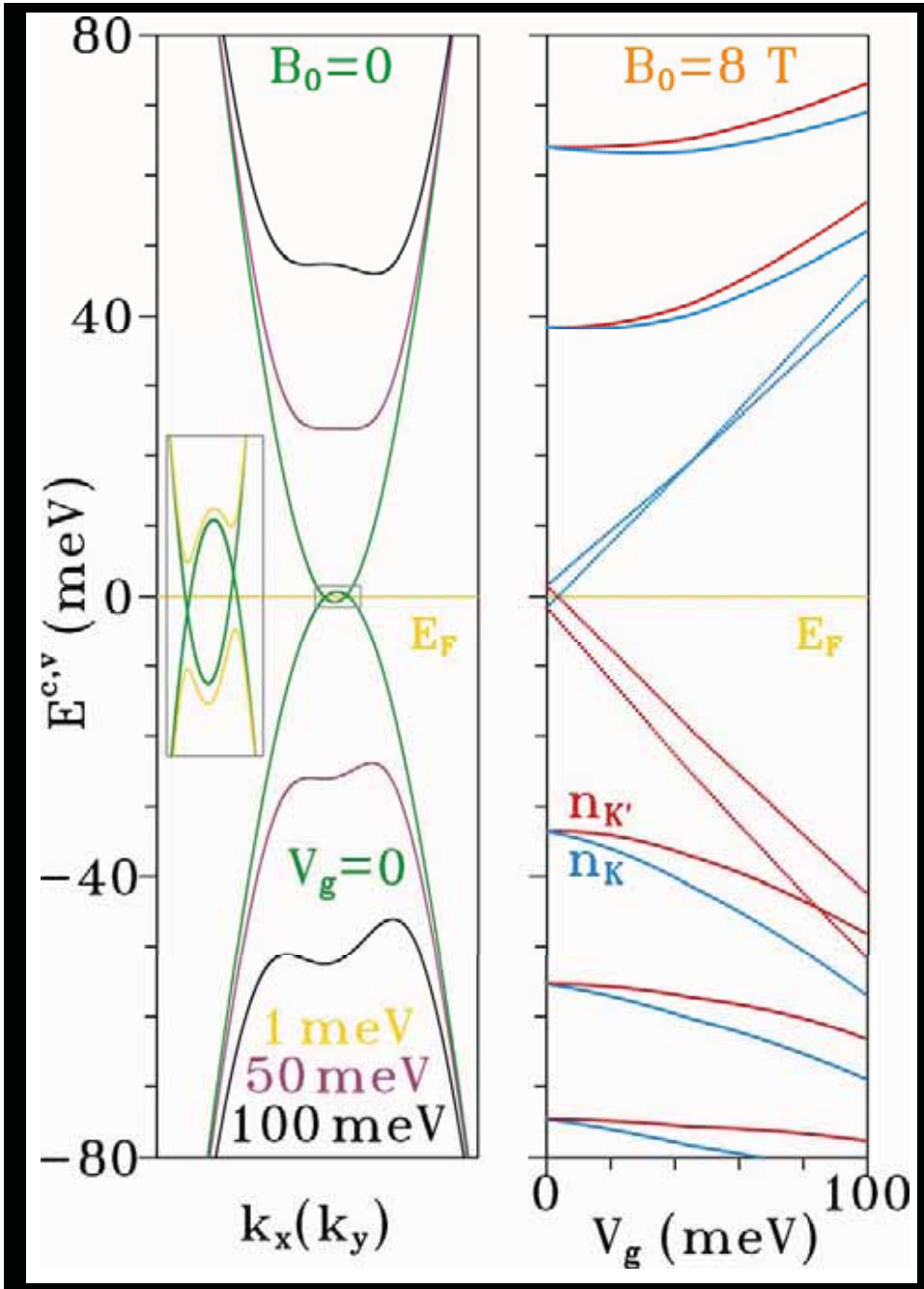
$$\Psi = \sum_{i=1}^{2R_B} c_{a,i}|A_{1,i}\rangle + c_{a',i}|A_{2,i}\rangle + c_{b,i}|B_{1,i}\rangle + c_{b',i}|B_{2,i}\rangle$$

