Electronic Structure 2018

Interaction Physics in Semimetals

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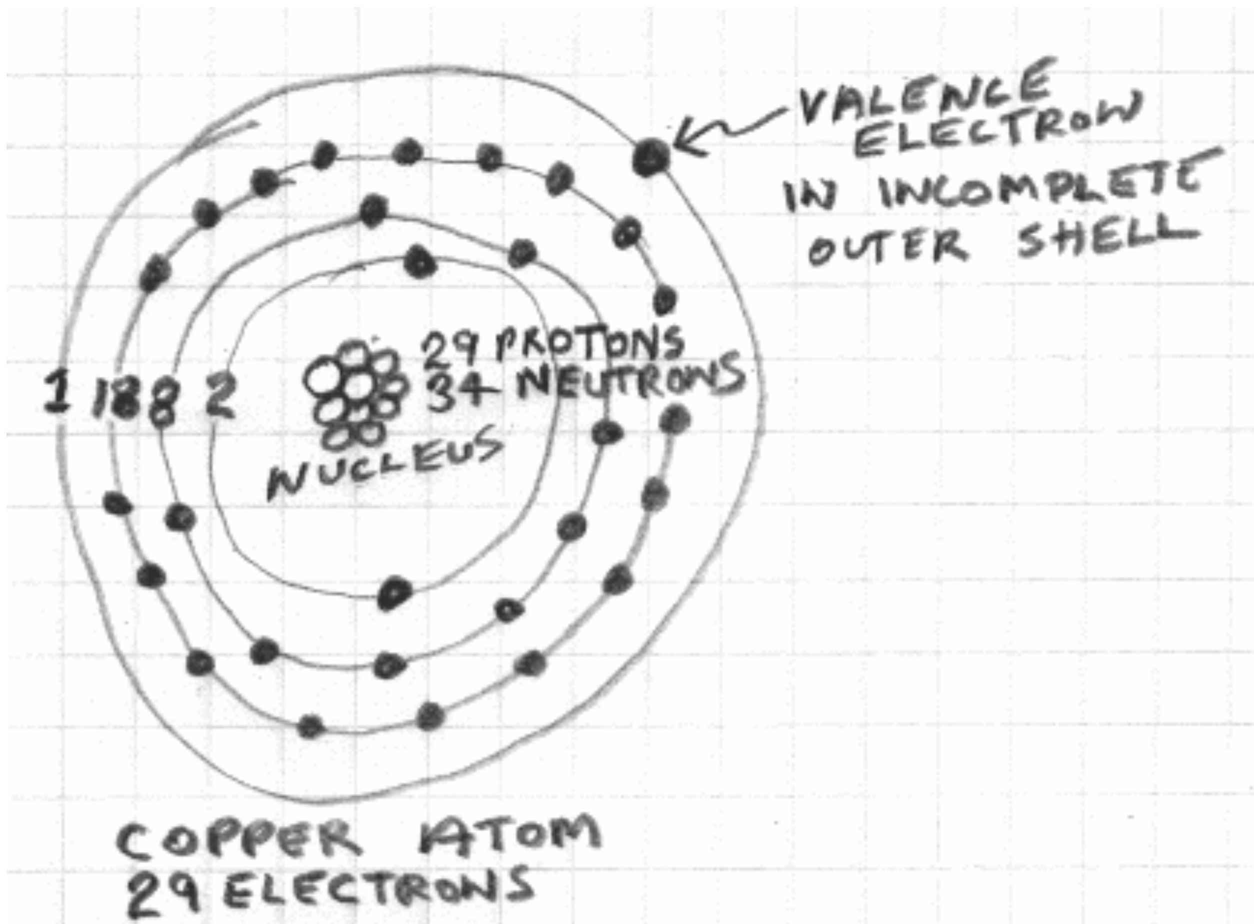
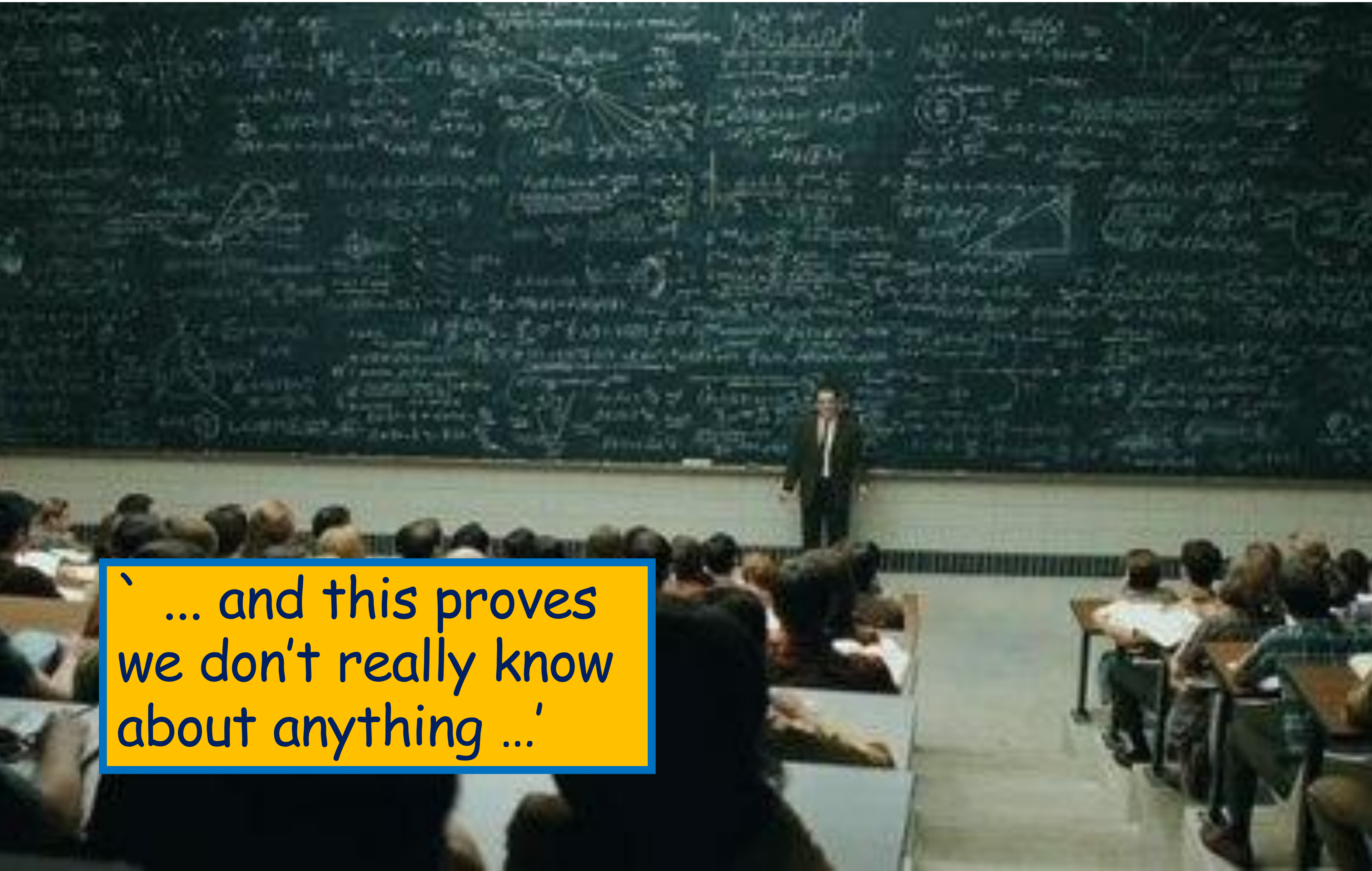
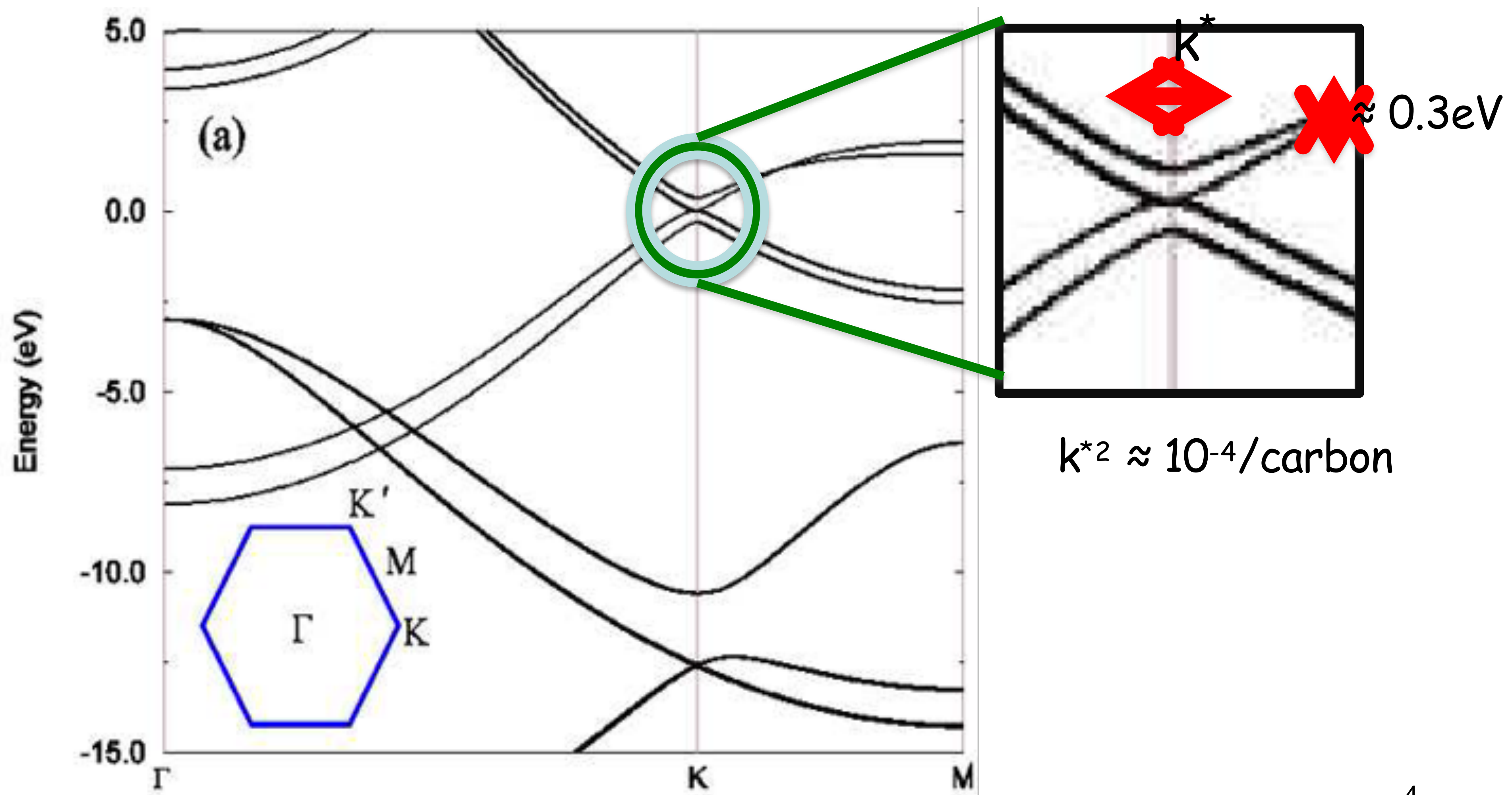
The Standard Model of Chemistry



