INTERACTION EFFECTS IN MoS_2

Alberto Cortijo
ICMM-CSIC

Correlations, criticality, and coherence in quantum systems- Évora 2014

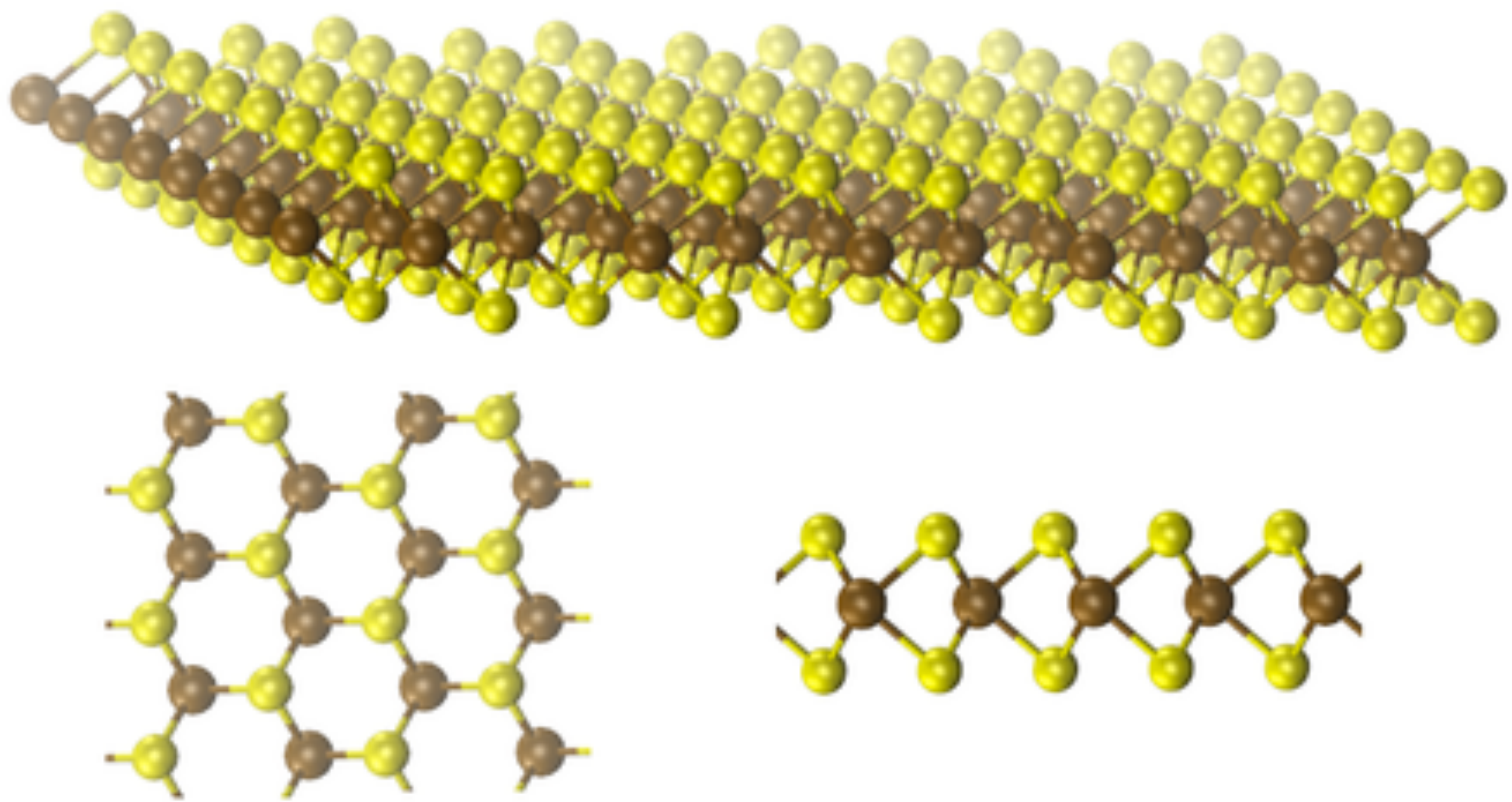
INTERACTION EFFECTS IN MoS_2

Alberto Cortijo
ICMM-CSIC

Correlations, criticality, and coherence in quantum systems- Évora 2014

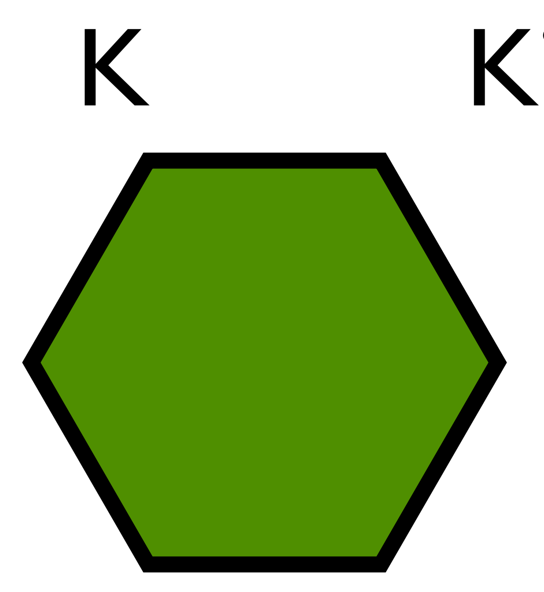
... with Yago Ferreiros

MoS_2:

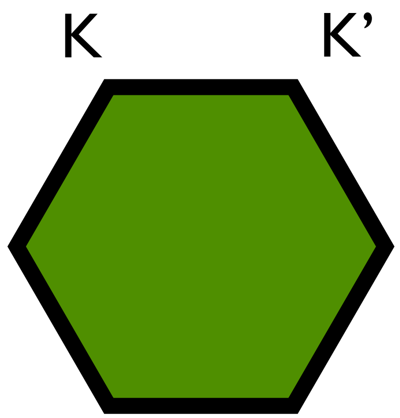


unit cell=1Mo atom +2 S atoms

hexagonal Brillouin zone



Low energy band structure:



$$\psi = \begin{pmatrix} |d_{z^2}\rangle \\ \frac{1}{\sqrt{2}}(|d_{x^2-y^2}\rangle + i\tau|d_{xy}\rangle) \end{pmatrix}$$

$m_l = 0$

$m_l = \pm 2$

valley index

$s = \pm 1$ ← spin$_z$ index

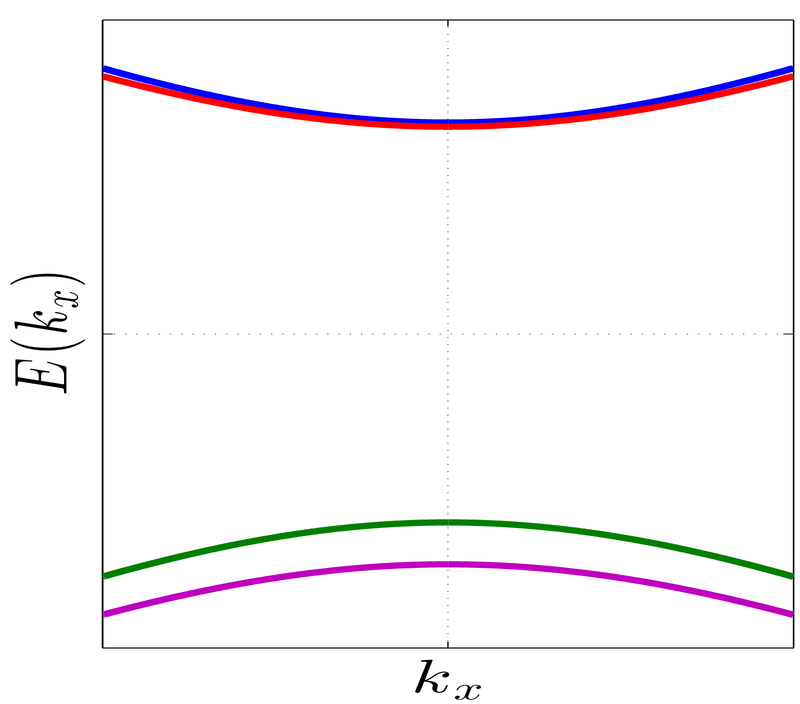
$\tau = \pm 1$

$$\mathcal{H}_0 = v_\tau \left(\tau\sigma_x k_x + \sigma_y k_y\right) + \frac{1}{2}s\tau\left(\lambda_c(\sigma_0 + \sigma_z) + \lambda_v(\sigma_0 - \sigma_z)\right) + \frac{\Delta}{2}\sigma_z$$

hopping term (through S p-like orbitals)

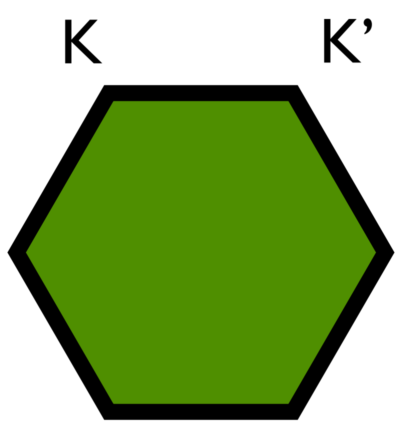
spin-orbit interaction

crystal field splitting



$$\lambda_c \simeq 0$$

Low energy band structure:



$$\psi = \begin{pmatrix} |d_{z^2}\rangle \\ \frac{1}{\sqrt{2}}(|d_{x^2-y^2}\rangle + i\tau|d_{xy}\rangle) \end{pmatrix}$$