2-D Energy bands B_0=0 to Landau levels at $B_0 \neq 0$

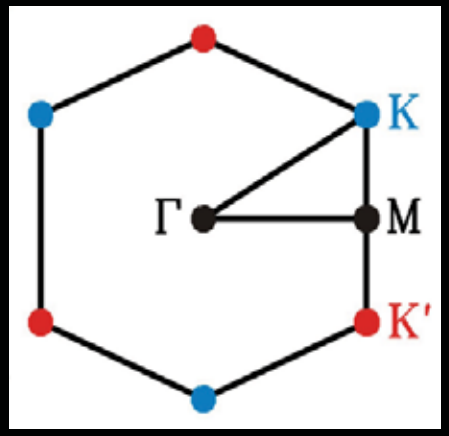


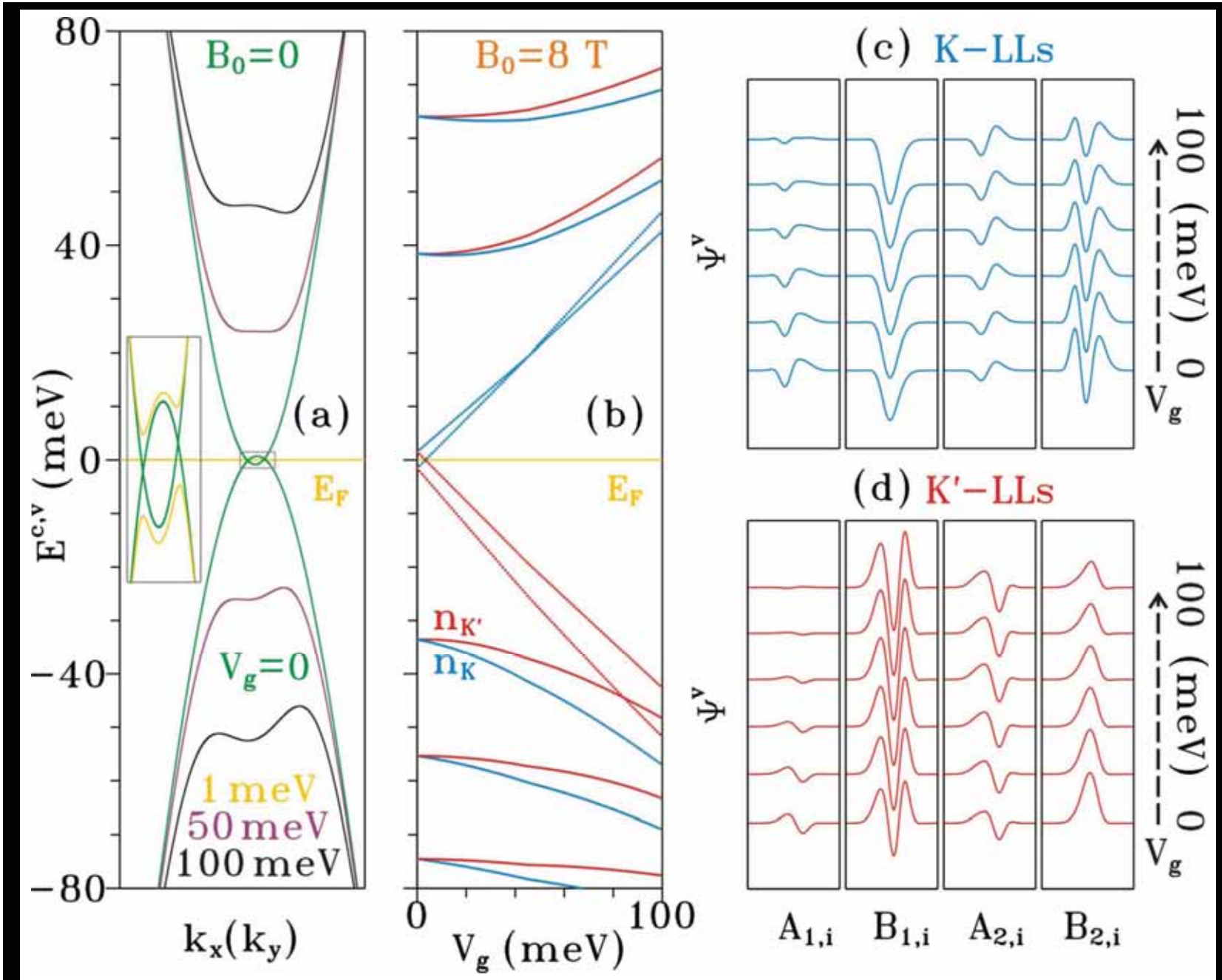


B≠0: Landau levels

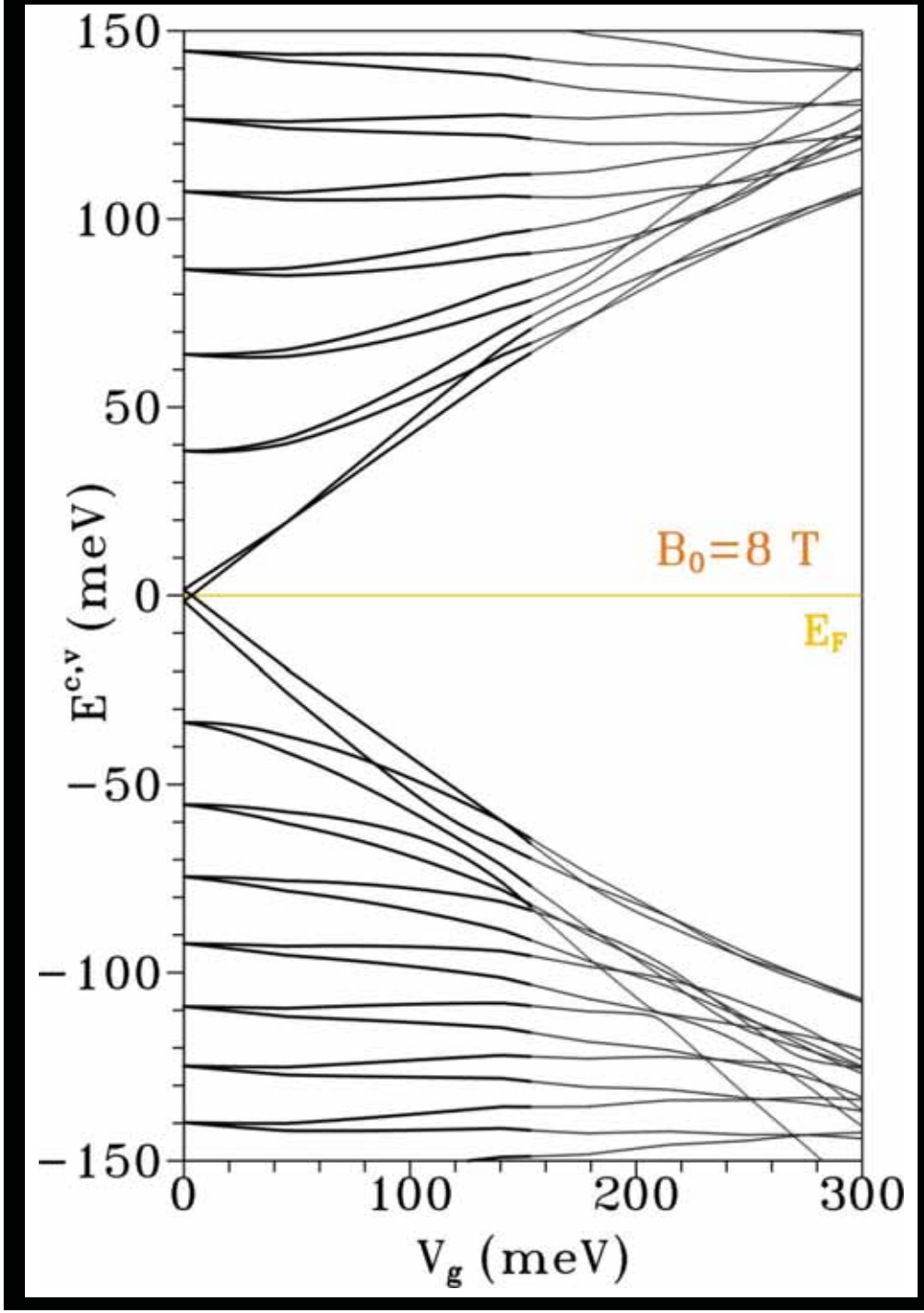


breaking of inter-valley degeneracy



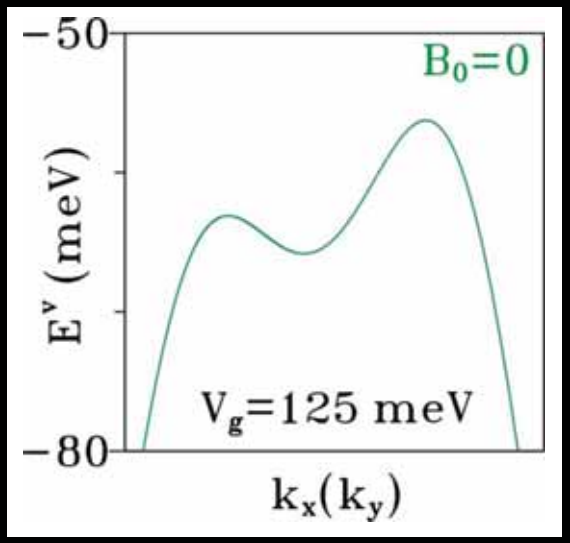