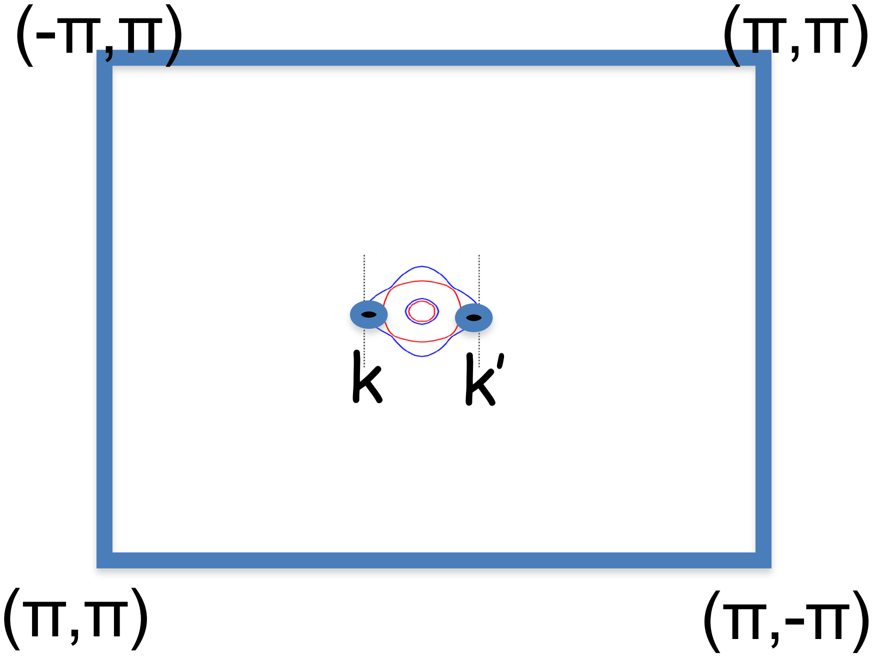
Many-Electron Quantum Mechanics



Electronic Structure of Bilayer Graphene



Coulomb Interactions and Continuum Models



$$\langle k'|V_{ee}|k\rangle \sim \sum_{|R|<k_F^{-1}} \frac{e^2}{R}\, e^{i(k-k')\cdot R}$$

1924-2018

David Pines

Random Phase Approximation

2D Topological Insulators

BHZ Model

Decoupled Time-Reversed Partners

$$\hat{H} = \sum_{\vec{k}} \psi^\dagger_{\vec{k}} \begin{pmatrix} H_{0,\uparrow} & 0 \\ 0 & H_{0,\downarrow} \end{pmatrix} \psi_{\vec{k}}$$

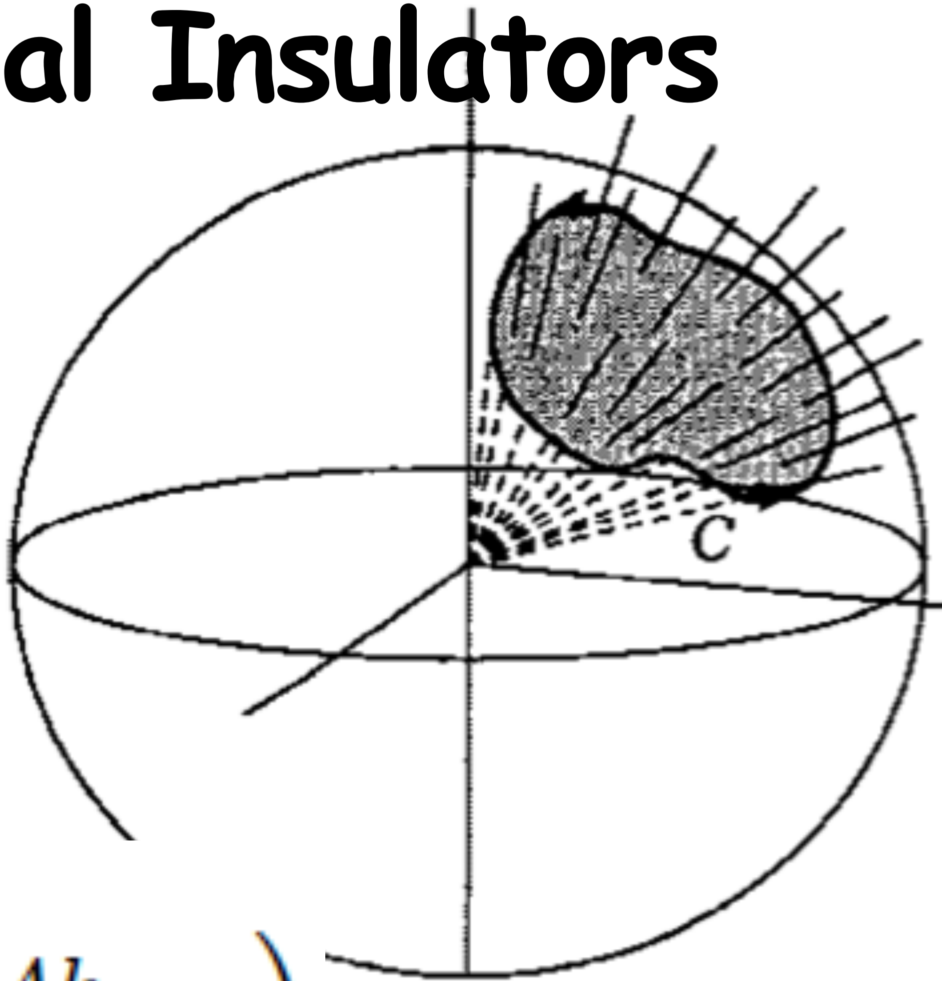
$S_z = 1/2$

$$H_{0,\downarrow} = \begin{pmatrix} \frac{\hbar^2 k^2}{2m_e} + E_c & -Ak_- \\ -Ak_+ & -\frac{\hbar^2 k^2}{2m_h} + E_v \end{pmatrix}$$

$J_z = 3/2$

2D Topological Insulators

BHZ Model



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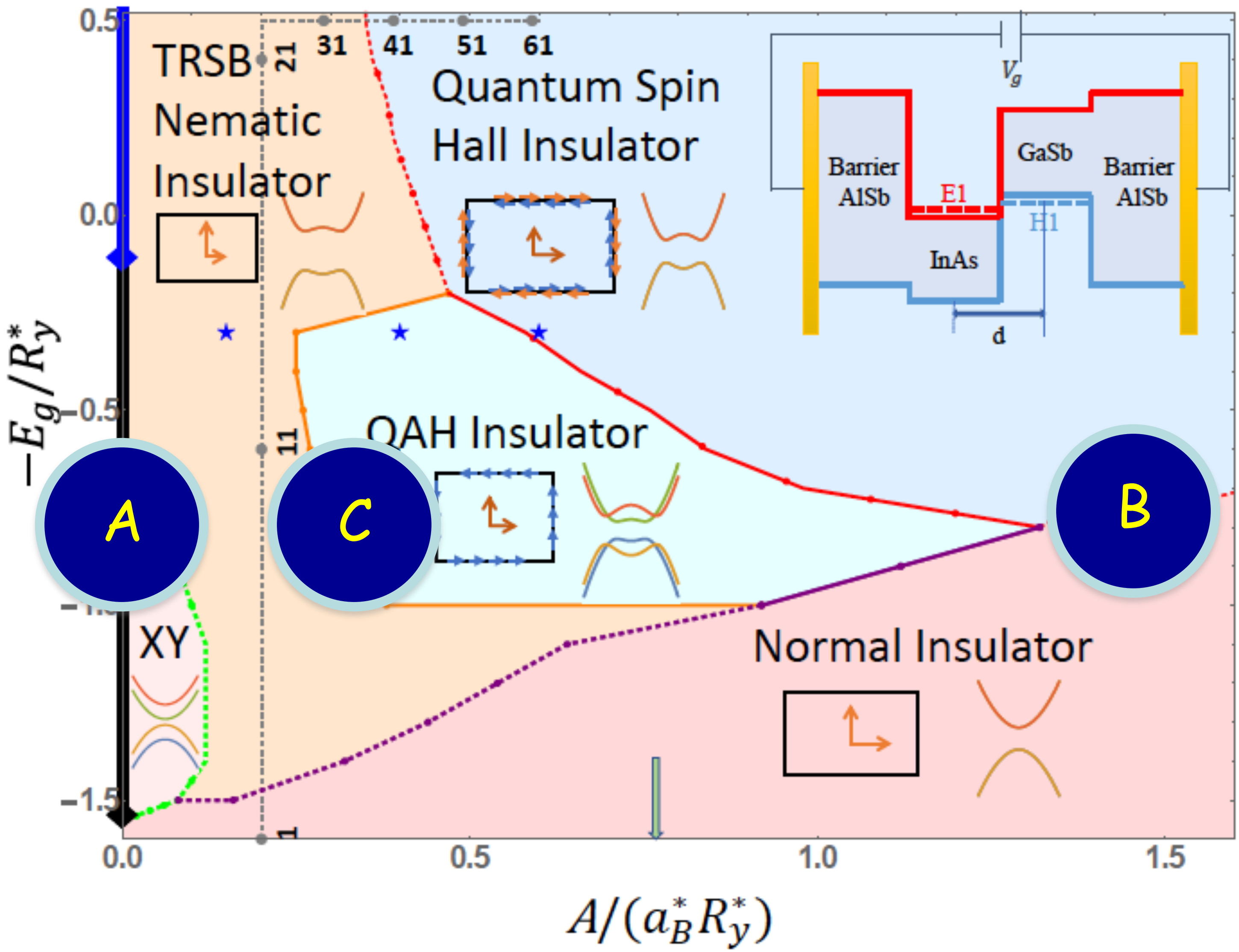
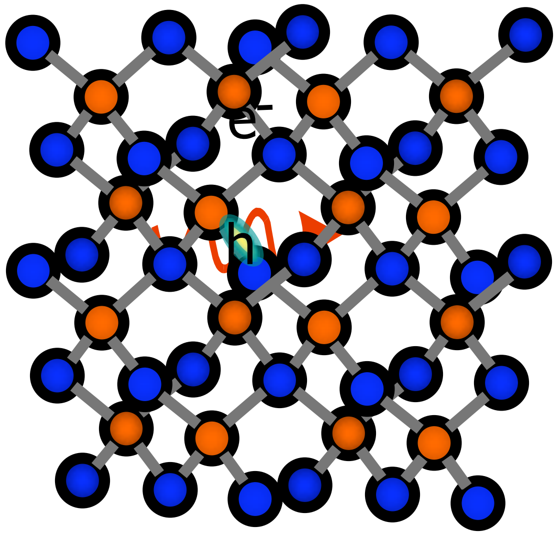
Xue & AHM, arXiv:1710.00410   PRL (2018)

