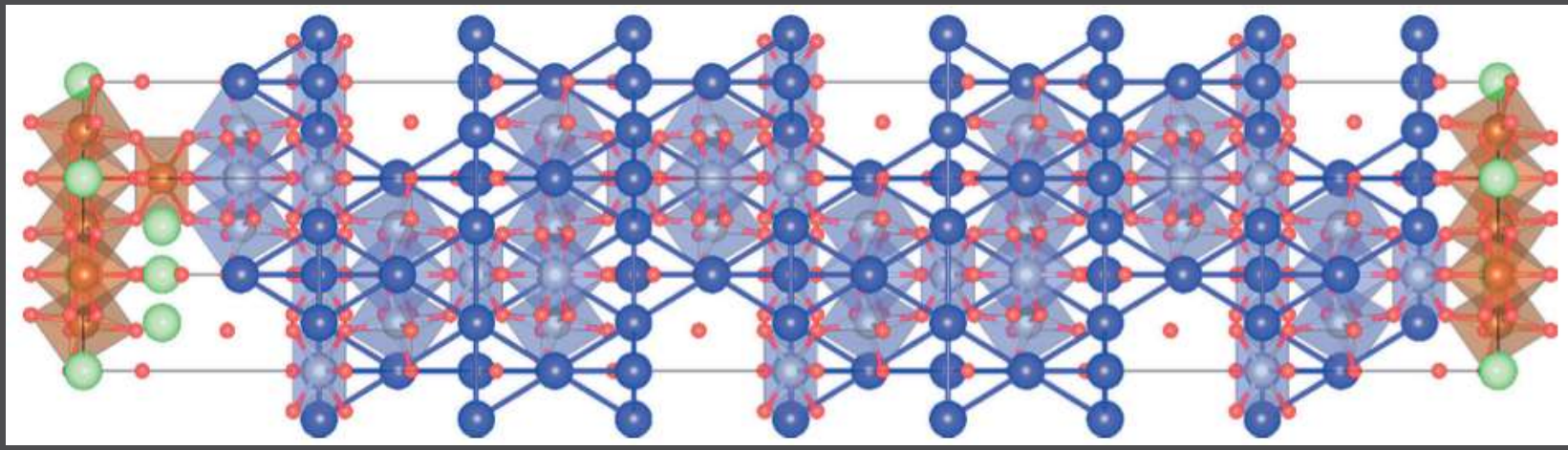
Interface Engineering?

Epitaxial Heterostructure

$$Pr_2Zr_2O_7/Y_2Sn_{2-x}Sb_xO_7 \quad (111)$$

Non-magnetic

s-electrons:
large overlap,
isotropic FS.

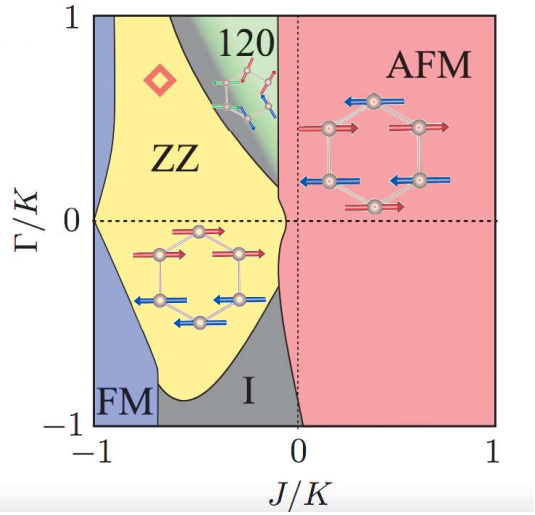


Other Quantum Paramagnets?

α-$RuCl_3$

- Layered spin-orbit assisted Mott insulator close to exotic quantum spin liquid ground state. Y.-J. Kim, K. S. Burch et al (2015)
- Candidate for honeycomb Kitaev model.