$$\langle\psi^*_{A_1}|\text{-}V_g|\psi_{A_1}\rangle+\langle\psi^*_{B_1}|\text{-}V_g|\psi_{B_1}\rangle+\langle\psi^*_{A_2}|V_g|\psi_{A_2}\rangle+\langle\psi^*_{B_2}|V_g|\psi_{B_2}\rangle$$



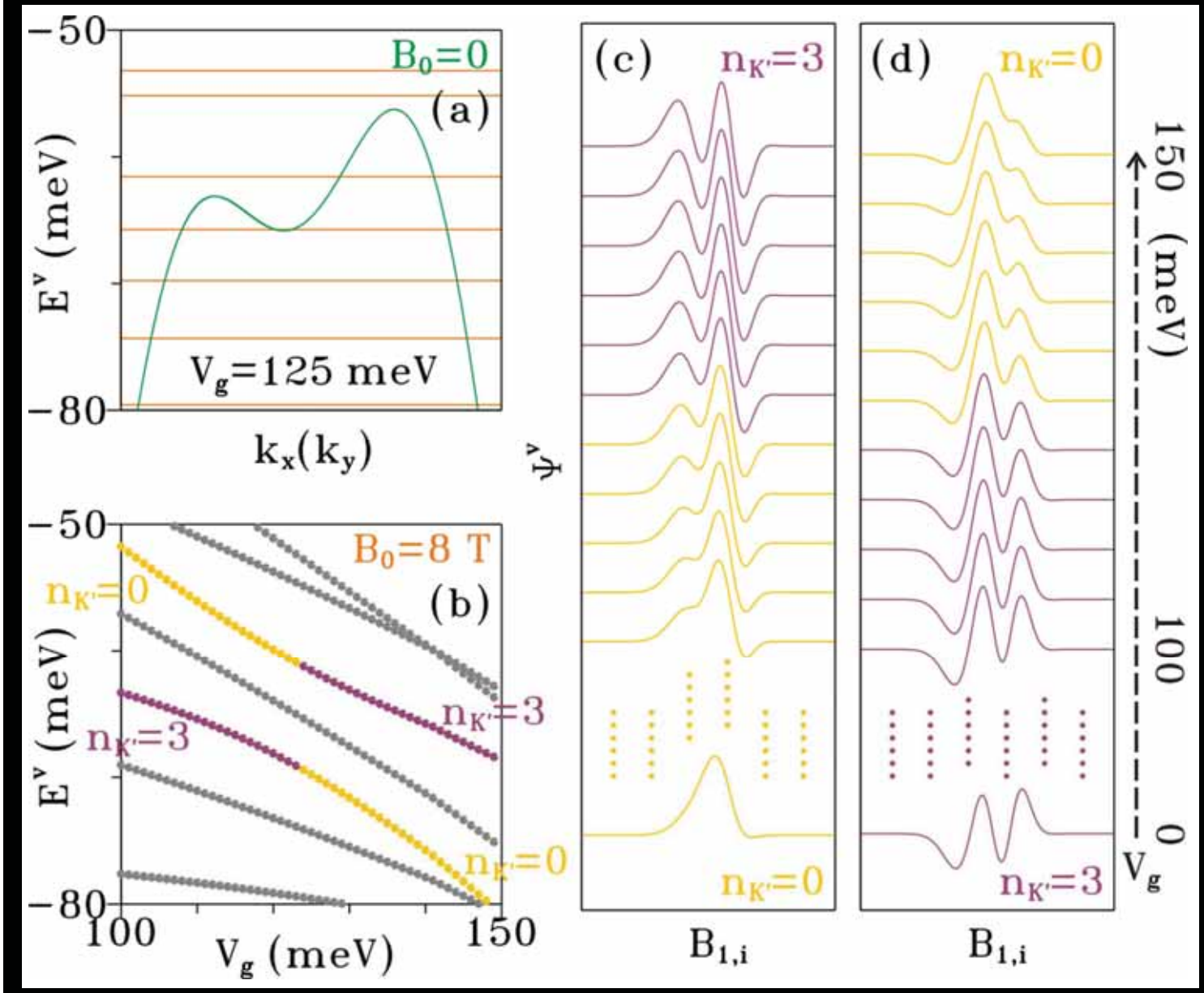
Landau levels for a wider range of energy & bias electric field