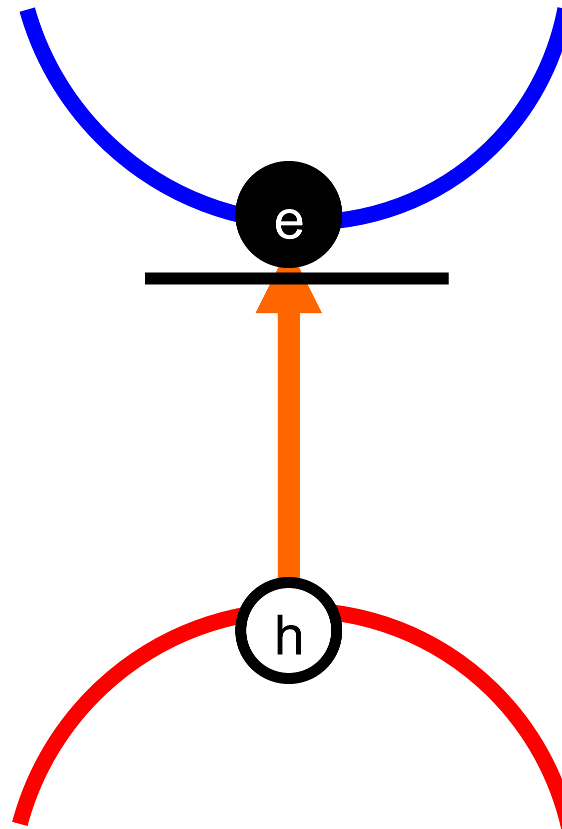


A

Exciton Superfluids

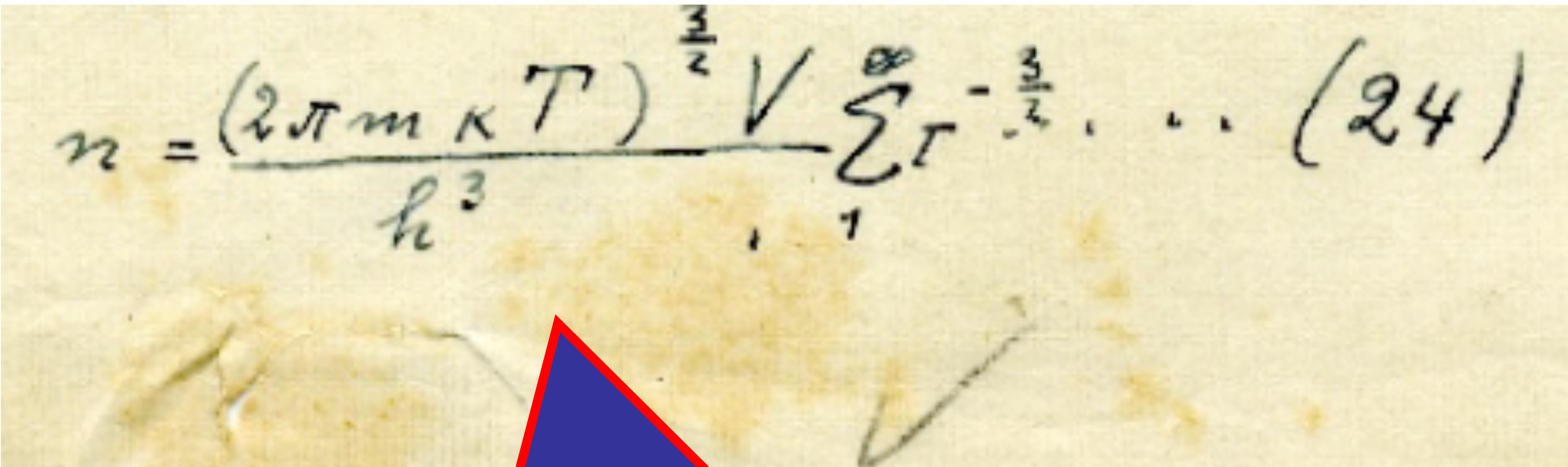
Excitons - Elementary Excitations of Intrinsic Semiconductors





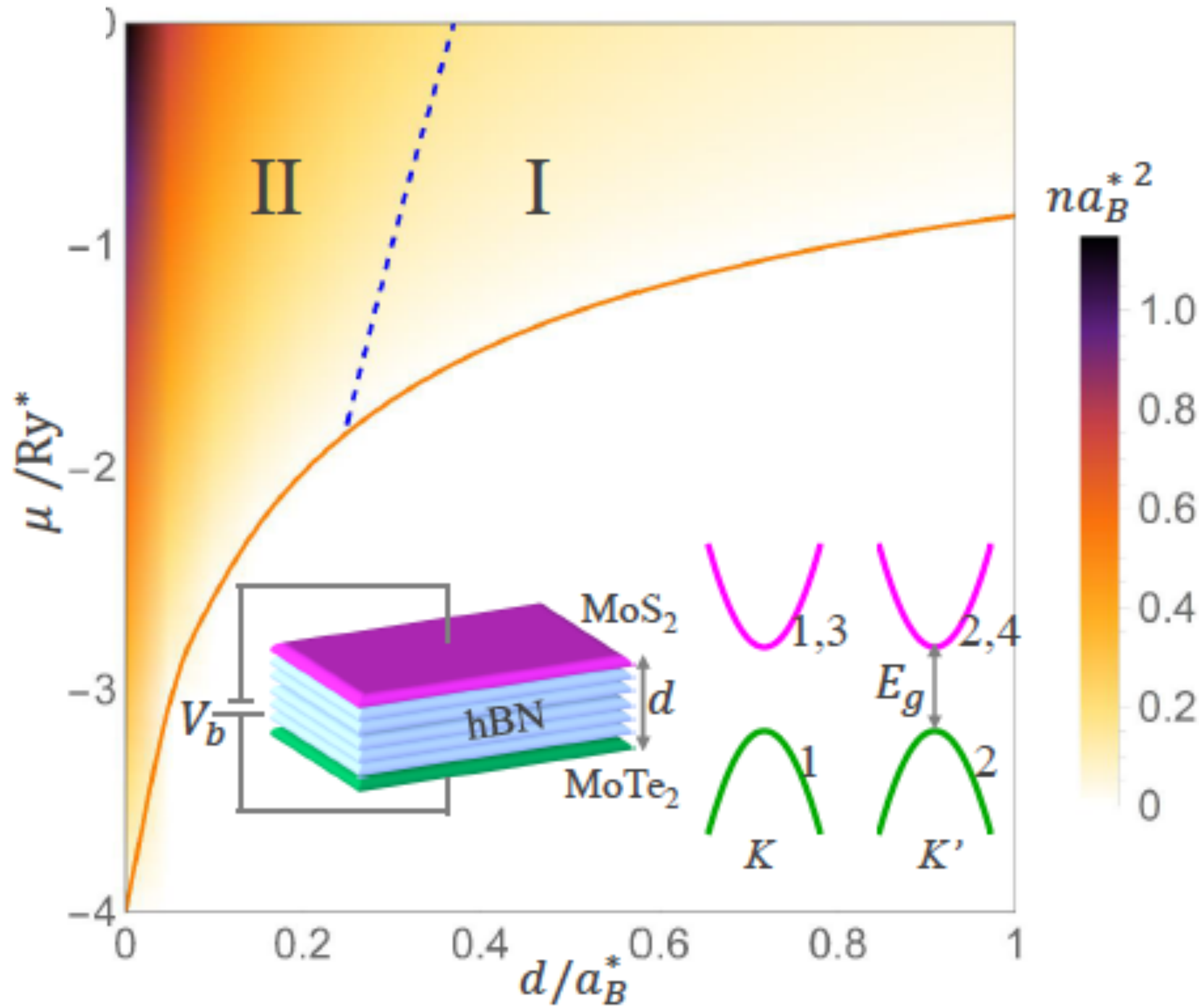
Bose-Einstein Condensation

Einstein 1925


$$n = \frac{(2\pi m \kappa T)^{\frac{3}{2}} V}{h^3} \sum_{1}^{\infty} \tau^{-\frac{3}{2}} \quad \ldots \quad (24)$$

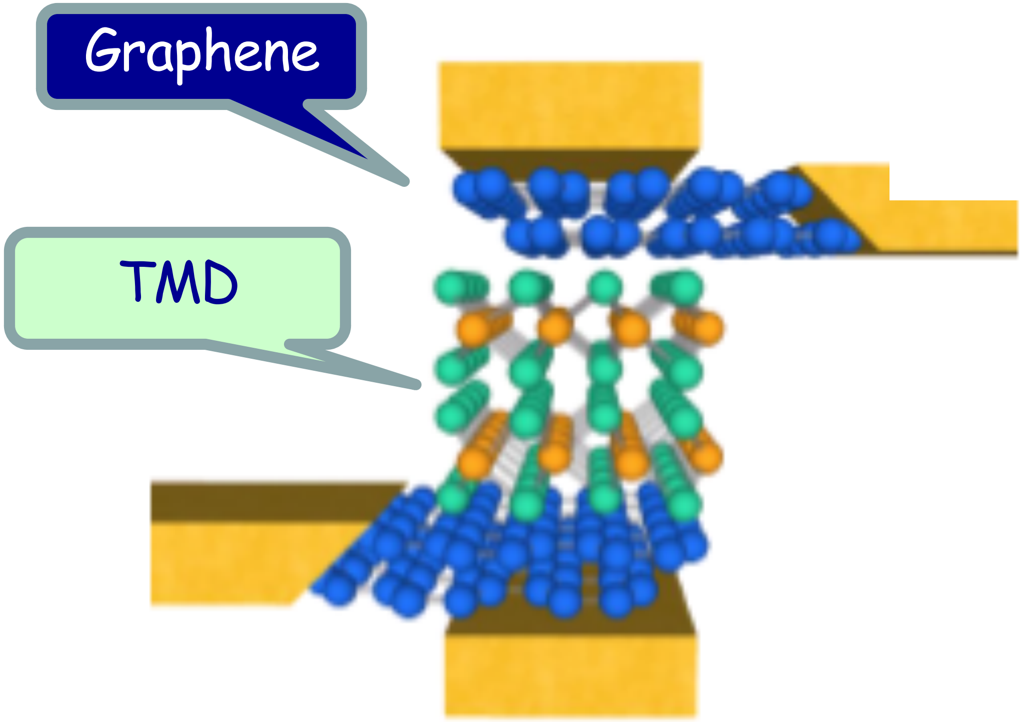
University of Leiden
Einstein Archive

TMD Bilayer XC Phase Diagram



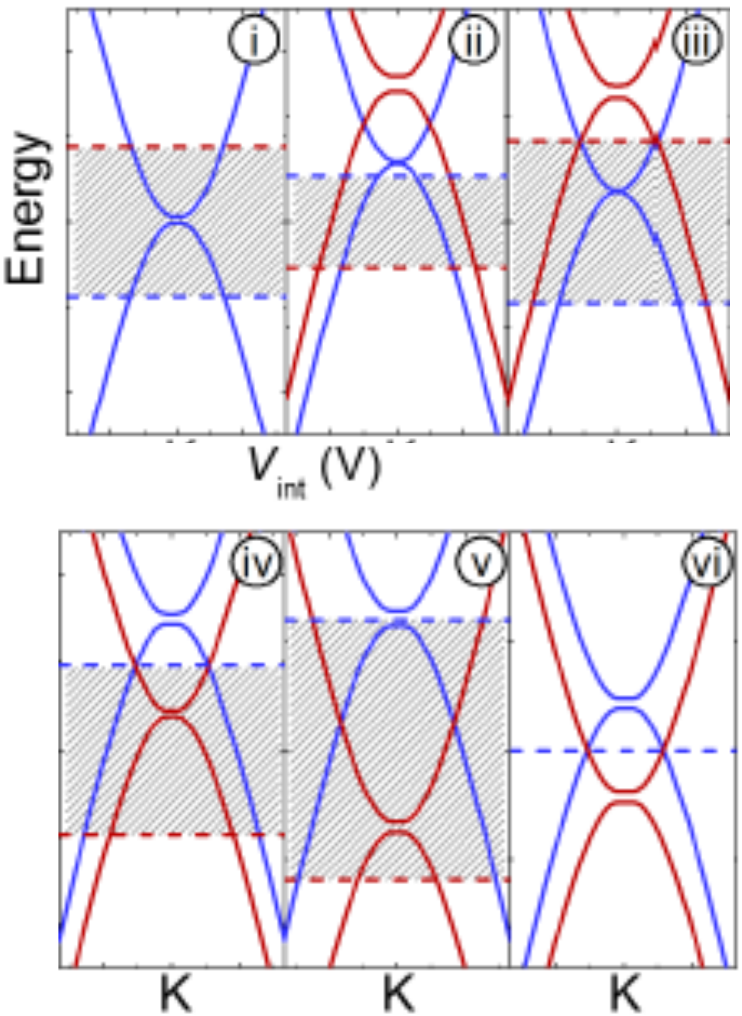
Wu & AHM PRB (2015)