$\leftarrow m_l = 0$

$\leftarrow m_l = \pm 2$

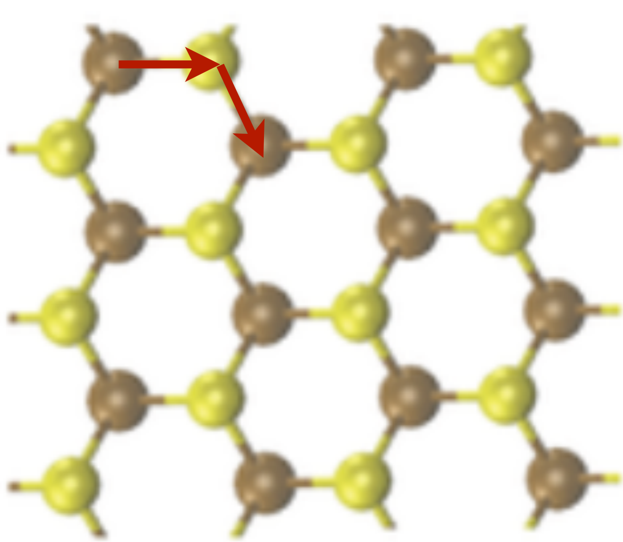
τ: valley index

$s = \pm 1 \leftarrow$ spin$_z$ index

$\tau = \pm 1$

$$\mathcal{H}_0 = v(\tau\sigma_x k_x + \sigma_y k_y) + \frac{\Delta}{2} s_0 \tau_0 \sigma_z + \frac{\lambda_c - \lambda_v}{2} s_z \tau_z \sigma_z + \frac{\lambda_c + \lambda_v}{2} s_z \tau_z \sigma_0$$

- $v(\tau\sigma_x k_x + \sigma_y k_y)$: hopping term (through S p-like orbitals)
- $\frac{\Delta}{2} s_0 \tau_0 \sigma_z$: staggered mass
- $\frac{\lambda_c - \lambda_v}{2} s_z \tau_z \sigma_z$: Kane-Mele mass
- $\frac{\lambda_c + \lambda_v}{2} s_z \tau_z \sigma_0$: "chiral" chemical potential

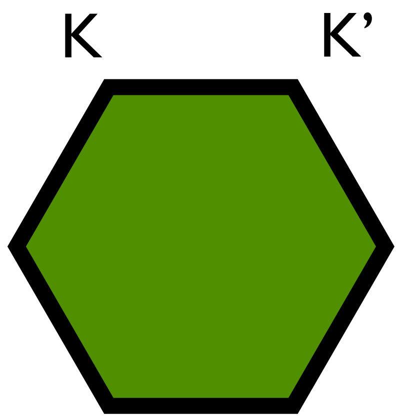


H. Ochoa, R. Roldán. PRB, 87, 245421(2013)

A. Kormányos et al. PRB, 88, 045416 (2013)

K. Kosmider et al. PRB, 88, 245436 (2013)

Low energy band structure:



$$\psi = \begin{pmatrix} |d_{z^2}\rangle \\ \frac{1}{\sqrt{2}}(|d_{x^2-y^2}\rangle + i\tau|d_{xy}\rangle) \end{pmatrix}$$

← $m_l = 0$

← $m_l = \pm 2$

↑ valley index

$s = \pm 1$ ← spin$_z$ index

$\tau = \pm 1$

$$\mathcal{H}_0 = v(\tau\sigma_x k_x + \sigma_y k_y) + \frac{\Delta}{2} s_0 \tau_0 \sigma_z + \frac{\lambda_c - \lambda_v}{2} s_z \tau_z \sigma_z + \frac{\lambda_c + \lambda_v}{2} s_z \tau_z \sigma_0$$

hopping term (through S p-like orbitals)

↑ staggered mass

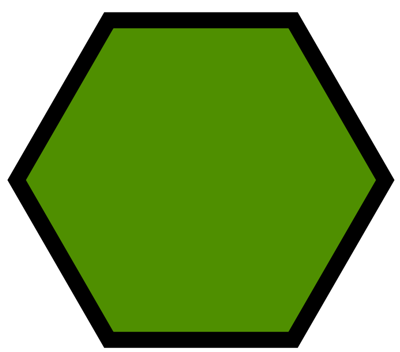
↑ Kane-Mele mass

↑ "chiral" chemical potential

The Hamiltonian form can be fixed by symmetry arguments

how do we fix the parameters?

Low energy band structure:



$$\psi = \begin{pmatrix} |d_{z^2}\rangle \\ \frac{1}{\sqrt{2}}(|d_{x^2-y^2}\rangle + i\tau|d_{xy}\rangle) \end{pmatrix}$$

$\leftarrow m_l = 0$

$\leftarrow m_l = \pm 2$

τ: valley index

$s = \pm 1$ ← spin$_z$ index

$\tau = \pm 1$

$$\mathcal{H}_0 = v(\tau\sigma_x k_x + \sigma_y k_y) + \frac{\Delta}{2} s_0\tau_0\sigma_z + \frac{\lambda_c - \lambda_v}{2} s_z\tau_z\sigma_z + \frac{\lambda_c + \lambda_v}{2} s_z\tau_z\sigma_0$$

hopping term (through S p-like orbitals)

staggered mass

Kane-Mele mass

"chiral" chemical potential

The Hamiltonian form can be fixed by symmetry arguments

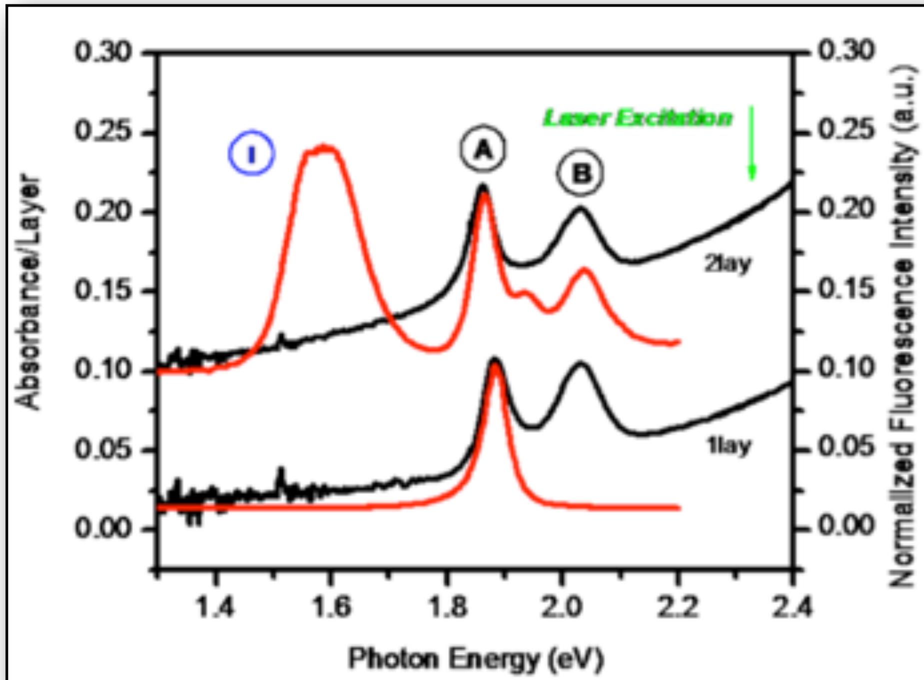
Role of interactions?