Alexei Kitaev (2006)



Kee et al (2015)

$$H = \sum_{\langle ij \rangle \in \alpha\beta(\gamma)} \left[K S_i^\gamma S_j^\gamma + J \mathbf{S}_i \cdot \mathbf{S}_j + \Gamma (S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) \right]$$

α-$RuCl_3$

- Layered spin-orbit assisted Mott insulator close to exotic quantum spin liquid ground state. Y.-J. Kim, K. S. Burch et al (2015)
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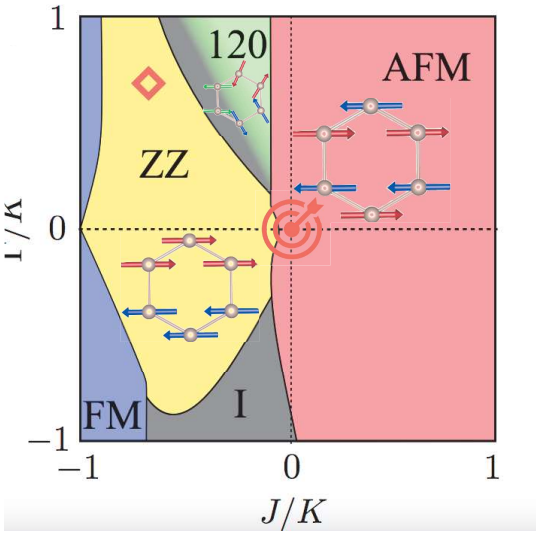


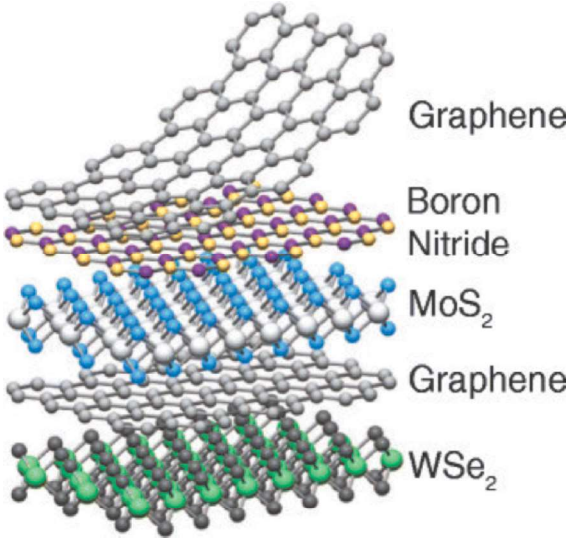
Kee et al (2015)

$$H = \sum_{\langle ij \rangle \in \alpha\beta(\gamma)} \left[K S_i^\gamma S_j^\gamma + J \mathbf{S}_i \cdot \mathbf{S}_j + \Gamma (S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) \right]$$

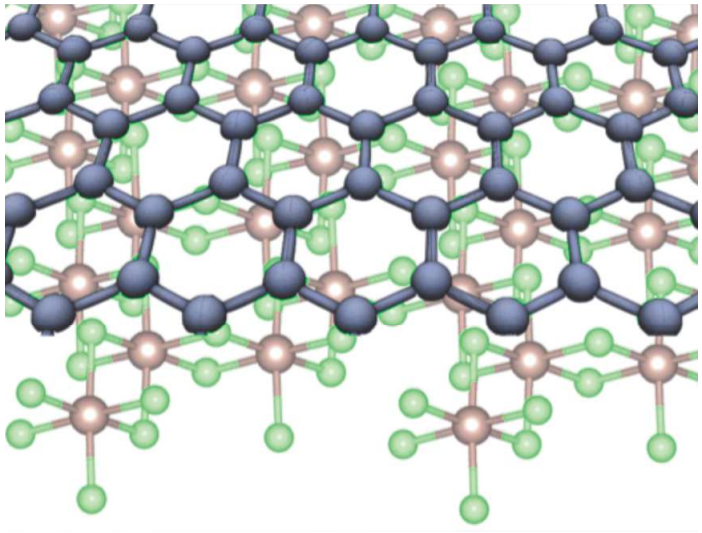
- Questions:
  - How to avoid ordering?
  - How to dope?

Mismatched Hetero-interfaces

- Experimental/fabrication developments offer rich new phase space of lattice-mismatched hetero-vdW interfaces



Geim & Grigorieva (2013)



graphene on α-$RuCl_3$

$$\left.\begin{aligned} a_{\mathrm{RuCl_3}} &= 5.96\ \text{Å} \\ a_{\mathrm{g}} &= 1.42\ \text{Å} \end{aligned}\right\} \approx 123\%$$ lattice mismatch.

Non-crystalline Interface?

- Twisted Homo-interfaces
  - Twisted multi-layer graphene and TMD's.
  - Moire superlattice provide approximate periodicity.