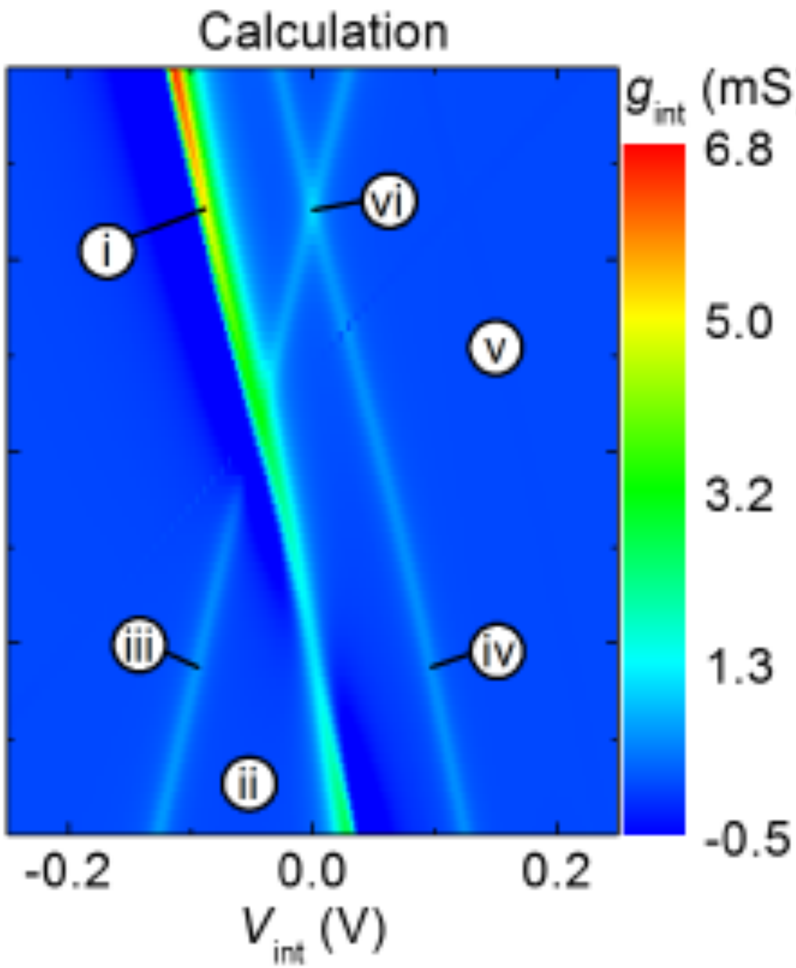
TMD Bilayer XC Phase Diagram



Burg et al. arXiv:1802.07331 – PRL (2018)