Lower LLs are more sensitive to Vg:
Shift toward higher energy
Splitting of K & K' states



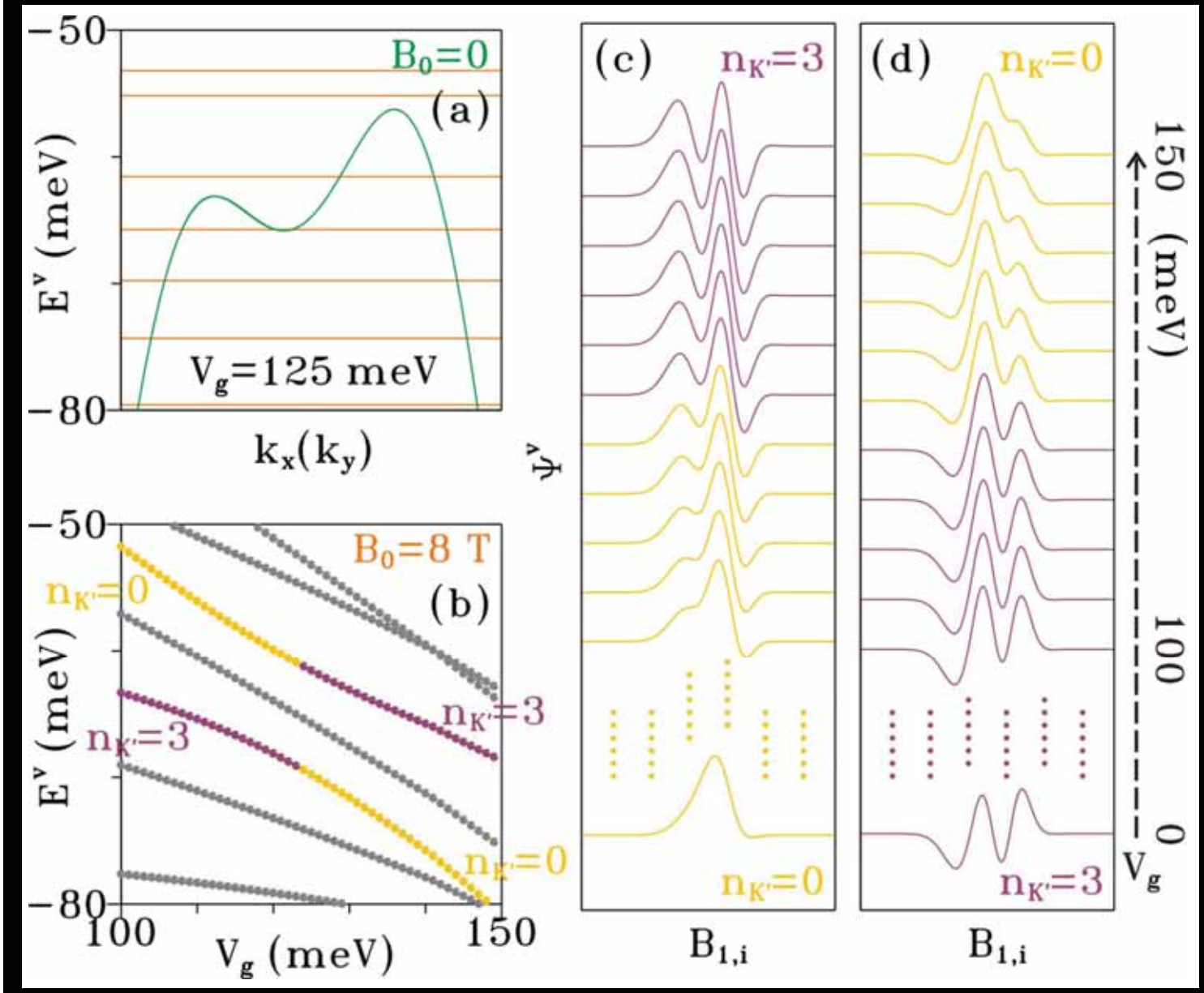
direct crossing
avoided crossing

Landau-level coupling → mixing of Landau wave functions



Even though WFs are severely mixed, but in energy, there're still well-quantized LLs