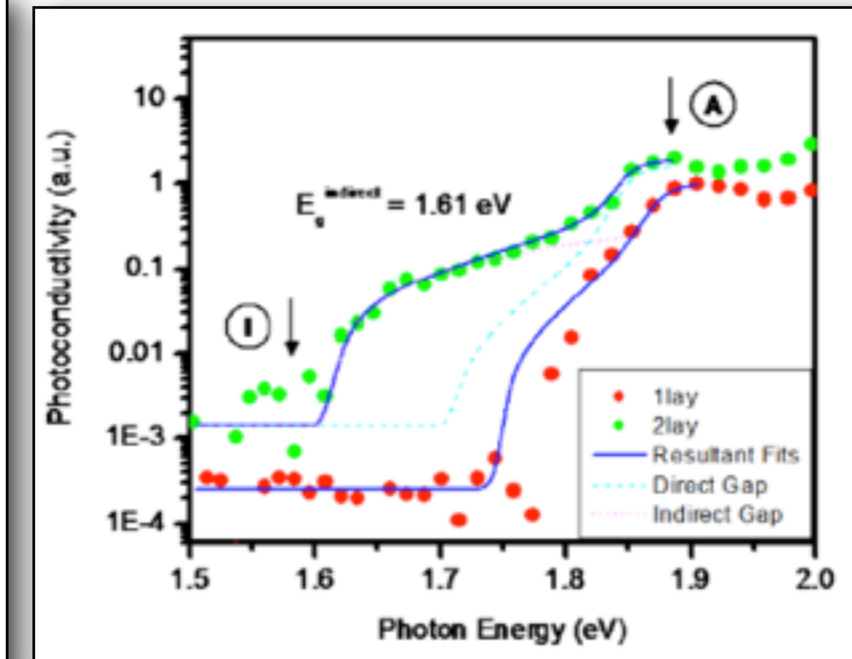
Important for spin relaxation studies

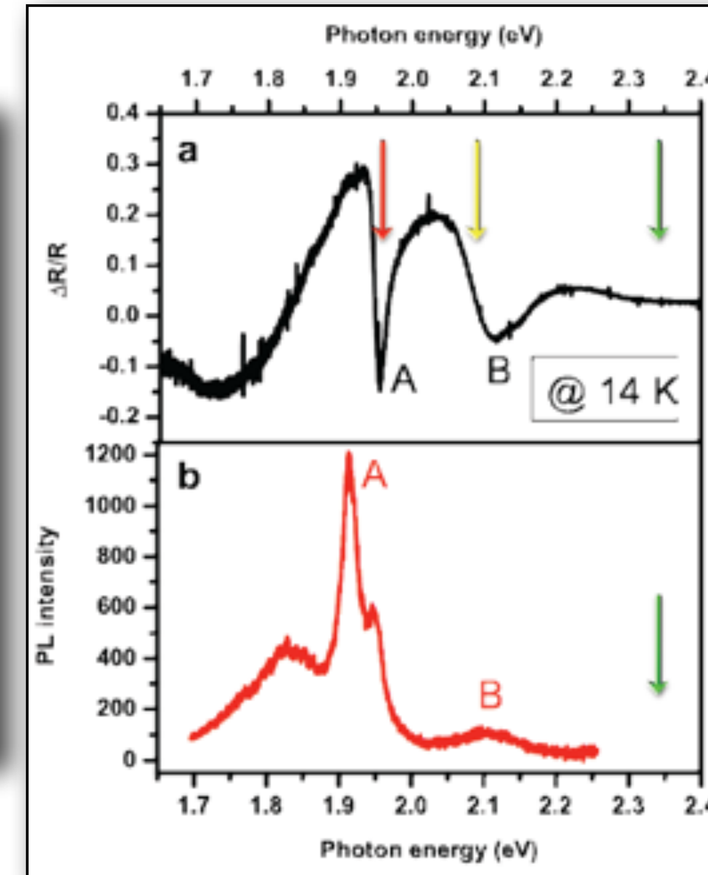
H. Ochoa, R. Roldán. PRB, 87, 245421(2013)

experiments...

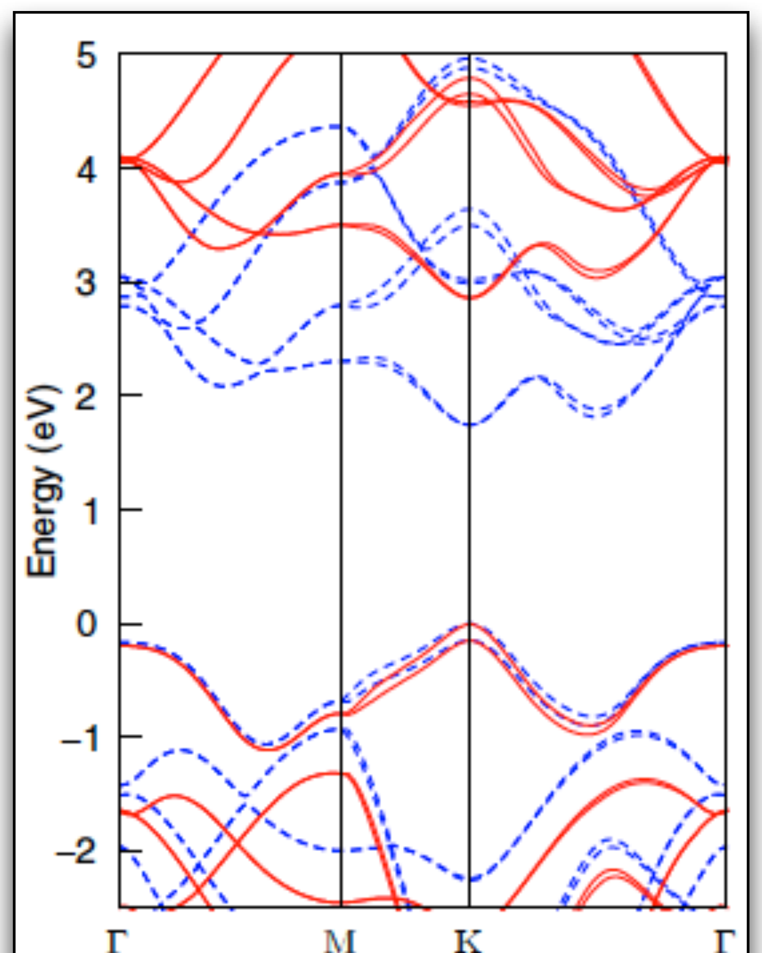
K. F. Mak et al. PRL, 105, 136805 (2010)

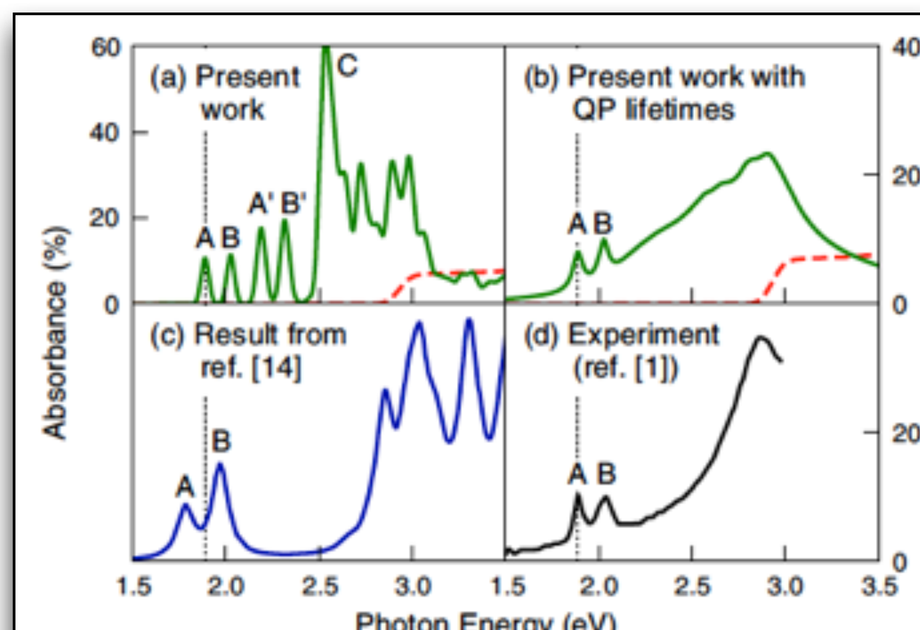






DFT...