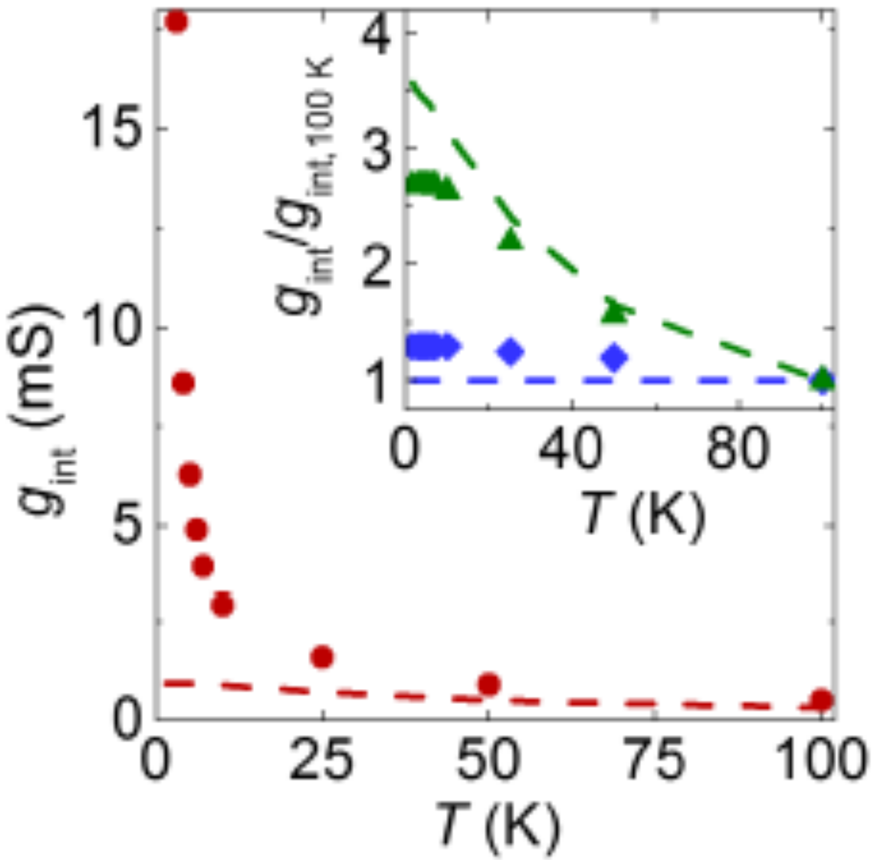
TMD Bilayer XC Phase Diagram

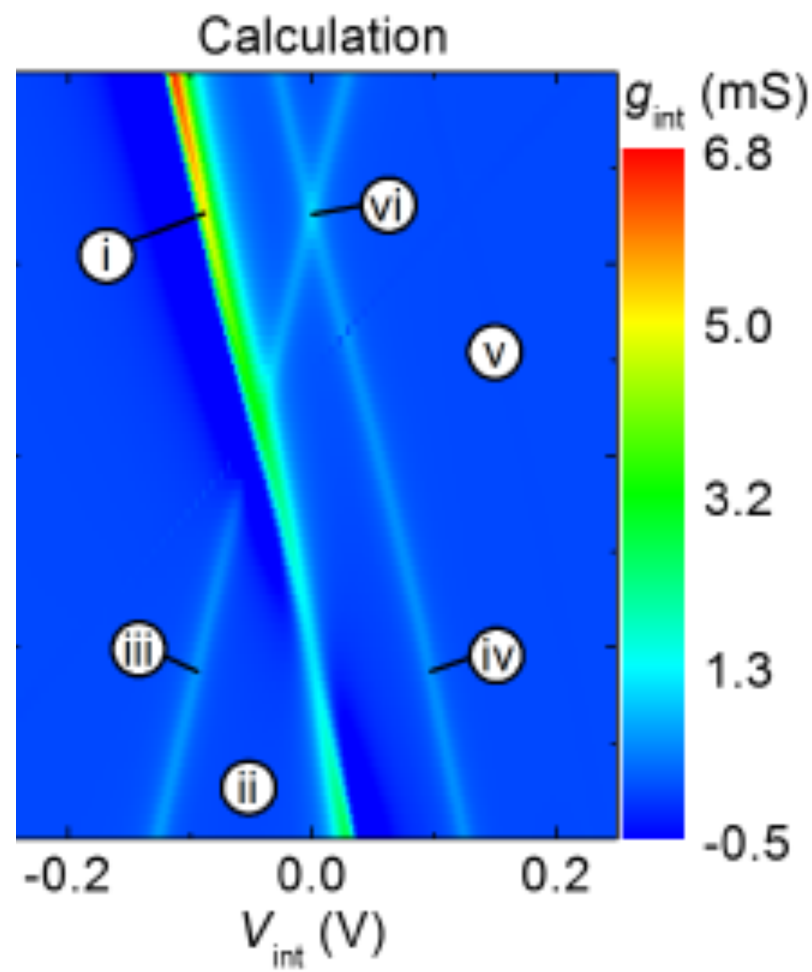




Burg et al. arXiv:1802.07331 – PRL – to appear

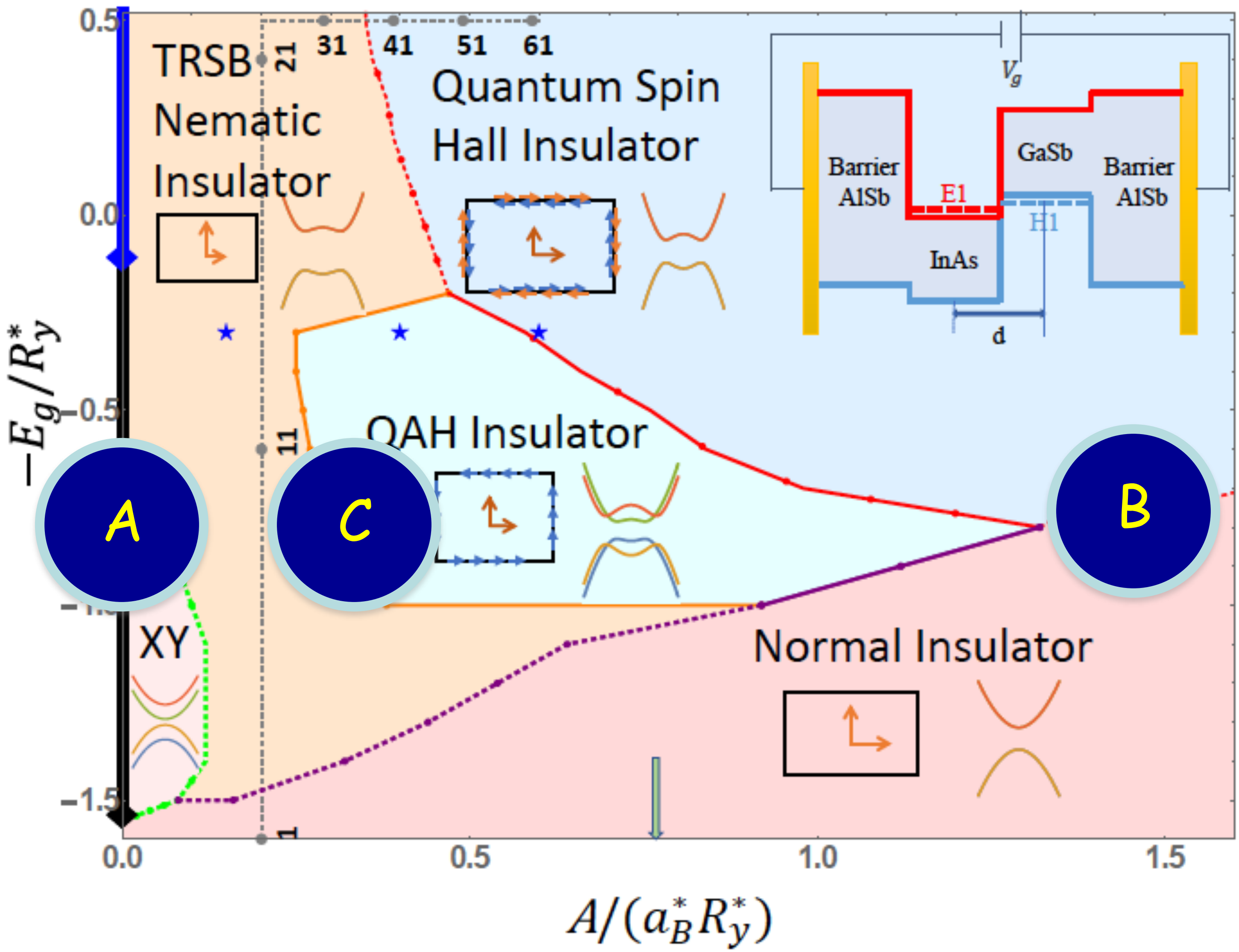
TMD Bilayer XC Phase Diagram

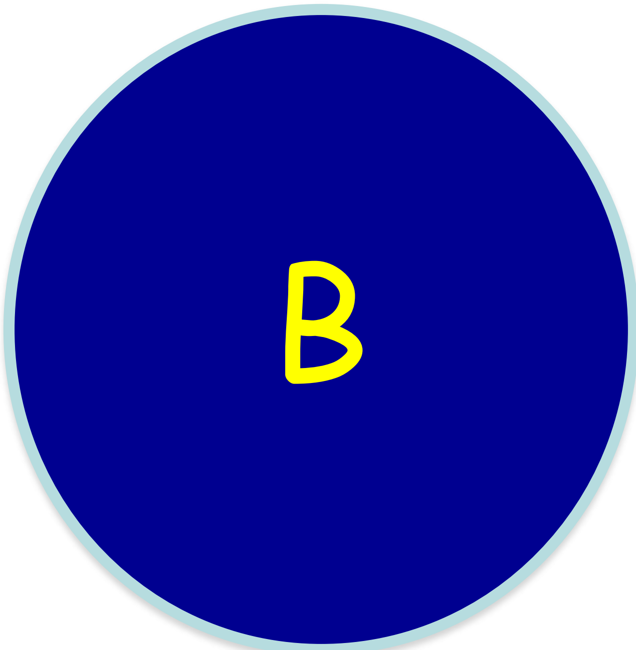




Burg et al. arXiv:1802.07331 – PRL (2018)

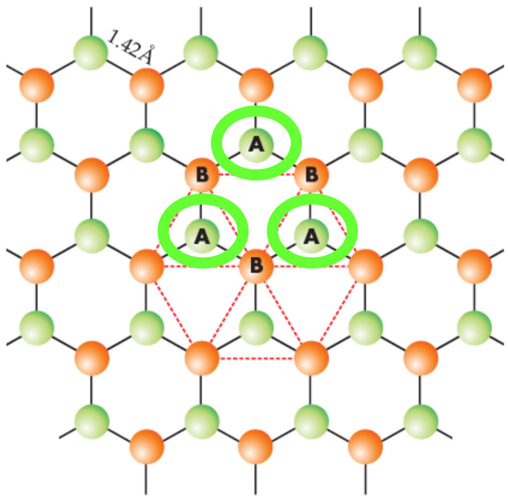
Xue & AHM, arXiv:1710.00410 PRL (2018)