Landau-level coupling → mixing of Landau wave functions



$\Delta n = 3l$

interlayer coupling γ_3

Optical absorption spectrum…

absorption rate: $W(\vec{q}\sim 0,\omega)=\sum_{i,j} P_{i\to j}-P_{j\to i}$

$$=\frac{2\pi}{\hbar}(\frac{eA_0}{mc})^2 2\sum_{i,j}|\langle\Phi_j|e^{i\vec{q}\cdot\vec{r}}\hat{e}\cdot\vec{p}|\Phi_i\rangle|^2\delta(E_j-E_i+\hbar\omega)[f(E_i)-f(E_j)]$$

dipole matrix element within the gradient approximation

$$\langle\Phi_j|\vec{p}|\Phi_i\rangle=\langle\Phi_j|\frac{im}{\hbar}[H,\vec{r}]|\Phi_i\rangle$$

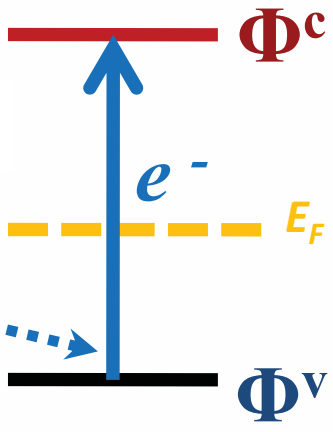
$$=\frac{im}{\hbar}(\vec{R}_i-\vec{R}_j)\langle\Phi_j|H|\Phi_i\rangle$$

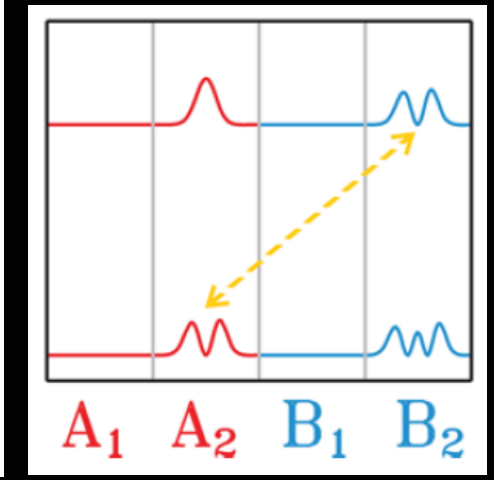
$$=\frac{m}{\hbar}\nabla_{\vec{k}}\langle\Phi_j|H|\Phi_j\rangle$$

$$|\langle A_i|\partial_{\mathbf{k}}H_{\in\gamma_0}|B_i\rangle|^2$$

Fermi-Dirac distribution function:

$$f(E_{i,j})=\frac{1}{\exp\{[E_{i,j}-\mu(T)]/k_BT\}+1}$$

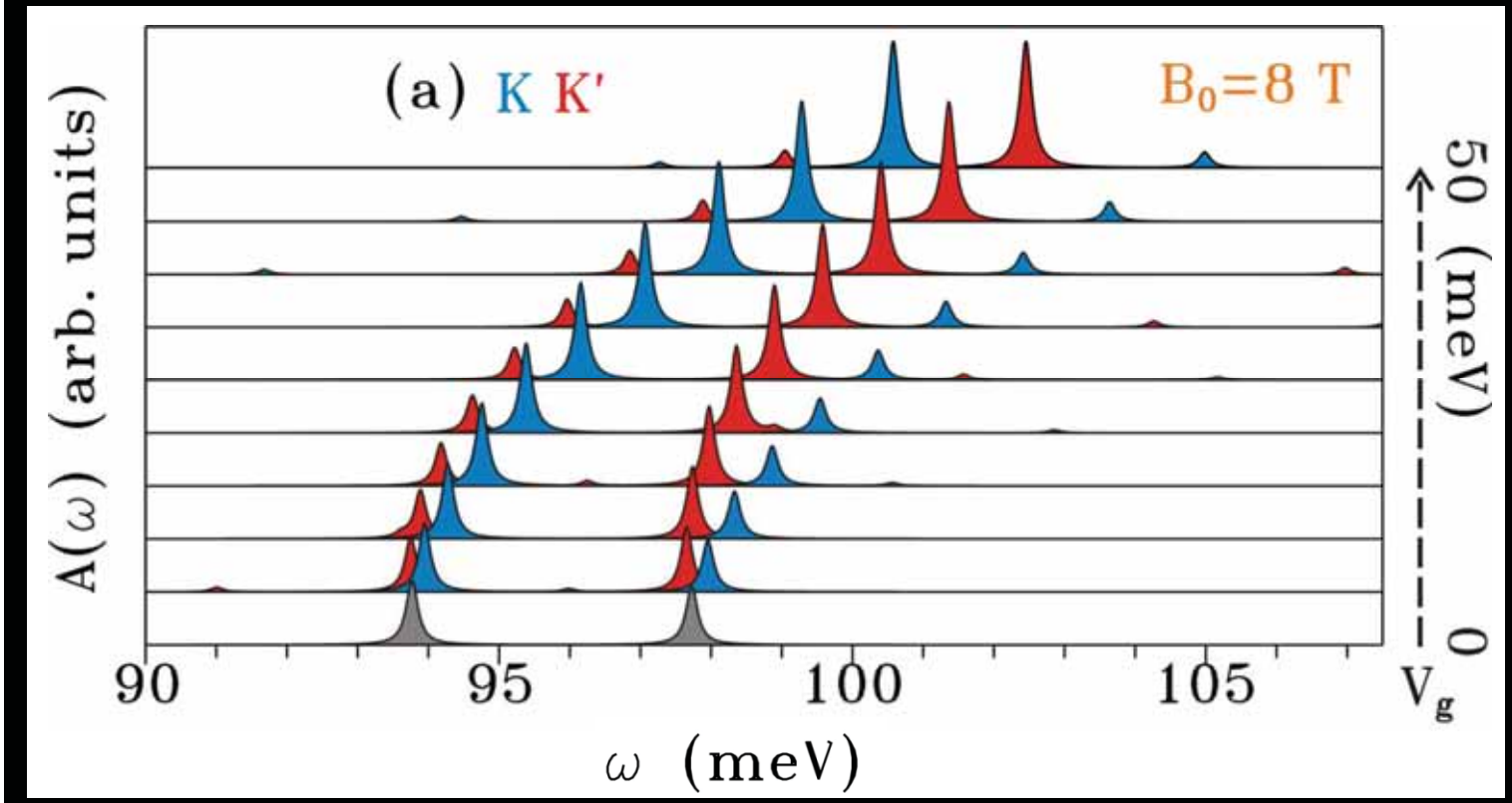




γ_0 :>> $\gamma_{1,3,4,6}$: Optical transitions are mainly determined by the terms related to γ_0, as well as the WF on the both sides.

Sublattices must have the same node number…
to satisfy the orthogonality relation of Hermite polynomial.

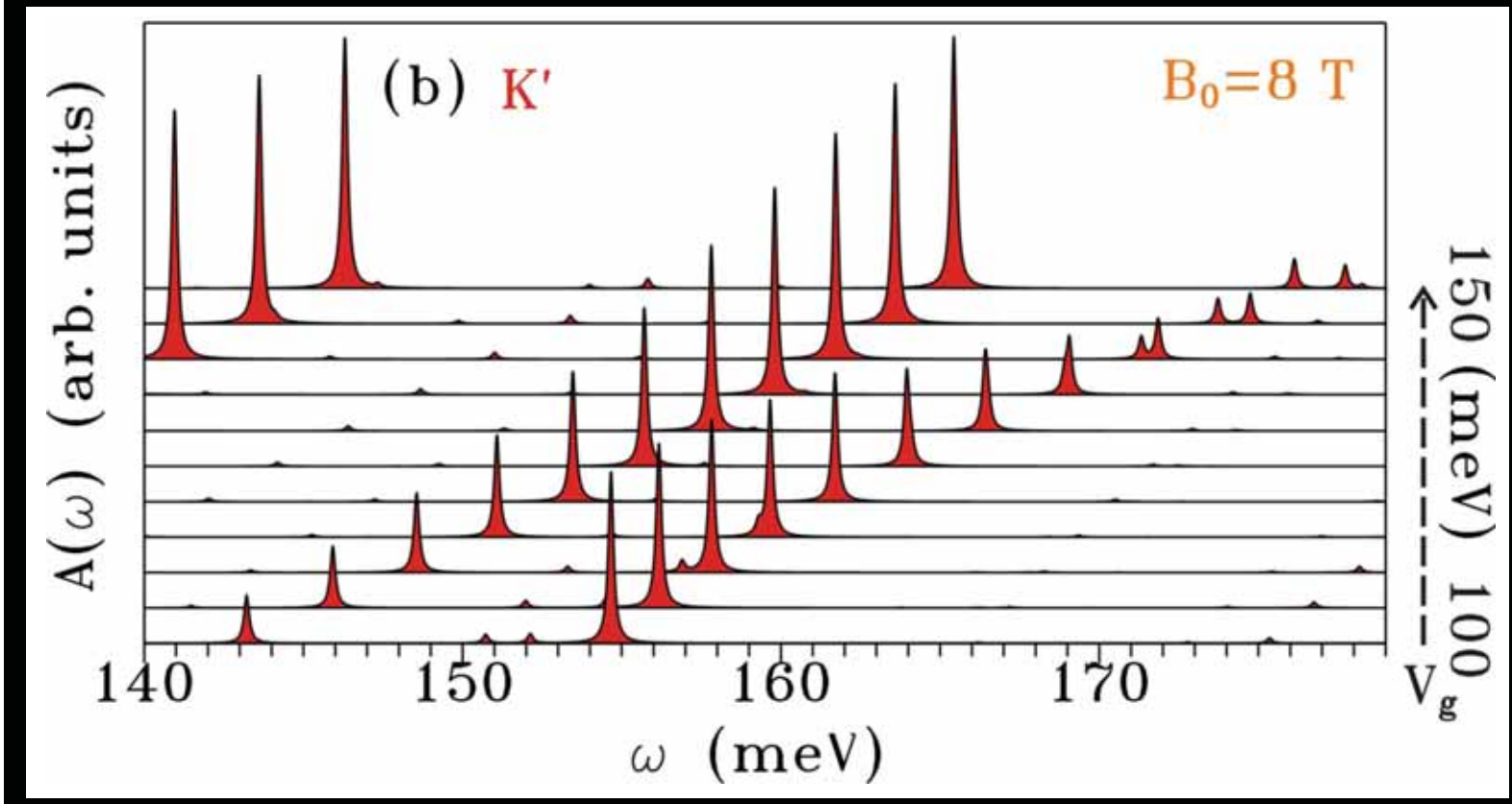
Magneto-optical spectra for breaking of inter-valley degeneracy