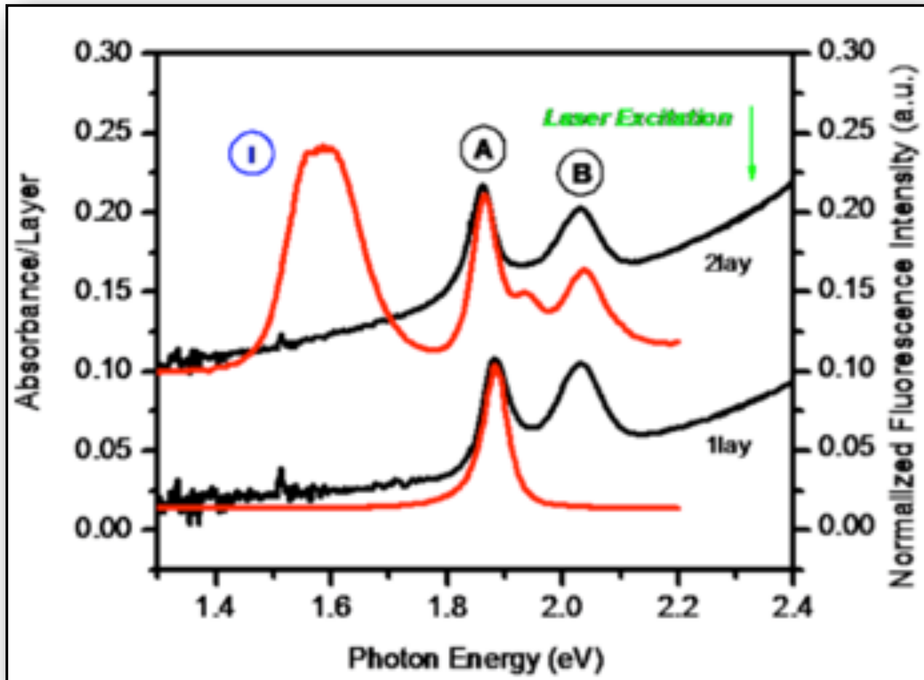


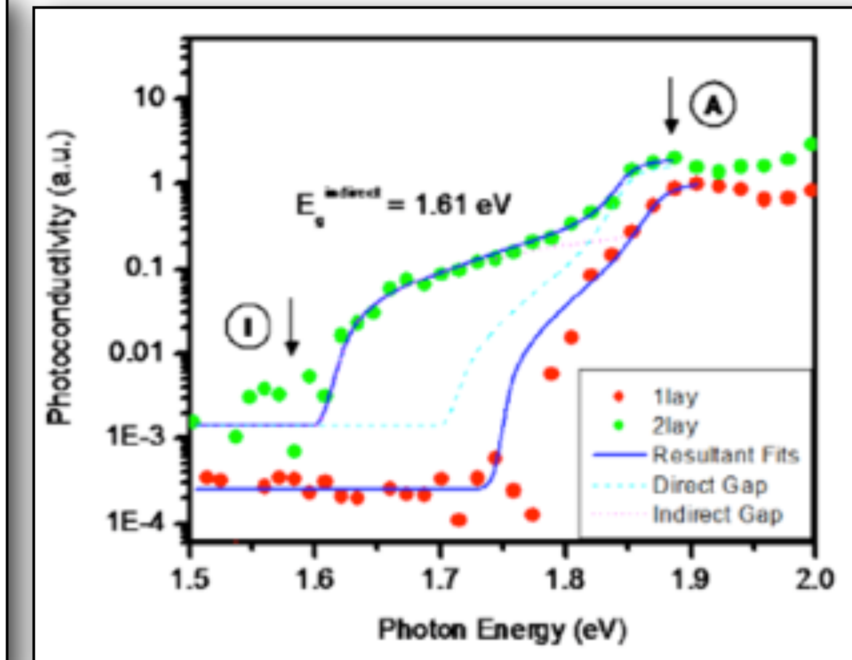


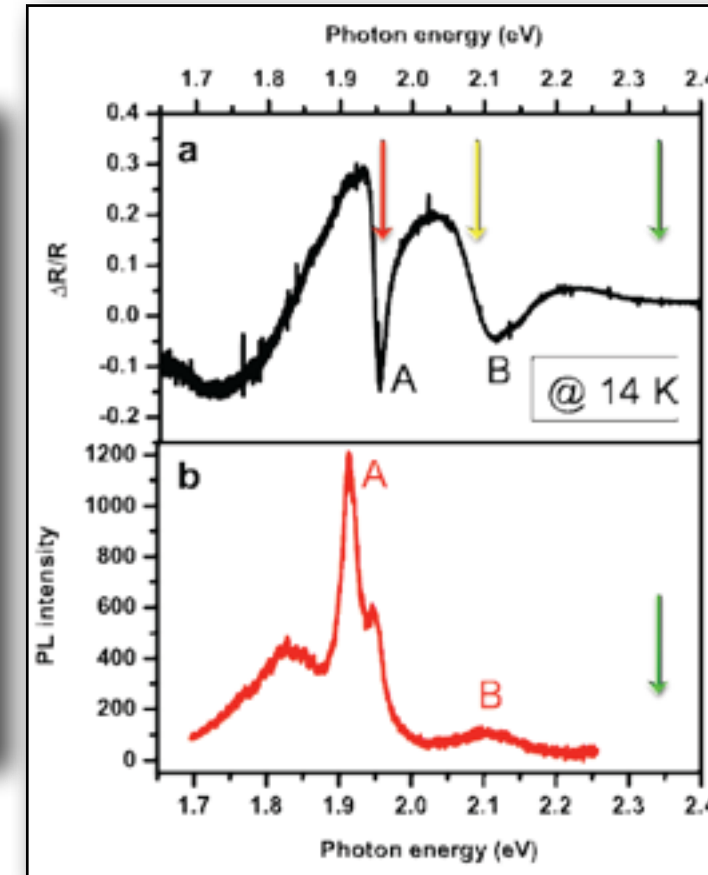
D.Y. Qiu et al. PRL, 111, 216805 (2013)

experiments...

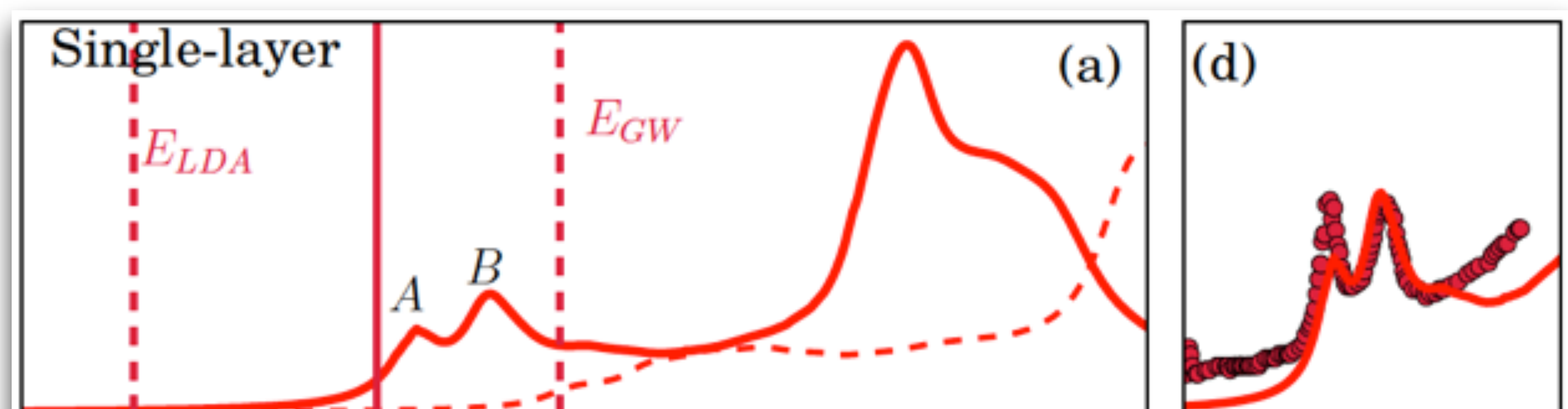
K. F. Mak et al. PRL, 105, 136805 (2010)







DFT...



finite k-point sampling. Panels (d)–(f): symbols: experimental absorption spectra[3,4] in comparison with the calculations (solid lines, shifted by about -0.2 eV).

A. Molina-Sanchez et al. PRB, 88, 045412 (2013)

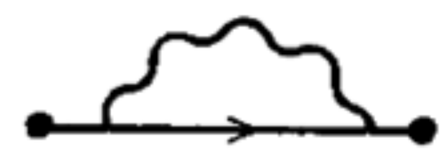
experiments...+ analytical GW calculation

$$G^{-1}(\omega, \mathbf{k}) = \omega - \mathcal{H}_0(\mathbf{k}) - \Sigma(\omega, \mathbf{k})$$

Unscreened Coulomb interaction:

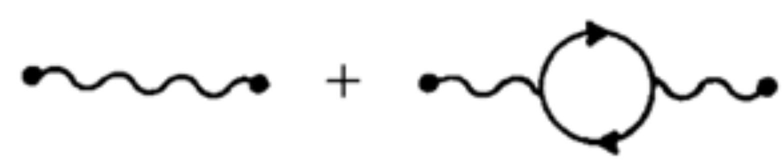
$$\mathcal{H}_{int} = e\psi^+(x)\psi(x)\varphi(x) + \epsilon\varphi(x)|\vec{\nabla}|\varphi(x)$$

$$D(q)_0 \equiv D_0(\mathbf{q}) = \frac{1}{4\pi\epsilon}\frac{1}{|\mathbf{q}|}$$



$\Sigma(k)$

$$\Sigma(k) = e^2 \int \frac{d^3q}{(2\pi)^3} D(q)G(k-q)$$



$D(q)$

$$D^{-1}(q) = 4\pi\epsilon(|\mathbf{q}| + \Pi(q))$$

$\Pi(q)$

$$\Pi(q) = \int \frac{d^3p}{(2\pi)^3} G(p)G(p-q)$$

Analytical GW calculation

$$\Sigma(k) = e^2 \int \frac{d^3q}{(2\pi)^3} D(q) G(k-q) \Gamma(p,q)$$

$$\Sigma(k) = e^2 \int \frac{d^3q}{(2\pi)^3} D(q) G(k-q)$$

$\Pi(q) \to \Pi(0, \mathbf{q})$ instantaneous approximation

no vertex corrections

$$\frac{\partial \Sigma(k)}{\partial \omega} = \gamma^0$$

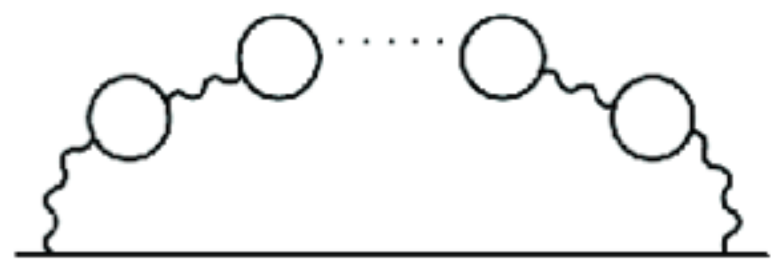
no wavefunction renormalization

$$\Sigma(k) = -(\tau\sigma_x k_x + \sigma_y k_y)\delta v_s - \frac{\delta\Delta}{2}\sigma_z - \frac{\delta\lambda_c}{2}\tau s(\sigma_0 + \sigma_z) - \frac{\delta\lambda_v}{2}\tau s(\sigma_0 - \sigma_z)$$

quantum corrections to be calculated

Analytical GW calculation

we wont restrict ourselves to small values of $g_s = \frac{e^2}{4\pi\epsilon v_s}$

$1/N$ expansion $\longrightarrow$  $\longrightarrow$ equivalent to a RPA expansion

$$\Pi(q) = \frac{e^2}{4\pi}|\mathbf{q}| \sum_{s=\pm} \left[\frac{2m_s}{q_s^2} + \frac{q_s^2 - 4m_s^2}{q_s^3} \arctan\left(\frac{q_s}{2m_s}\right)\right]$$

$$q_s^2 = q_0^2 + v_s^2|\mathbf{q}|^2$$

$$m_s = (\Delta + s(\lambda_c - \lambda_v))/2$$

$$\Delta = \Delta^0 + \delta\Delta$$

$$\lambda_{c,v} = \lambda_{c,v}^0 + \delta\lambda_{c,v}$$

$$e^2 \int \frac{d^3q}{(2\pi)^3} D(q) G(k-q) = \tau_z \begin{pmatrix} I_\uparrow & 0 \\ 0 & I_\downarrow \end{pmatrix}$$

$$I_s = I_s^z \sigma_z + I_s \vec{\sigma} \cdot \vec{k} + \mathcal{O}(k^2)$$

$$I_s = \frac{3m_r}{4m_s} \ln\left(1 + \frac{2g_s m_s}{3m_r}\right) + \frac{g_s}{4 + 2\pi g_r} \ln\left(\frac{v_s\Lambda}{m_s}\right)$$

$$I_s^z = \frac{3m_r}{4} \ln\left(1 + \frac{2g_s m_s}{3m_r}\right) + \frac{g_s m_s}{2 + \pi g_r} \ln\left(\frac{v_s\Lambda}{m_s}\right)$$

logarithmic divergent cut-off Λ

Analytical GW calculation

we have 5 (nonlinear) algebraic equations for 11 parameters!