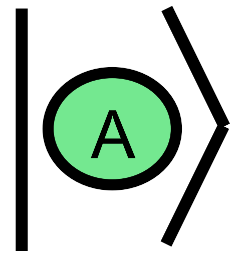


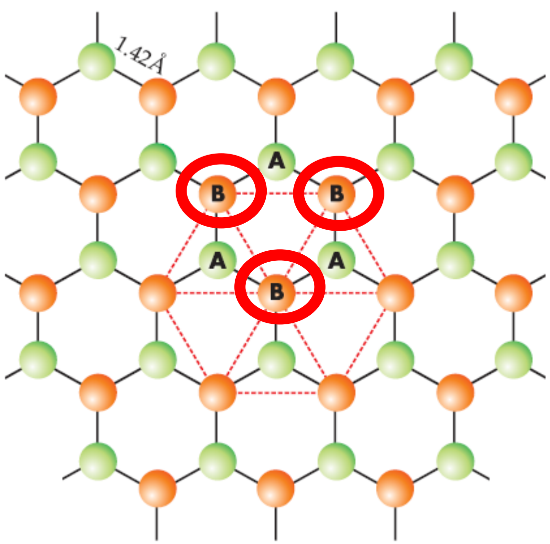


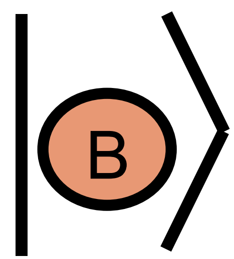
Quantum Anomalous Hall Effect

Sublattice-Pseudospins

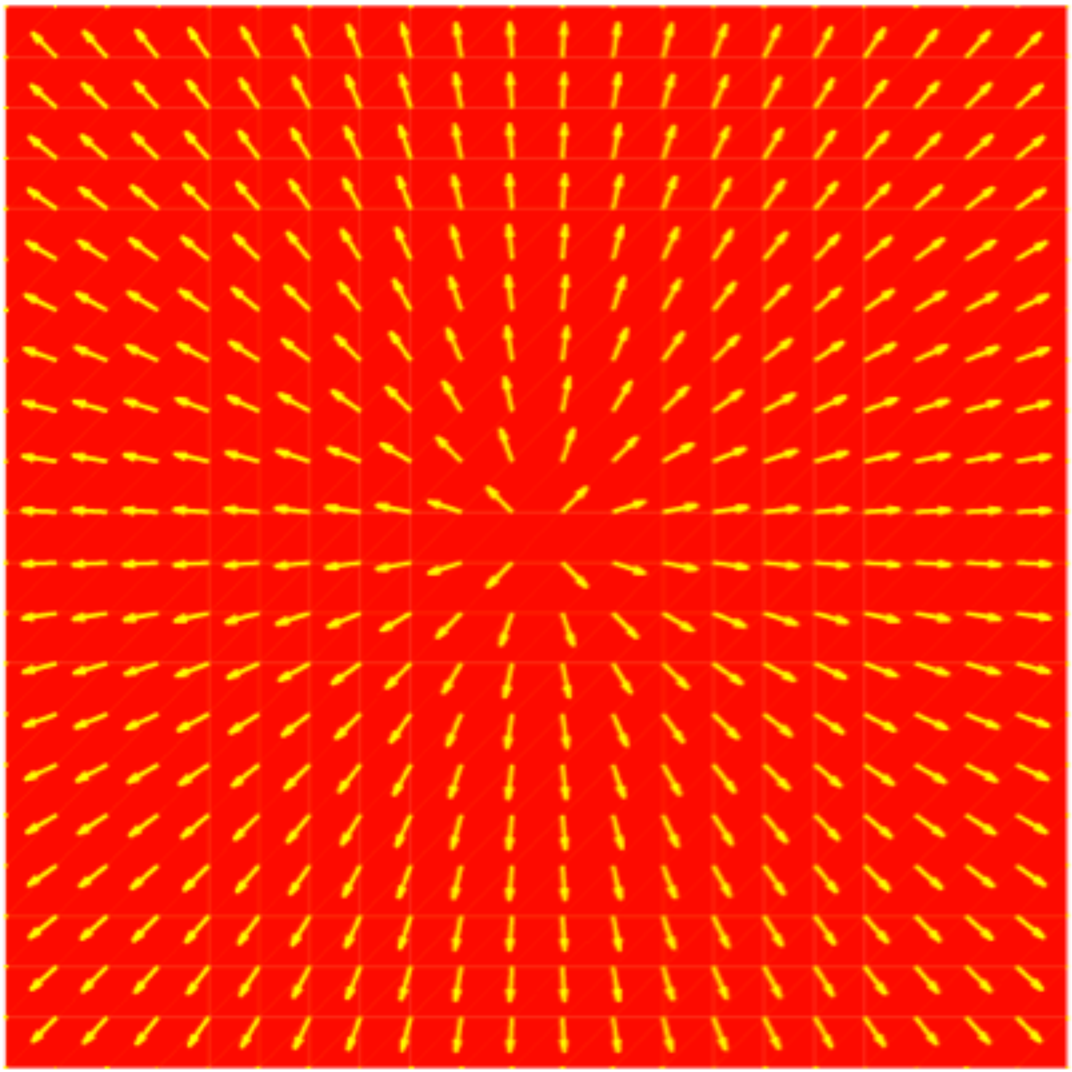




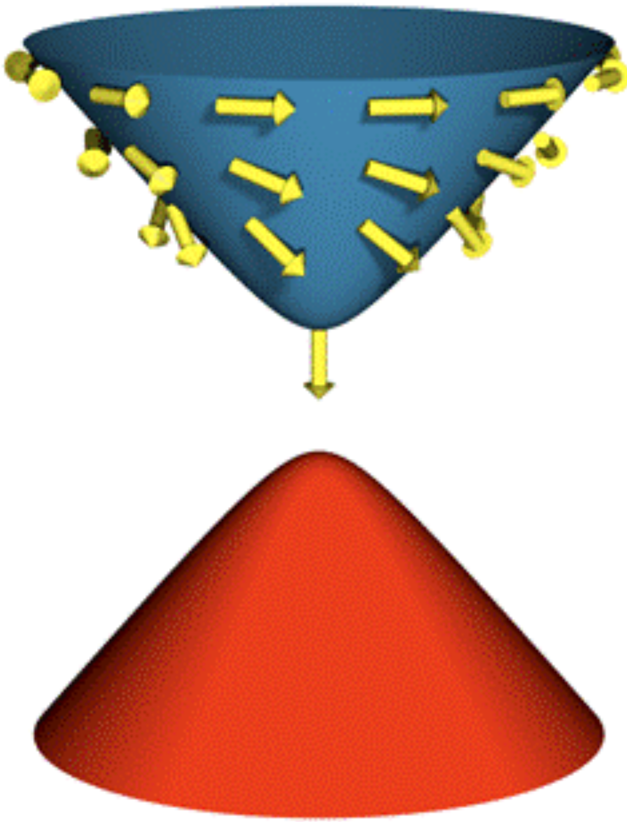




Band Eigenstate Pseudospins



Band Eigenstate Pseudospins



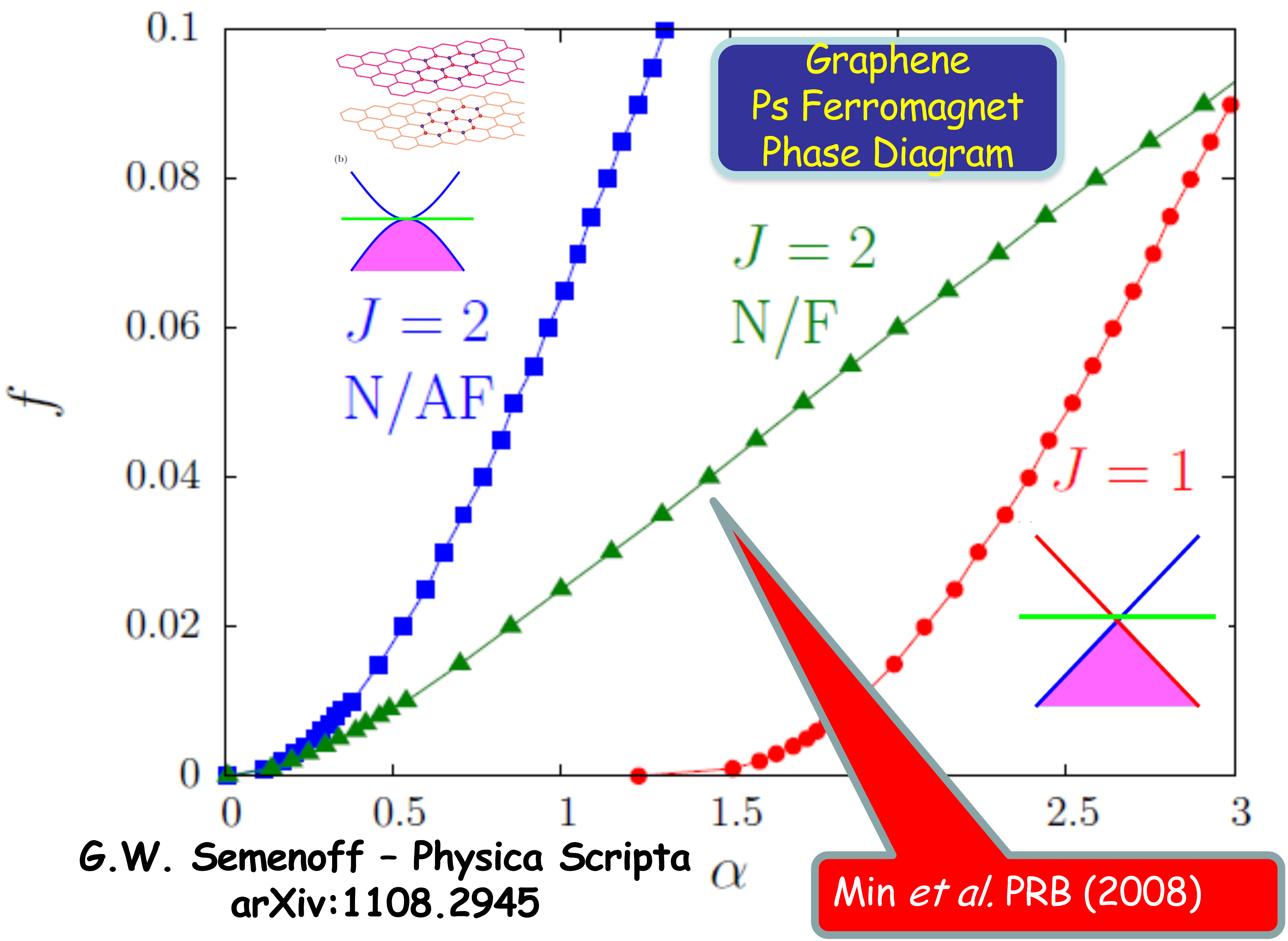
$$\mathcal{H} = \beta mc^2 + \hbar c\vec{\alpha}\cdot\vec{k}$$

Massive Dirac Equation – 3D

Sublattice Staggered Potential

$$\mathcal{H} = \tau_z mv^2 + \hbar v\vec{\tau}\cdot\vec{k}$$

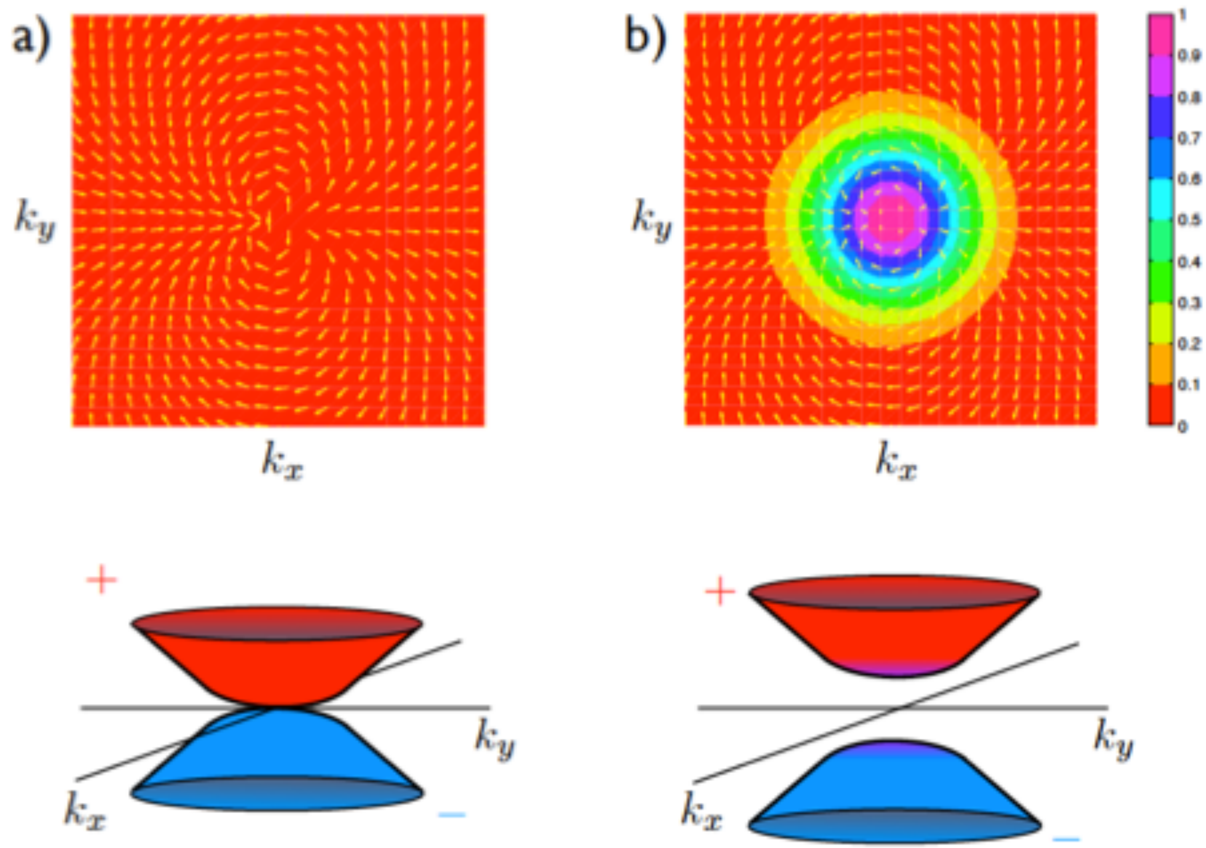
Massive Dirac Equation -2D



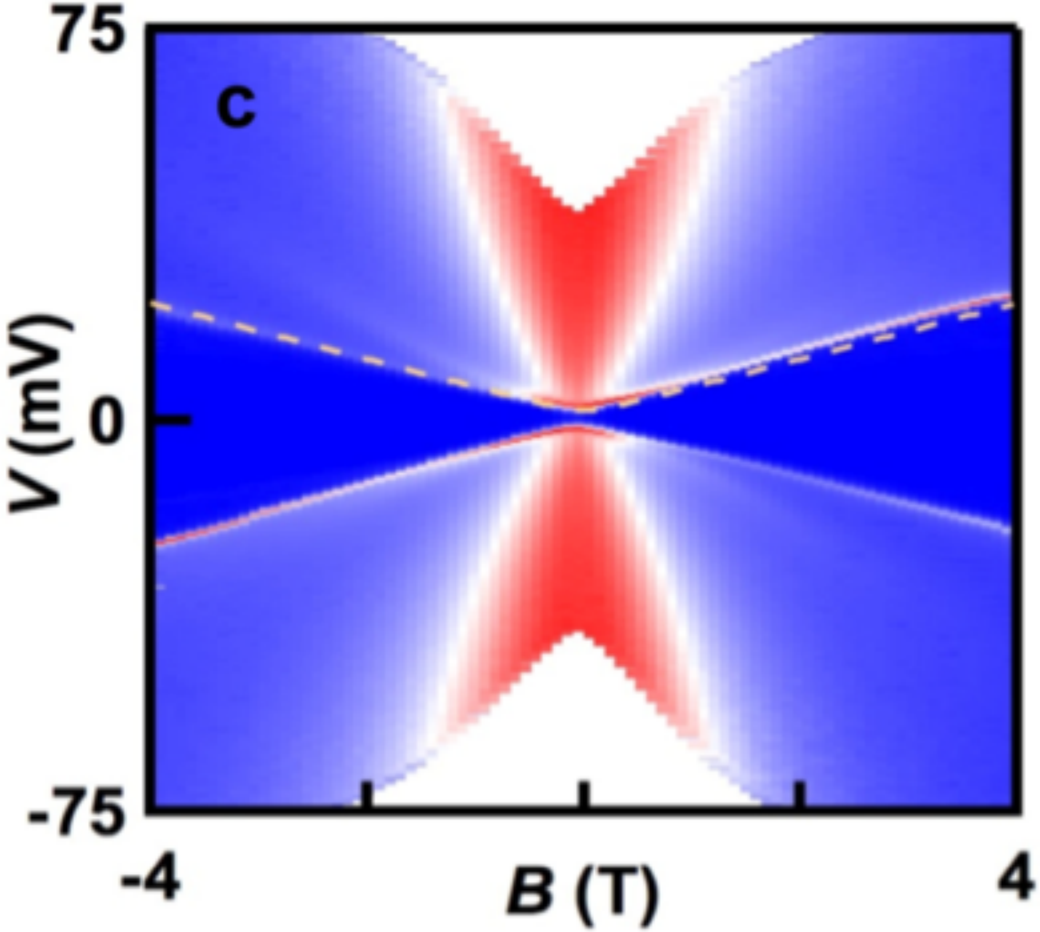
G.W. Semenoff – Physica Scripta
arXiv:1108.2945