Electron-hole asymmetry: $n^v+1 \rightarrow n^c$ $n^v \rightarrow n^c+1$

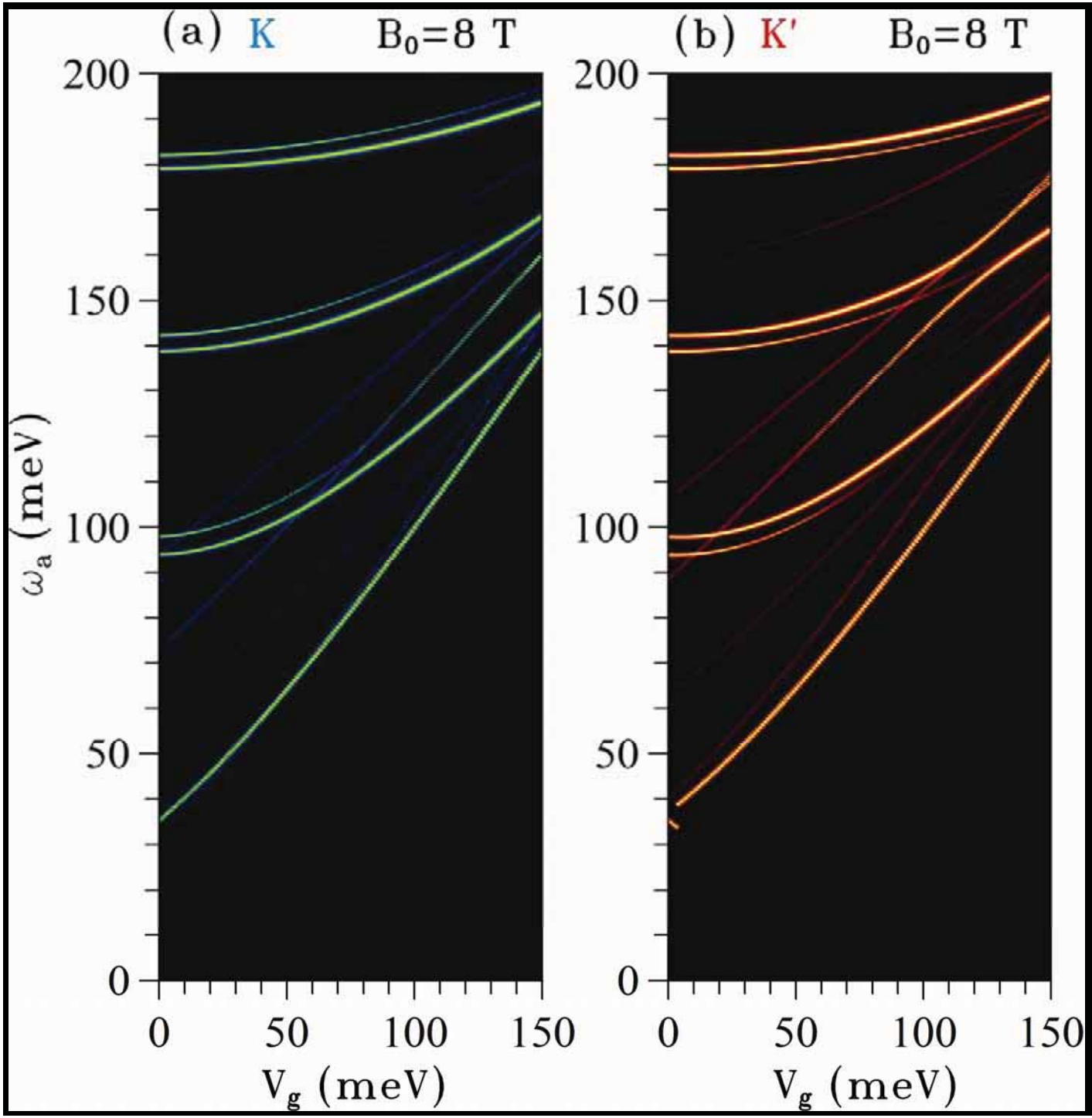
Lift inter-valley degeneracy: energy splitting and intensity changes

Magneto-optical spectra for Landau-level couplings



the changes in peak position & peak intensity, the occurrence of minor peaks.

Selection rules & transition rates by Landau wave functions.