$$\Sigma(k) = e^2 \int \frac{d^3q}{(2\pi)^3} D(q) G(k-q)$$

$$\delta v_{\uparrow\downarrow} = I_{\uparrow\downarrow} \quad \frac{1}{2}\delta\Delta + \delta\lambda_c = I^z_\uparrow \quad \frac{1}{2}\delta\Delta + \delta\lambda_v = I^z_\downarrow \quad \delta\lambda_c + \delta\lambda_v = 0$$

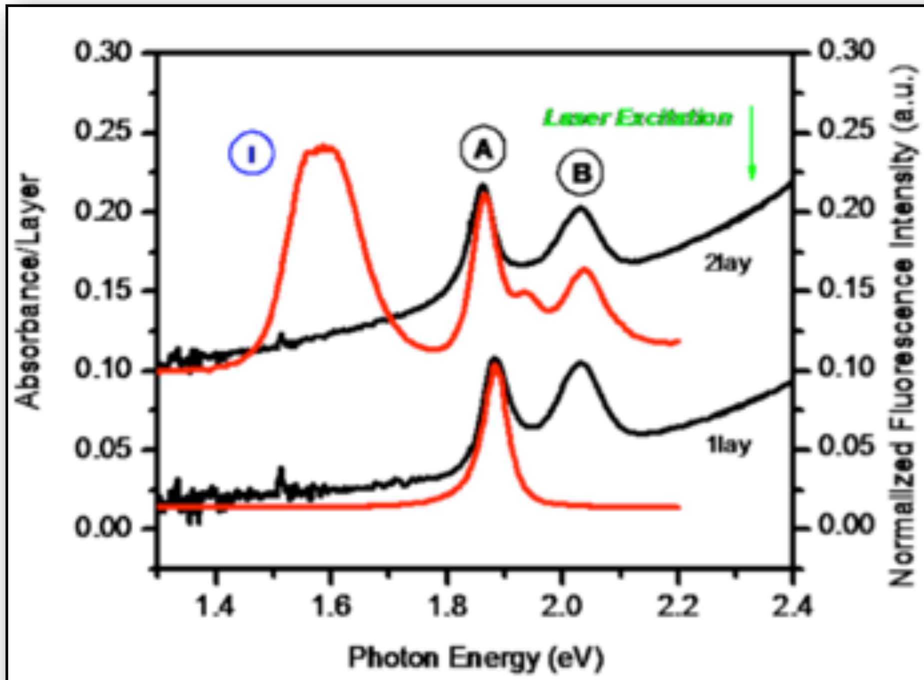
$\delta\lambda_c, \delta\lambda_v, \delta\Delta, \delta v_\uparrow, \delta v_\downarrow$ ⟵ quantum corrections

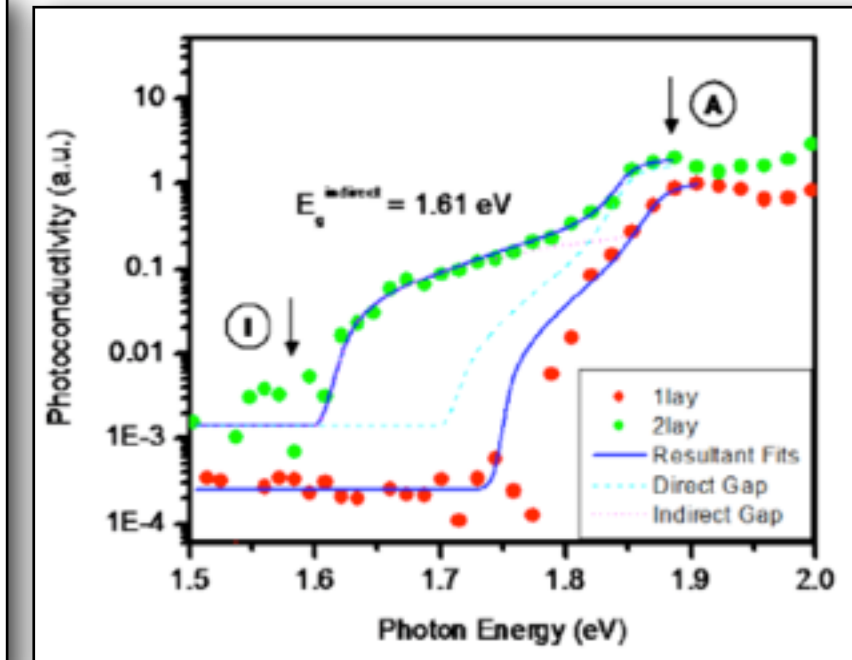
$\lambda^0_c, \lambda^0_v, \Delta^0, v^0_\uparrow, v^0_\downarrow,$ ⟵ bare parameters that are also unknown!

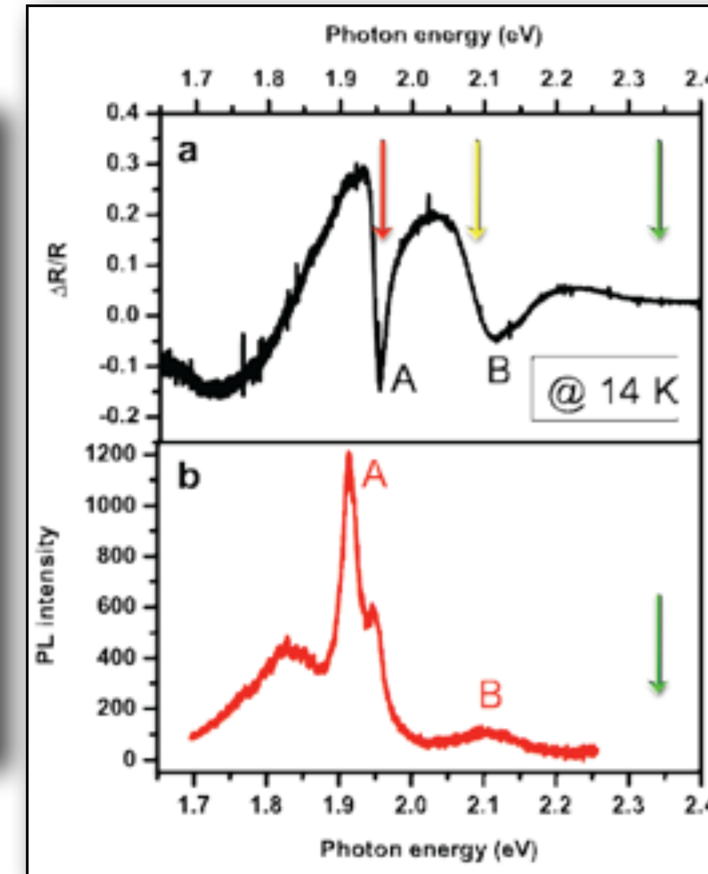
Λ ⟵ cut-off

we need 6 extra conditions to solve the problem!
"renormalization" conditions

experiments...







Absorption experiments see <u>two</u> exciton peaks

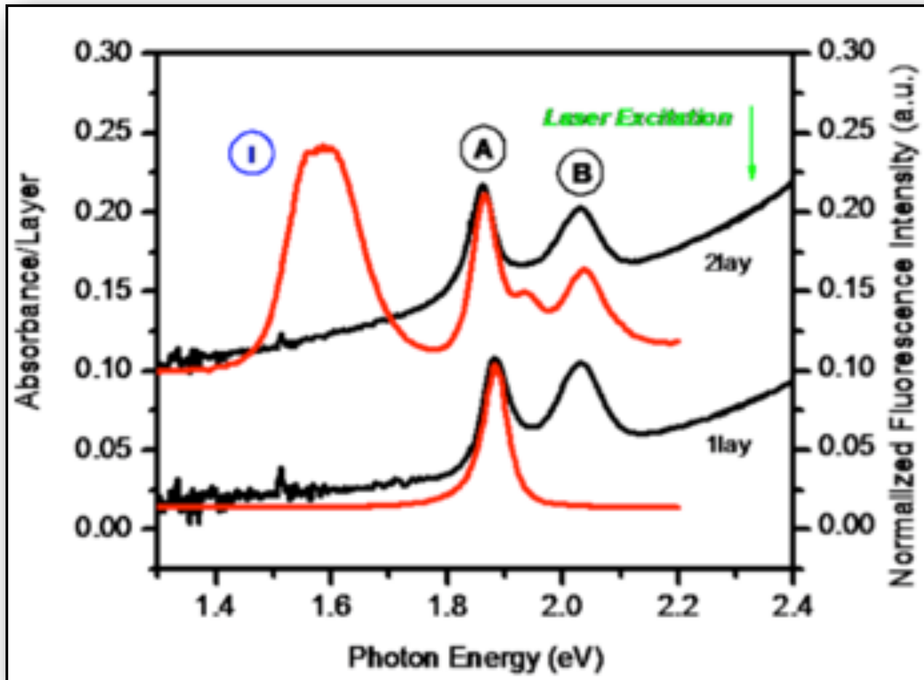
$$E_s(n,j) = m_s \left(1 + \frac{n + \sqrt{j^2 - g_s^2/4}}{\sqrt{g_s^2/4 + (n + \sqrt{j^2 - g_s^2/4})}} \right)$$