Momentum Space Vortex Core

- $\delta n \approx 10^{-5}/C$
- $\Delta \approx 10^{-2}$ eV

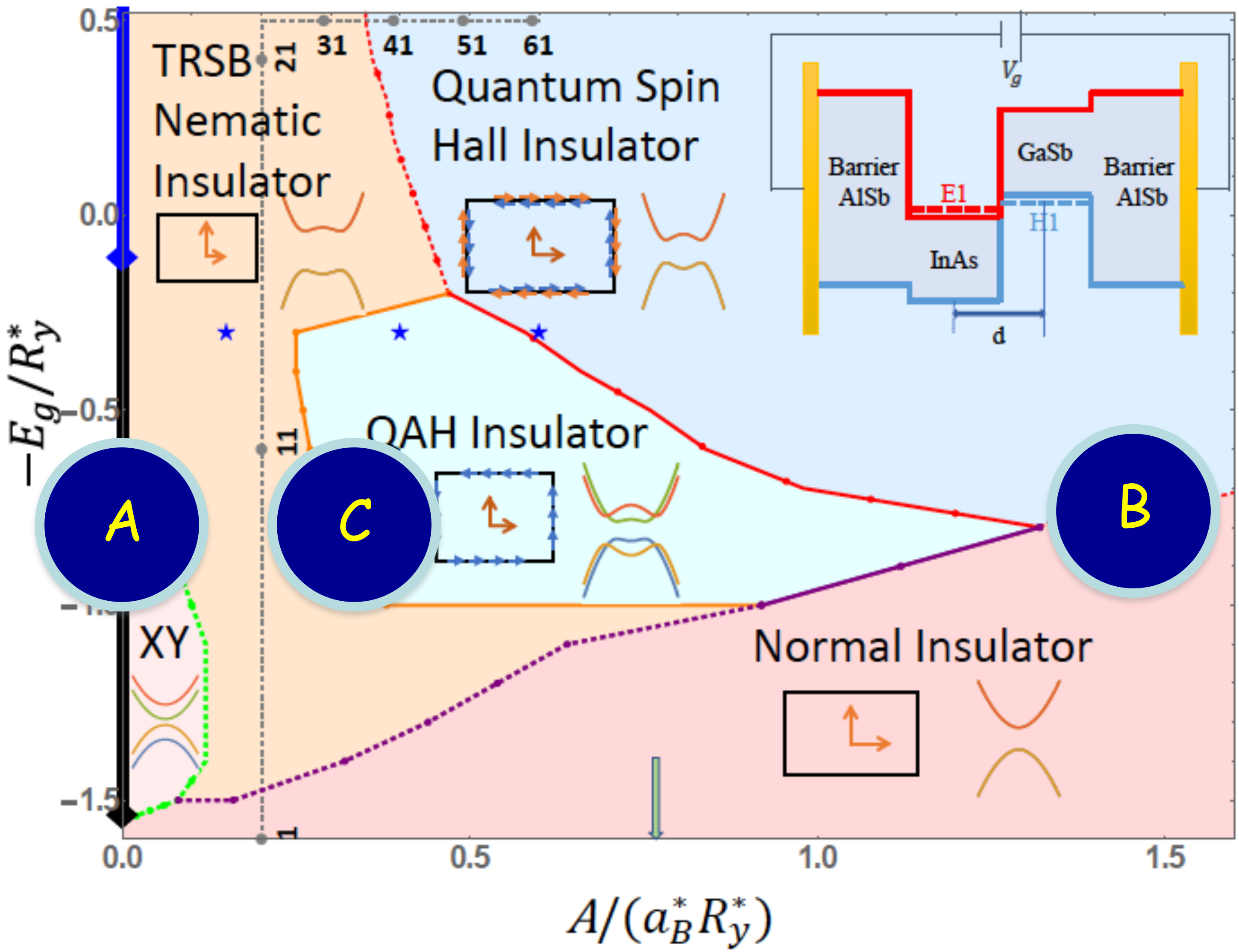


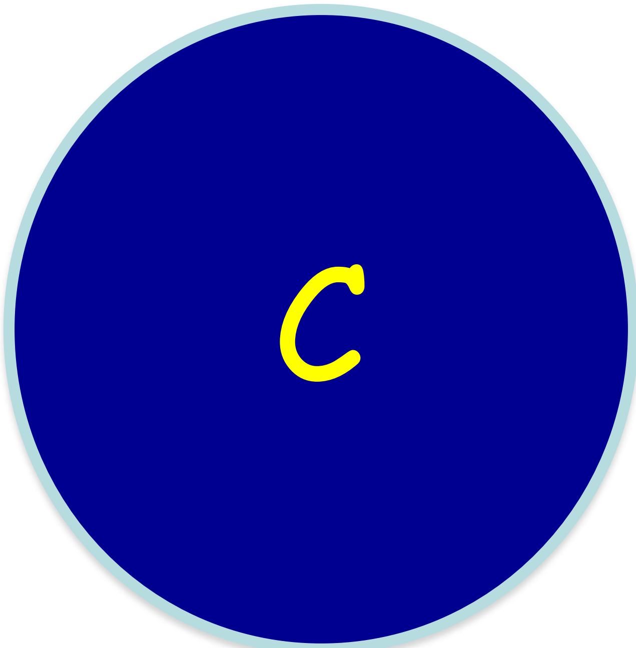
Gapped States in Bilayer Graphene



Bao, Velasco Nature Phys. (2011), arXiv:1108

Xue & AHM, arXiv:1710.00410 PRL (2018)





Nematic and Chern Insulators

Excitonic Insulator to BHZ model

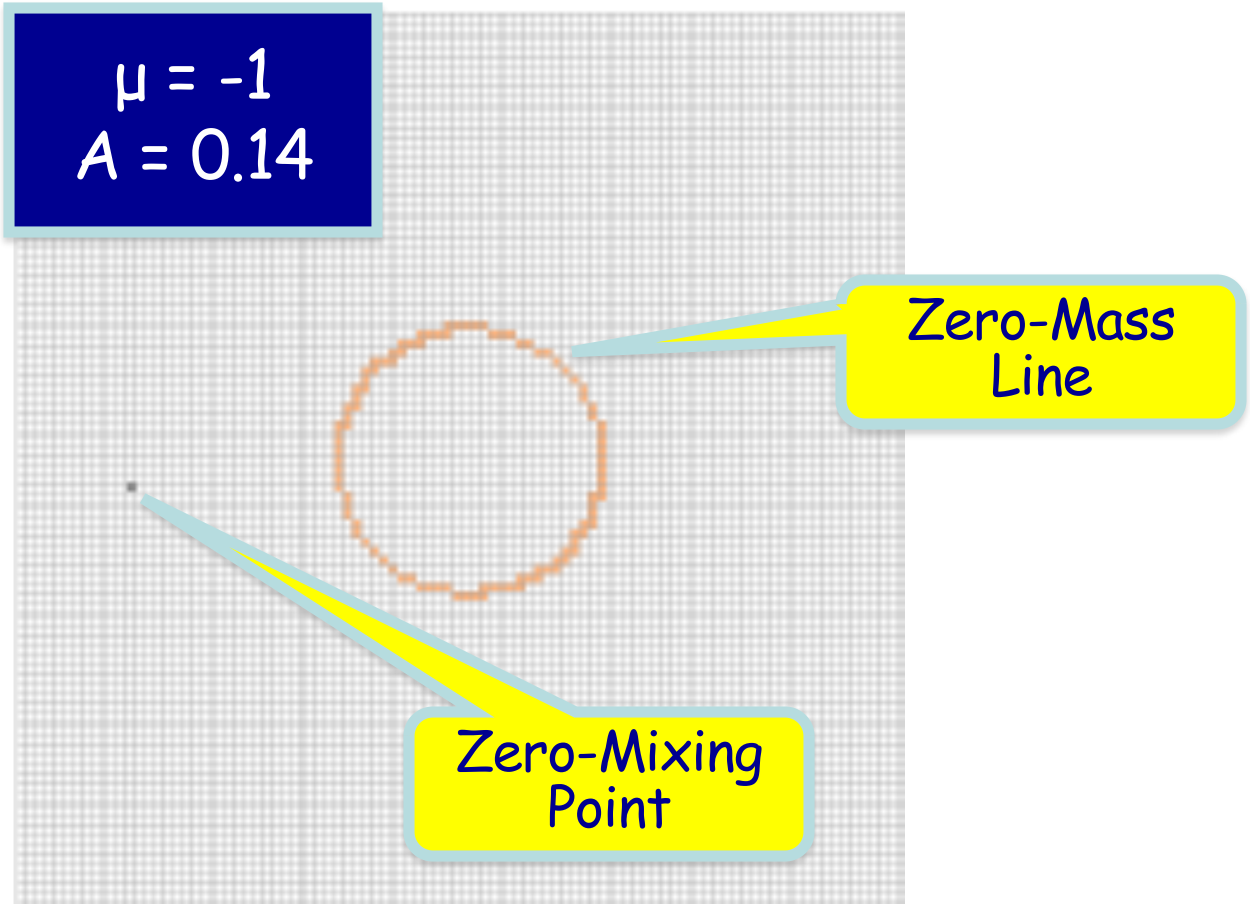
k-dependent
gap

$$\mathcal{H}_{\rm BHZ} = (\frac{\hbar^2 k^2}{2m} + \frac{E_{gap}}{2})\tau_z + A(k_x \tau_x \sigma_z - k_y \tau_y)$$