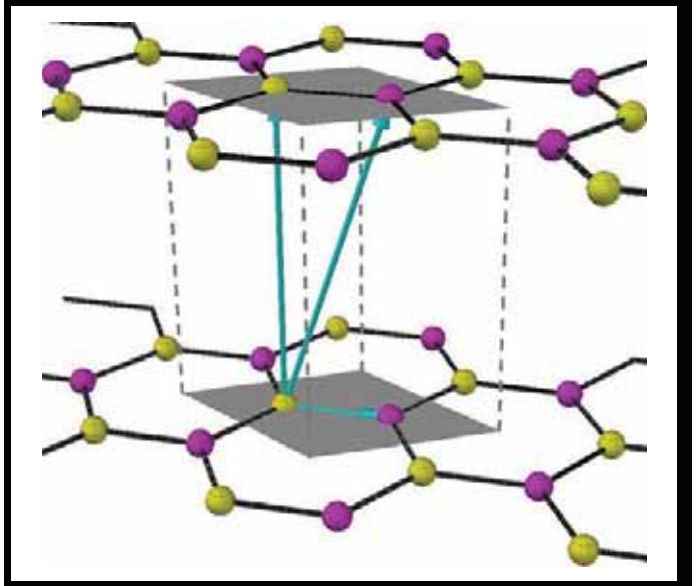
Contour plot of optical spectra: K & K' states

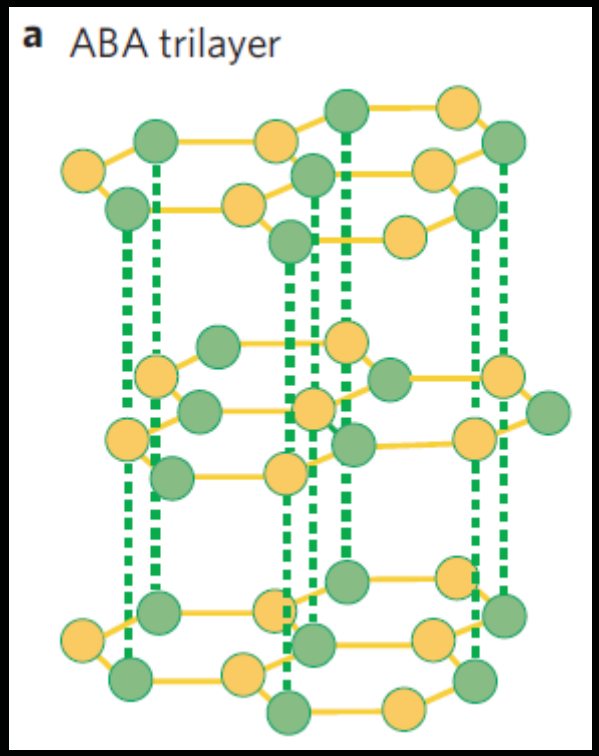
Breaking of inter-valley degeneracy

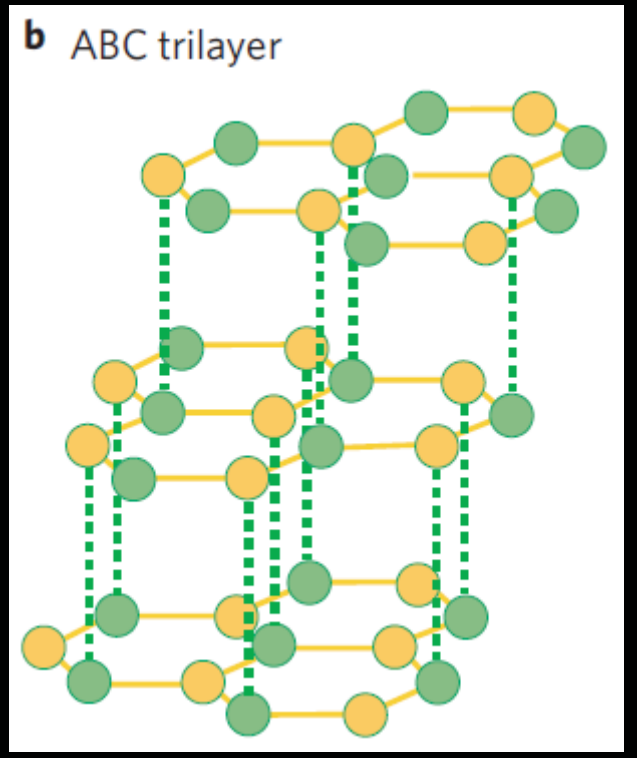
Landau level couplings

Peak intensities: Changes in the WFs.

Whether the 2 valley states split and whether the LL couplings appear depend on the stacking order and the layer numbers.

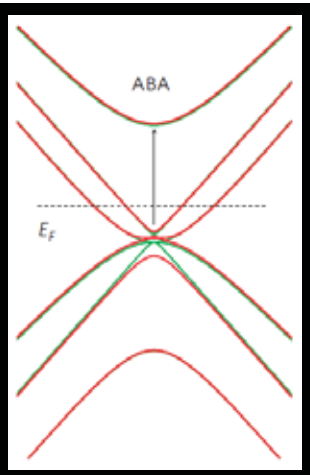


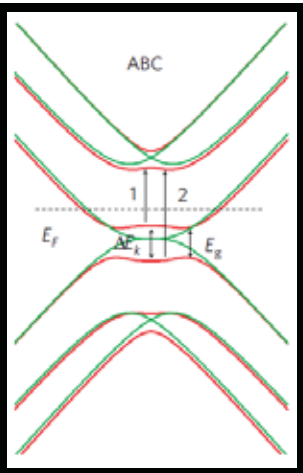




Valley states split:
top & bottom must be asymmetric

LL couplings:
depends on stacking order





Summary ...

We use a complete tight-binding model to study the Landau level structures in biased bilayer graphene. The changes of weight in Landau wave function enable us to characterize the breaking of inter-valley degeneracy and the appearance of unusual Landau levels, which have their direct counterpart in magneto-optical spectra.

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