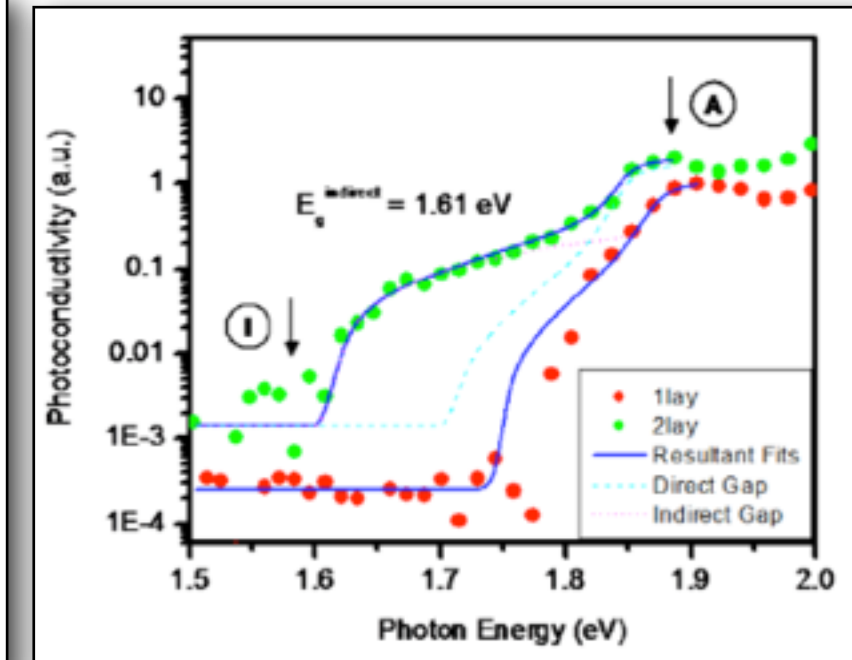
A. S. Rodin, A. H. Castro-Neto, PRB, 88, 195437 (2013)

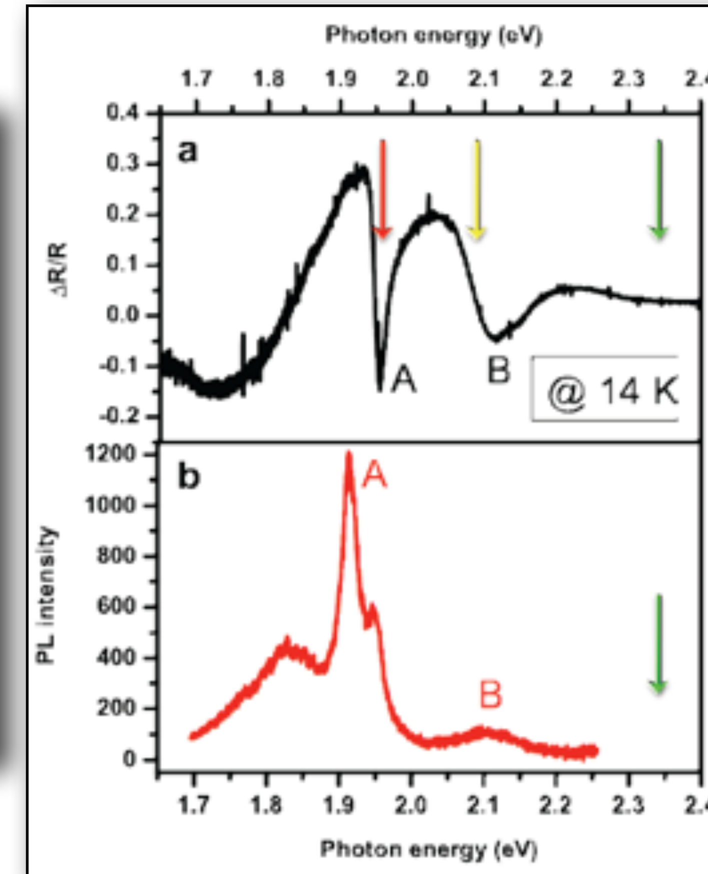
no more peaks are usually observed

the electron-hole continuum is hardly observed!

experiments...







Absorption experiments see two exciton peaks

$$E_s(n,j) = m_s \left(1 + \frac{n + \sqrt{j^2 - g_s^2/4}}{\sqrt{g_s^2/4 + (n + \sqrt{j^2 - g_s^2/4})}} \right)$$

$E_A = 1.85eV$ A. S. Rodin, A. H. Castro-Neto, PRB, 88,195437 (2013)

$E_A = 1.98eV$ A. Splendiani et al. Nanolett, 10, 1271 (2010)

physical insight?

(1). In absence of interactions the hopping process does not depend on spins

$$v_{\uparrow}^{0} = v_{\downarrow}^{0}$$

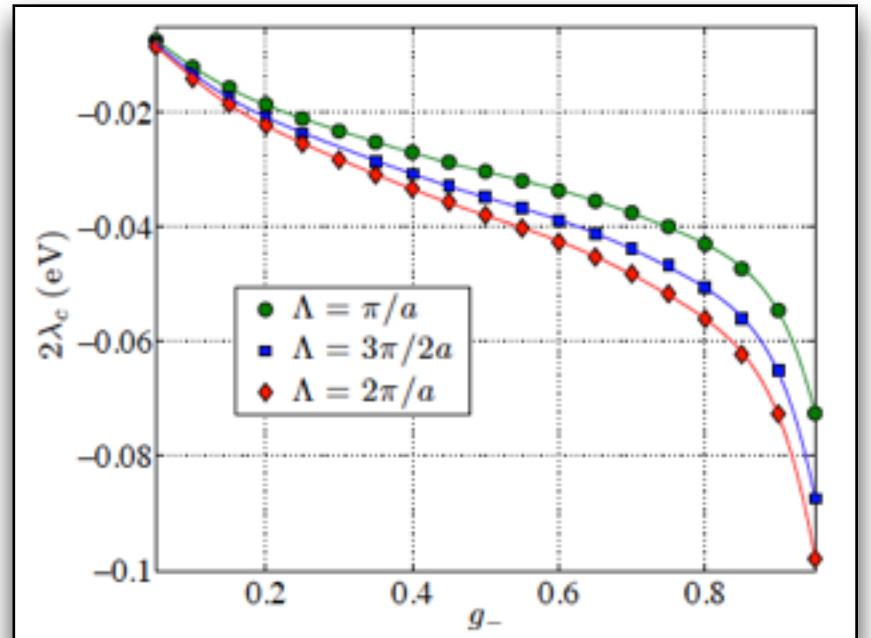
(2). In absence of interactions the spin orbit interaction for m_z=0 is (almost) zero

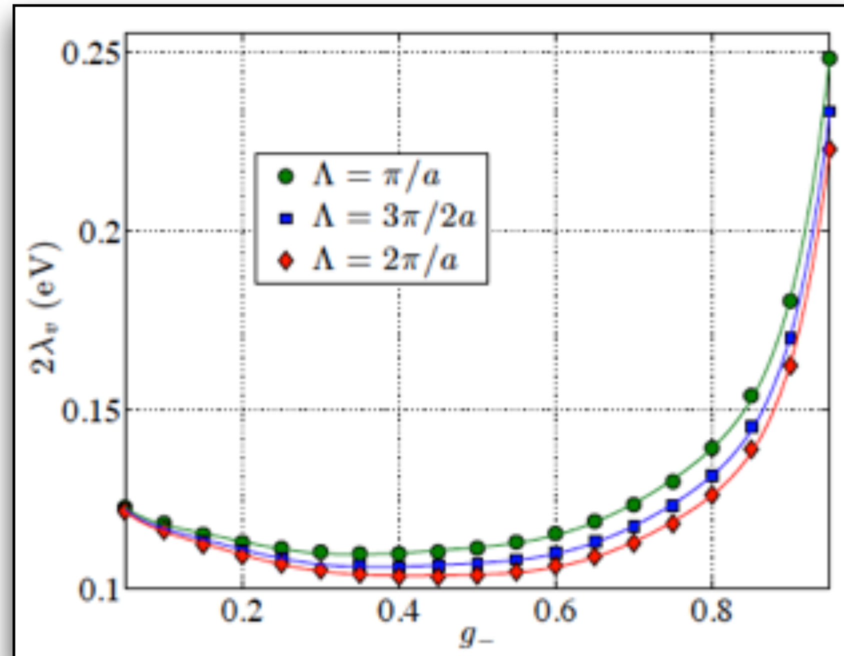
$$\lambda_c^0 \simeq 0$$

11- 5 - 4 = 2 still unknown parameters in the theory

?