k-dependent
Band-Pseudospin
Effective Magnetic
Field

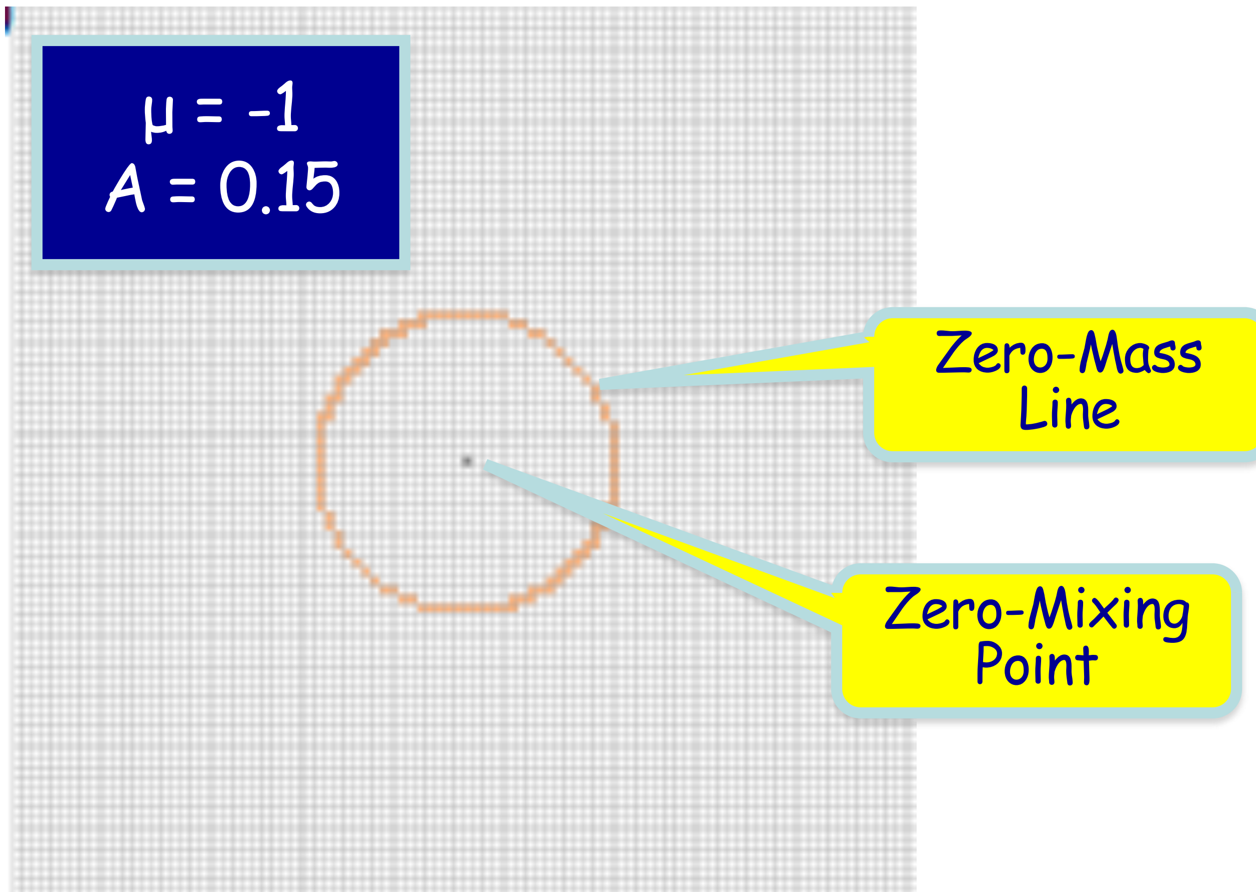
Mean-Field Theory - QSHI/NI

Nematic Insulator



Mean-Field Theory - QSHI/NI

QSH Insulator



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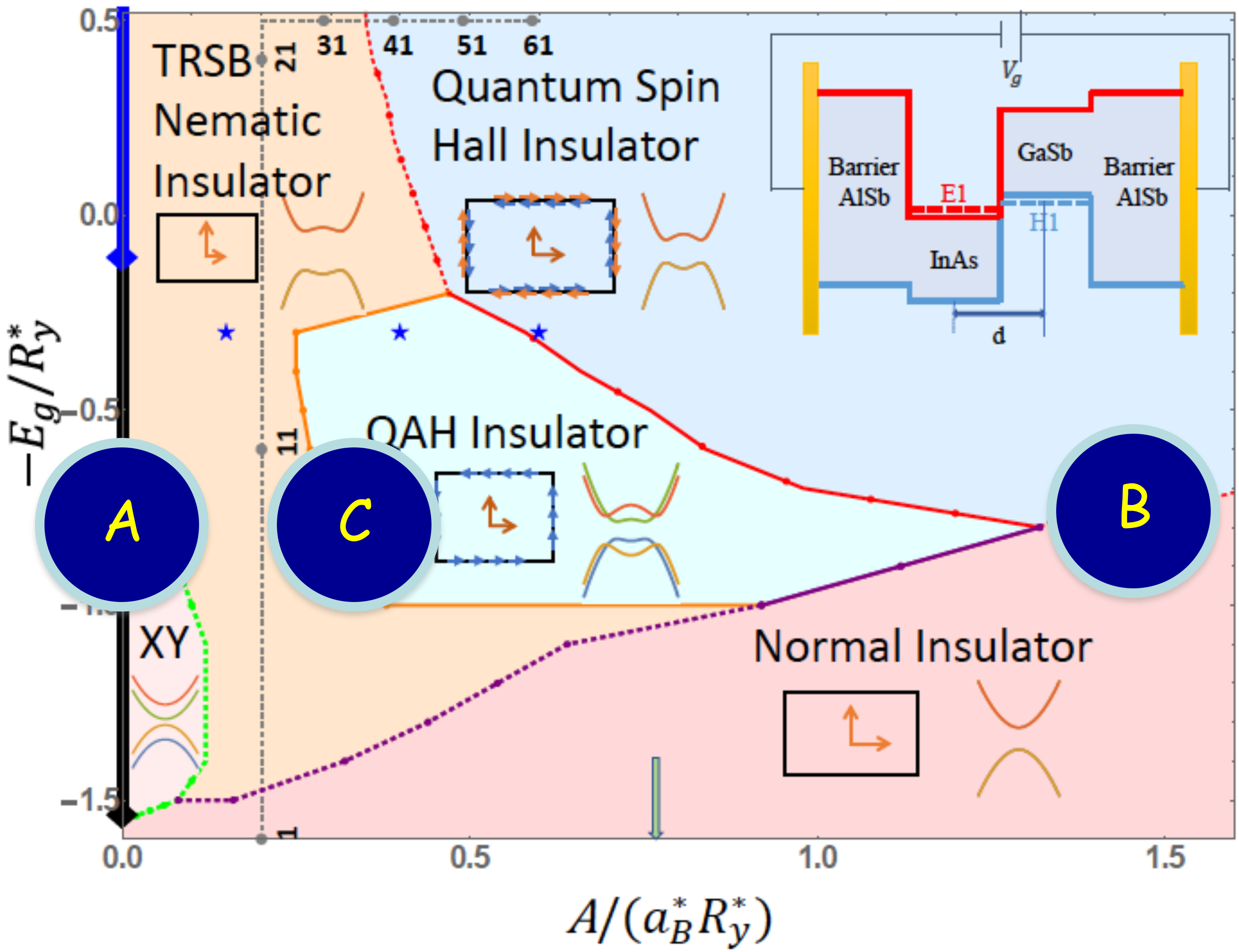
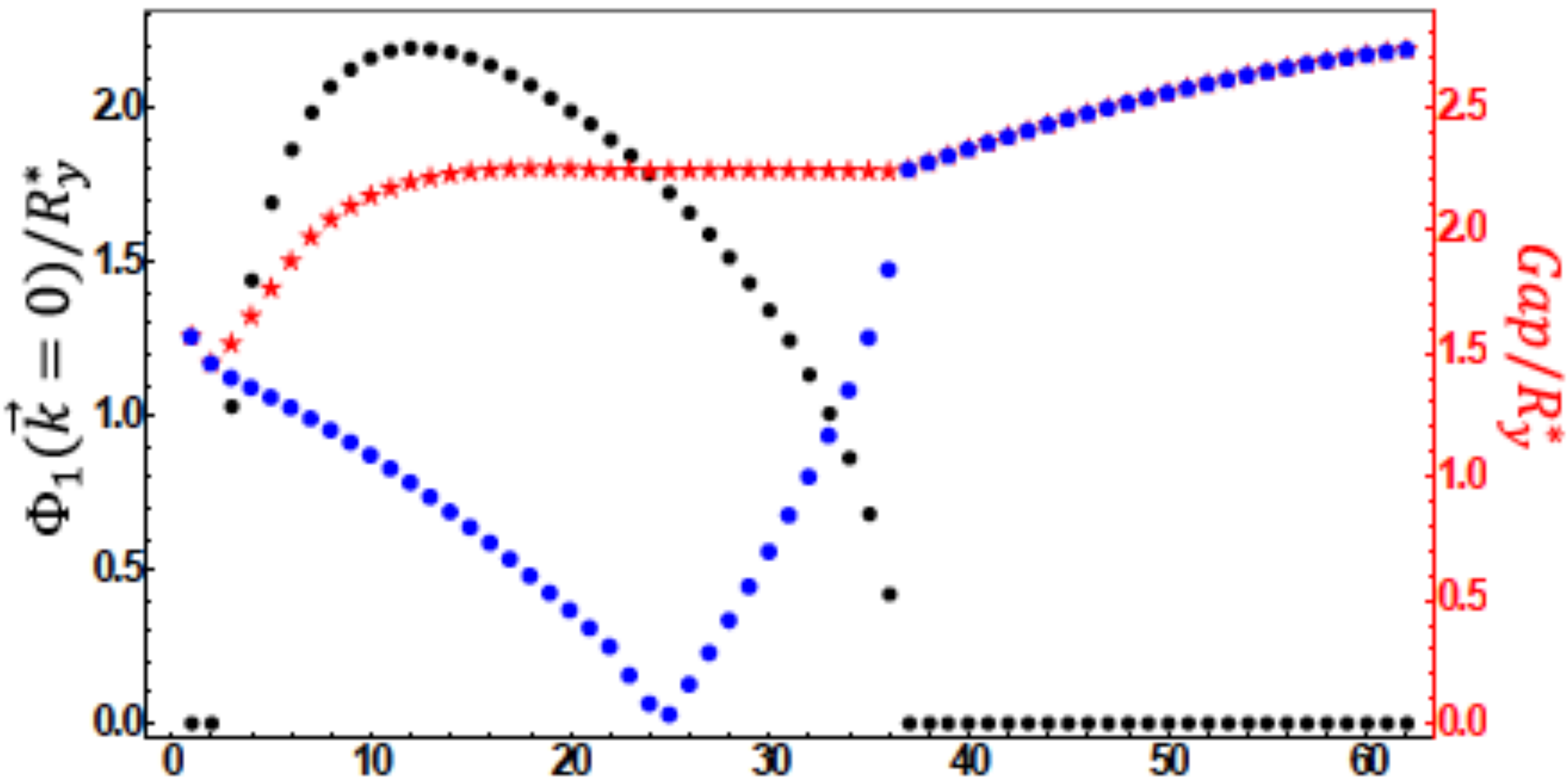
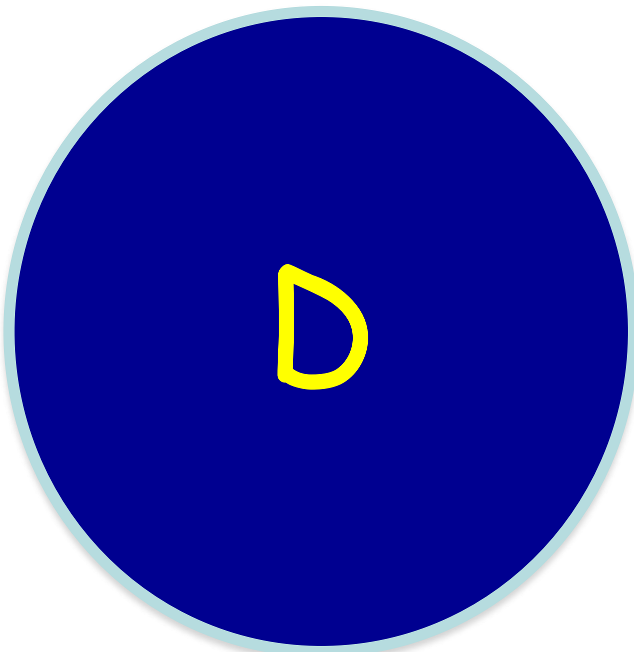


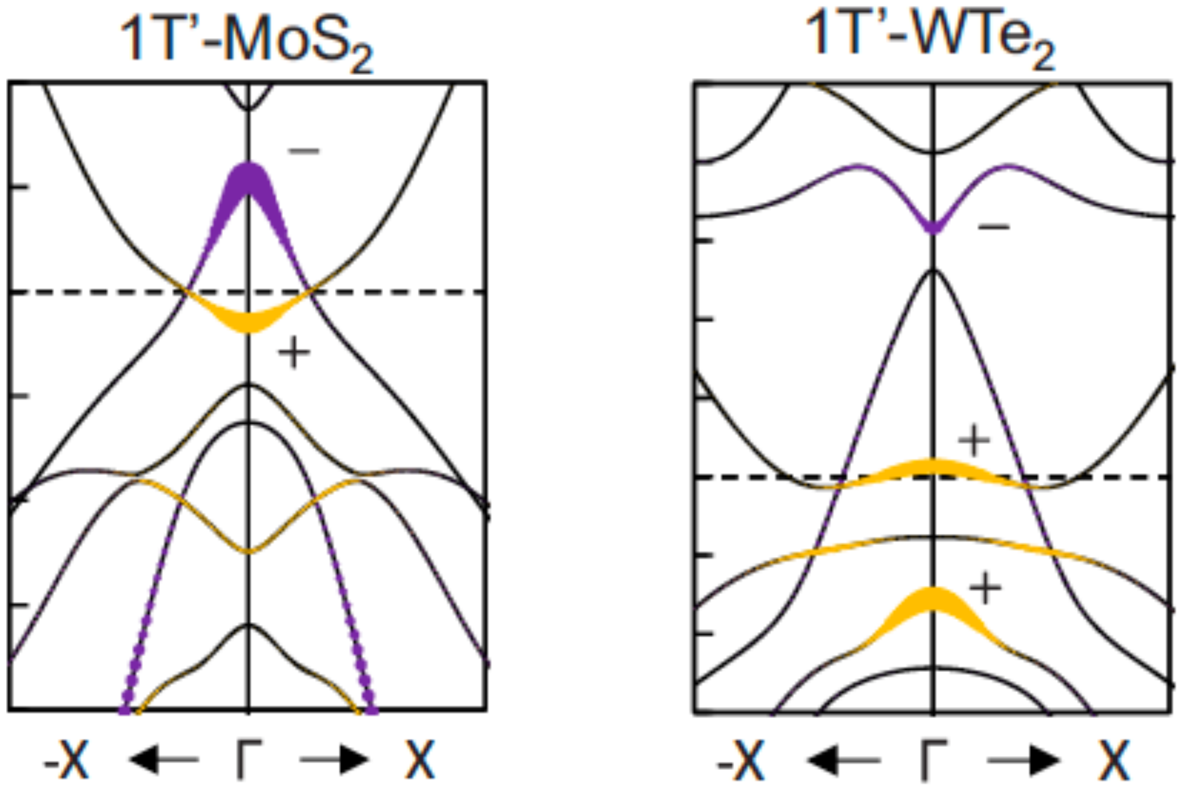
Mind the Gap





Less Simple Systems

The 1T' TMDs



Qian et al. Science (2014)
Choe et al. PRB, 93, 125109 (2016)
Meuchler et al. PRX, 6, 041069 (2016)

- ✓ The Coulomb interaction's long range must be retained in the theory of interaction effects in semiconductors and semi-metals and are often accurately described by GW approximations

- ✓ Broken Symmetries are Common in weakly correlated semiconductors and semimetals – especially in candidate topological materials

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