Let's see the outcome $g_- < 1$

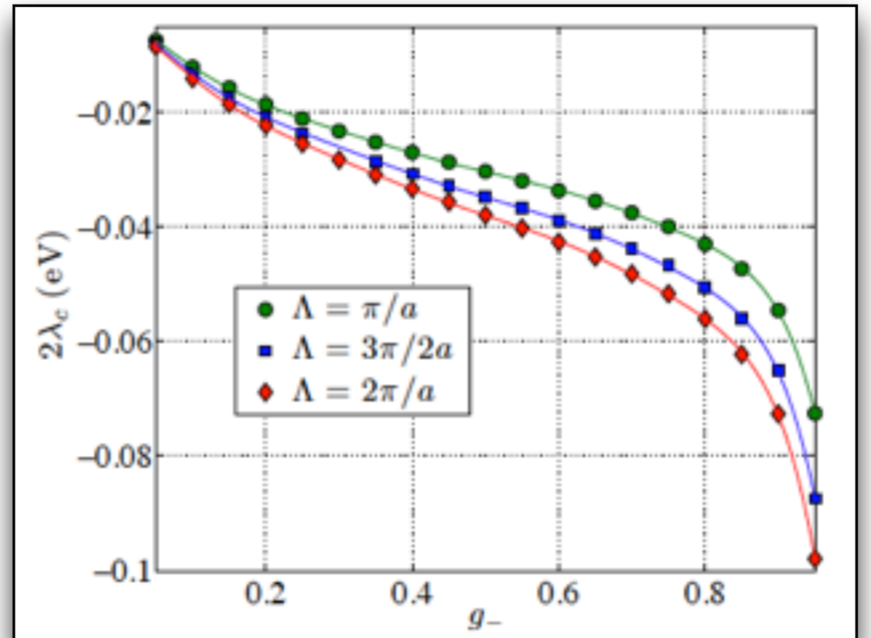


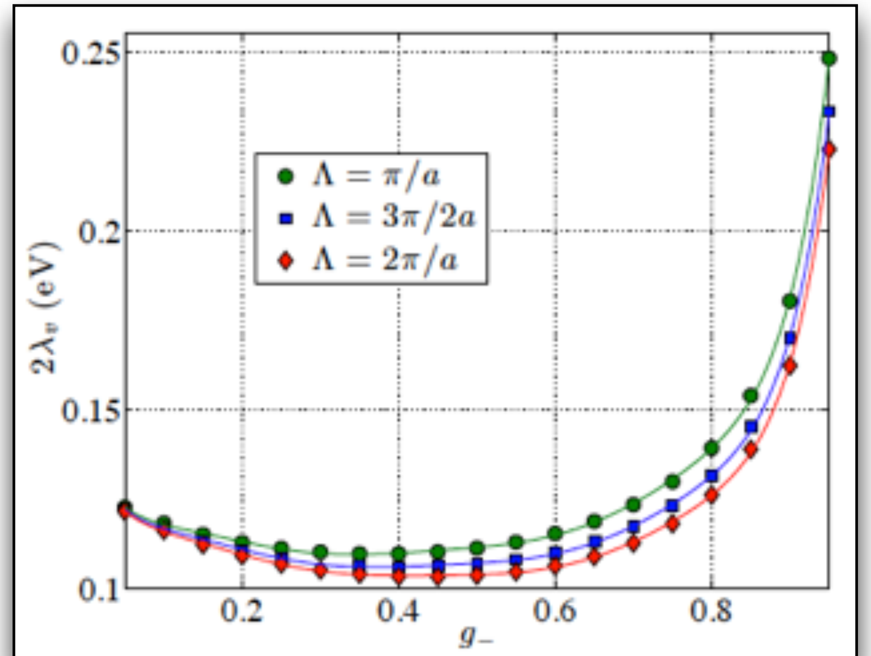


spin splittings
are cutoff dependent

qualitatively λ_c (λ_v)
grows (decreases)
with Λ
they compensate

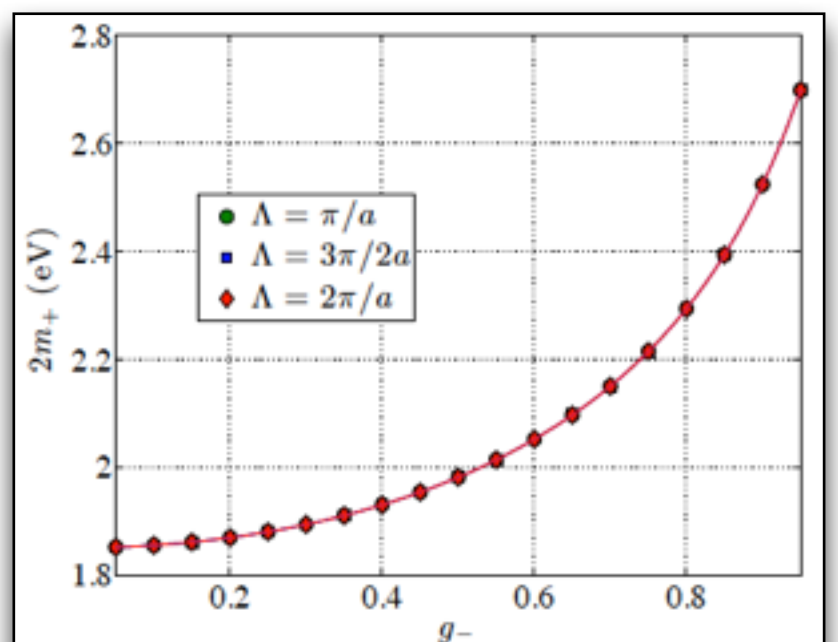
Let's see the outcome $g_- < 1$

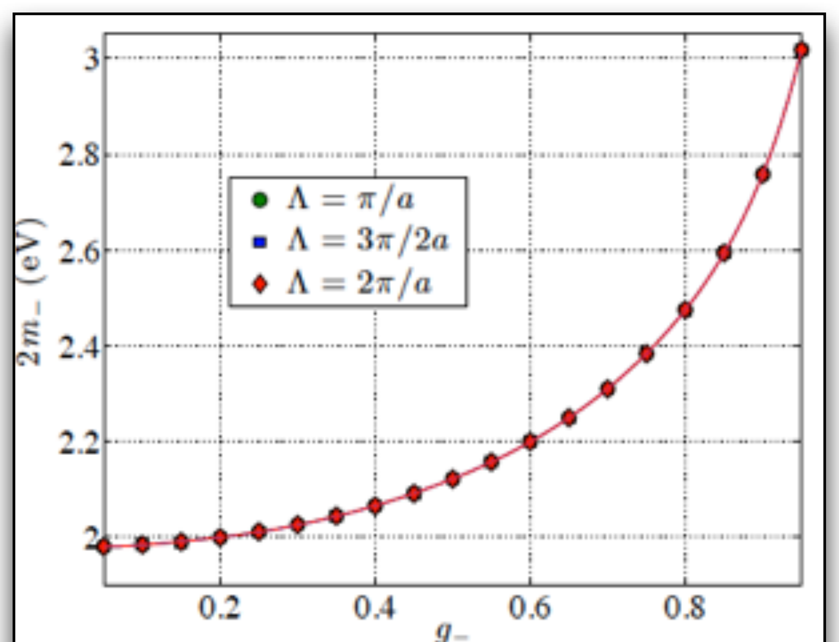


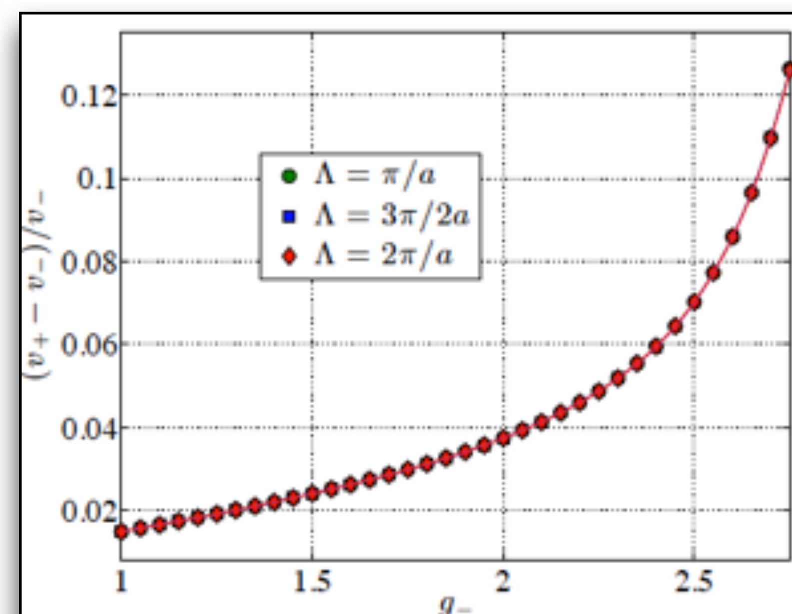


spin splittings
are cutoff dependent

qualitatively λ_c (λ_v)
grows (decreases)
with Λ
they compensate







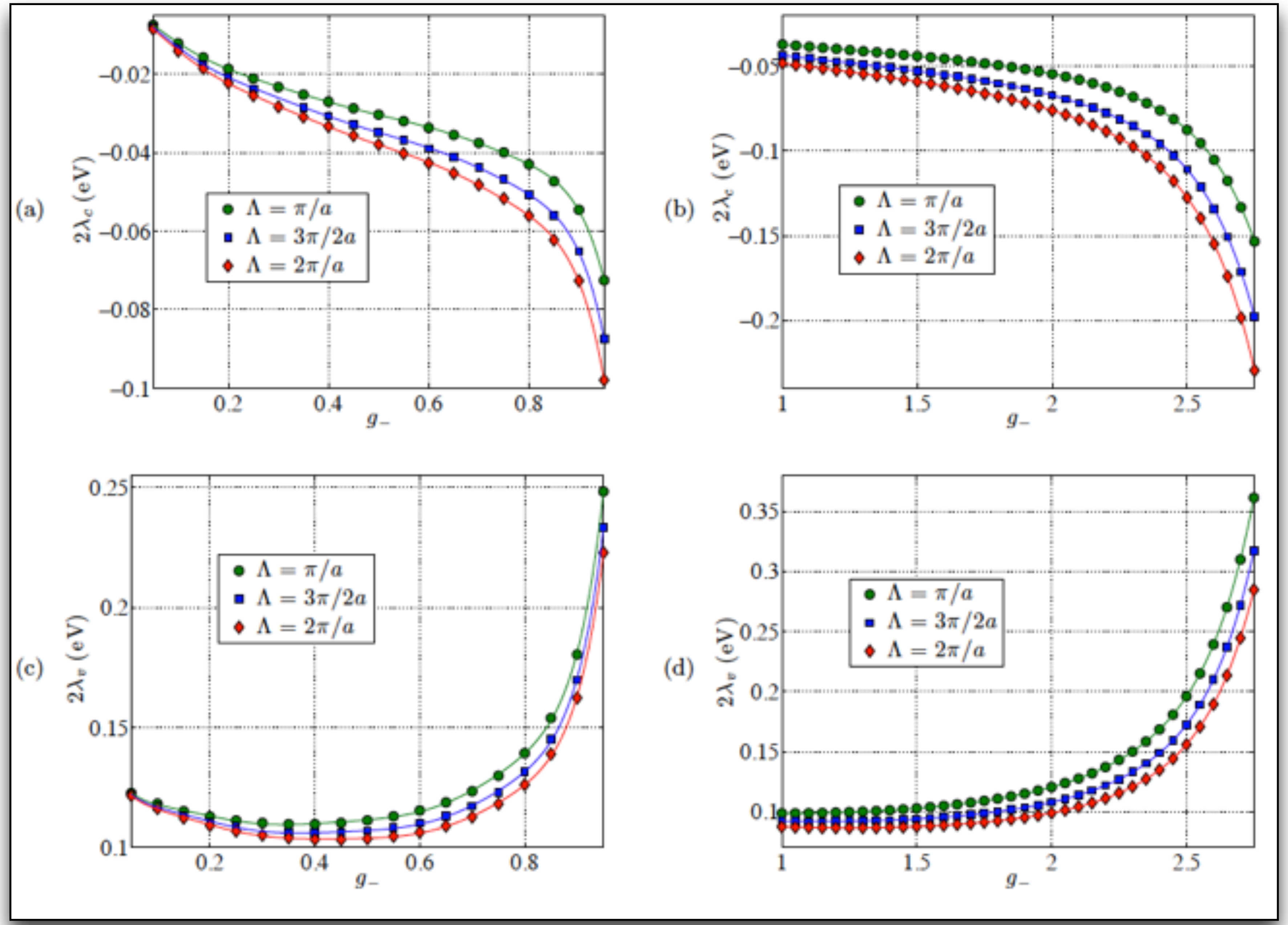
gaps are cutoff independent

spin dependent velocity
“renormalization”

Let's see the outcome

$g_- > 1$

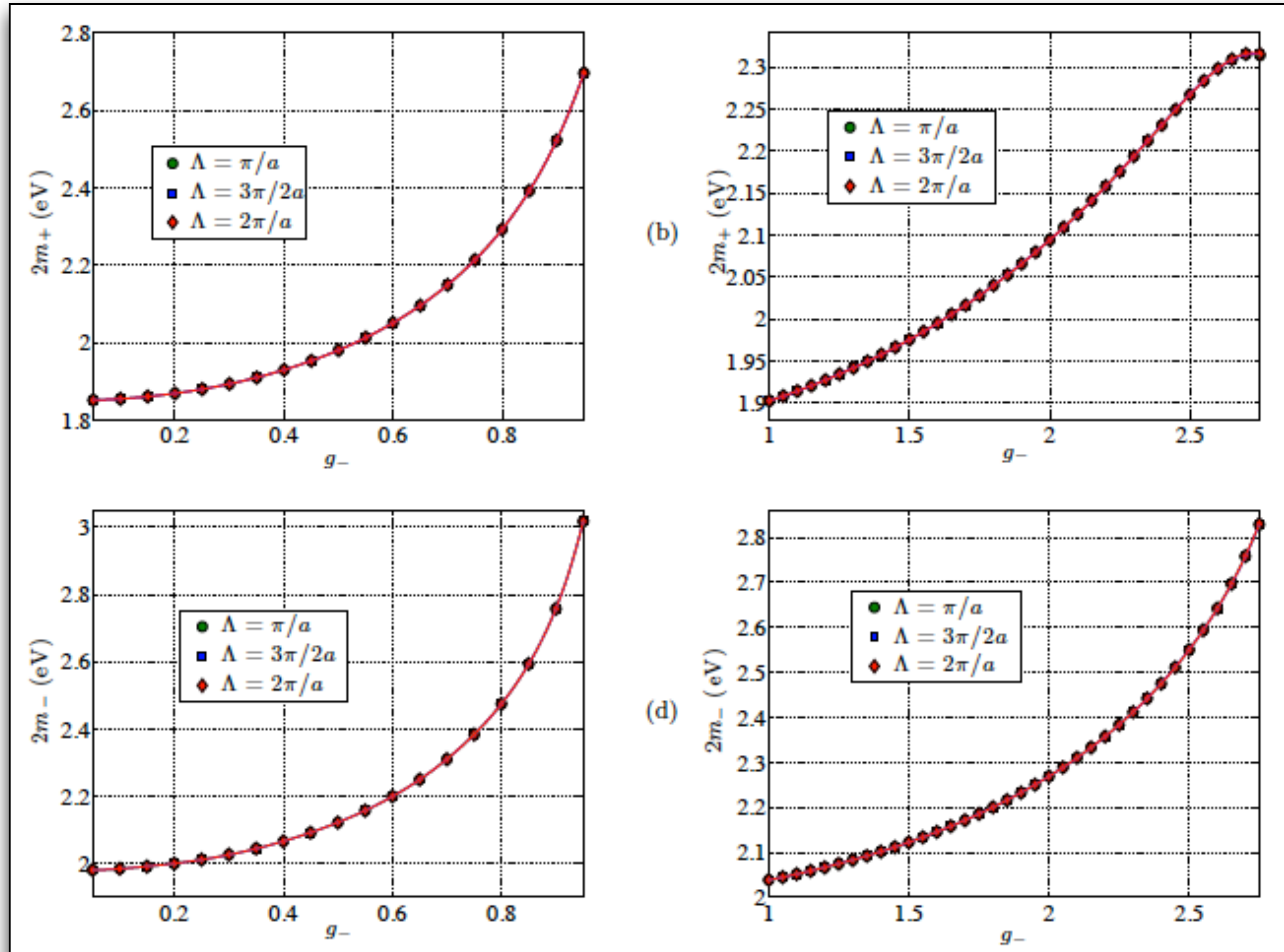
We can go beyond small couplings



at large g's the exciton gs can merge the valence band!

Let’s see the outcome

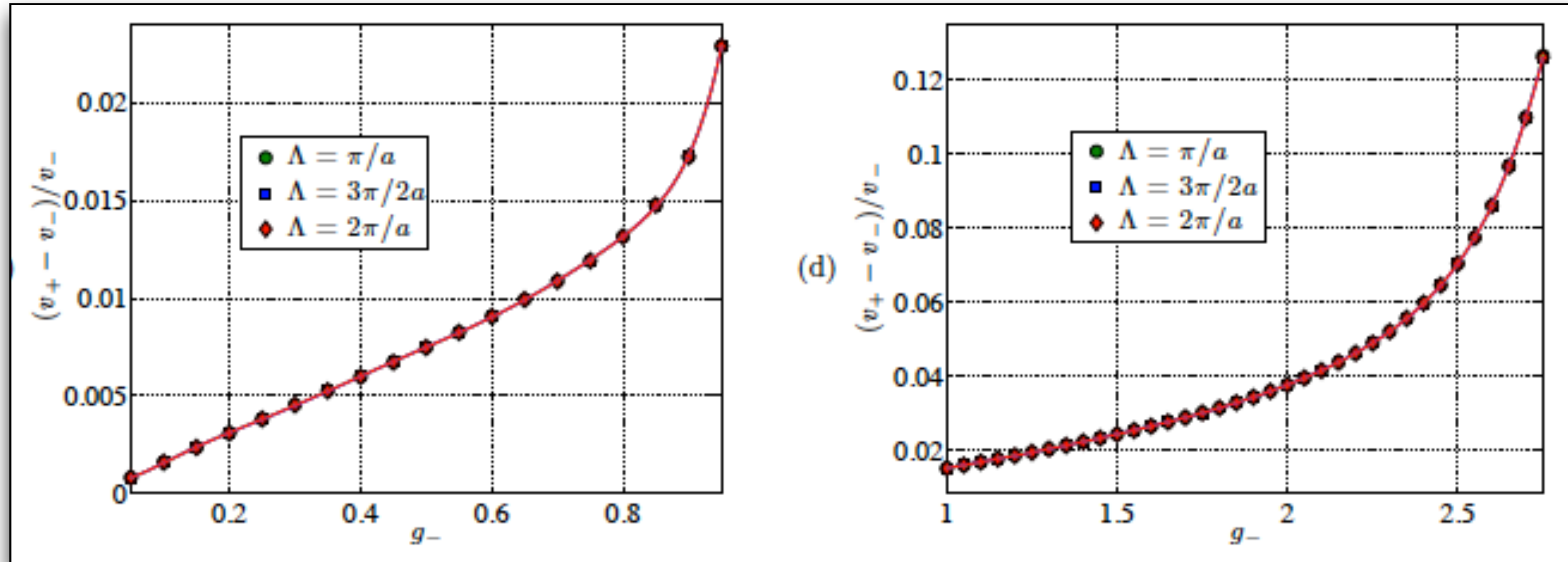
$g_- > 1$



exciton peaks correspond to higer exciton levels (?)

Let's see the outcome

$g_- > 1$



The trends do not match cause the exciton levels are not accurate close to a merging transition!

$$¿ \quad E_s(n,j) = m_s\left(1 + \frac{n + \sqrt{j^2 - g_s^2/4}}{\sqrt{g_s^2/4 + (n + \sqrt{j^2 - g_s^2/4})}}\right) \quad ?$$

A. S. Rodin, A. H. Castro-Neto, PRB, 88, 195437 (2013)

Conclusions:

1. The Coulomb interaction will modify the nominal value of the spin orbit splittings.
2. The conduction band can be significantly larger than the expected from DFT.
3. There is a spin dependent Fermi velocity renormalization can be observed?
4. Vertex corrections? Static approximation?
5. Redo the calculations in the doped regime. Screening effects.
6. Quantum corrections of quadratic terms.

Thank you for listening!