Large supercell calculation with strain:

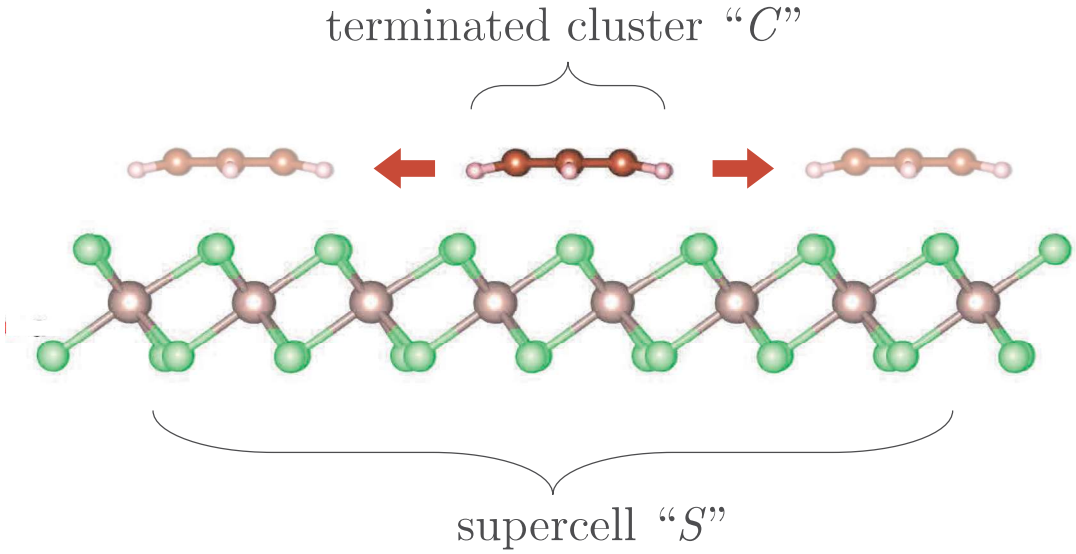
: Mismatched Interface Theory (MINT), Gerber, Arias, EAK, arXiv: https://arxiv.org/abs/1902.09550

Mismatched INterface Theory (MINT)

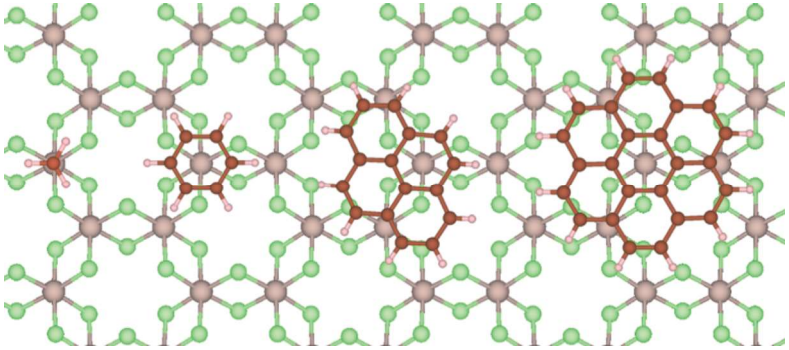
Step 1: construct "MINT representation" of heterostructure using increasingly large clusters "*C*" averaged over "*S*".

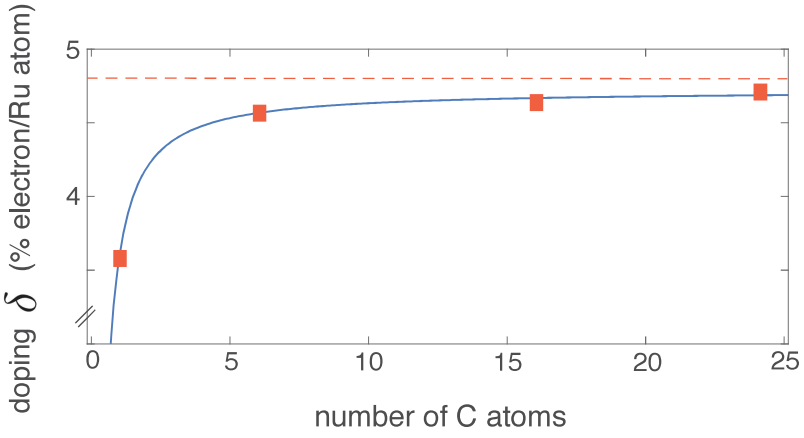
- Perform *ab initio* calculations for each reduced system.
- Scale to atomic density of ideal system, look for convergence.

Step 2: use this MINT representation, in which "*C*" is replaced by its averaged impact on "*S*", to predict electronic properties of an infinite heterostructure.



MINT: graphene on α-$RuCl_3$ (doping)

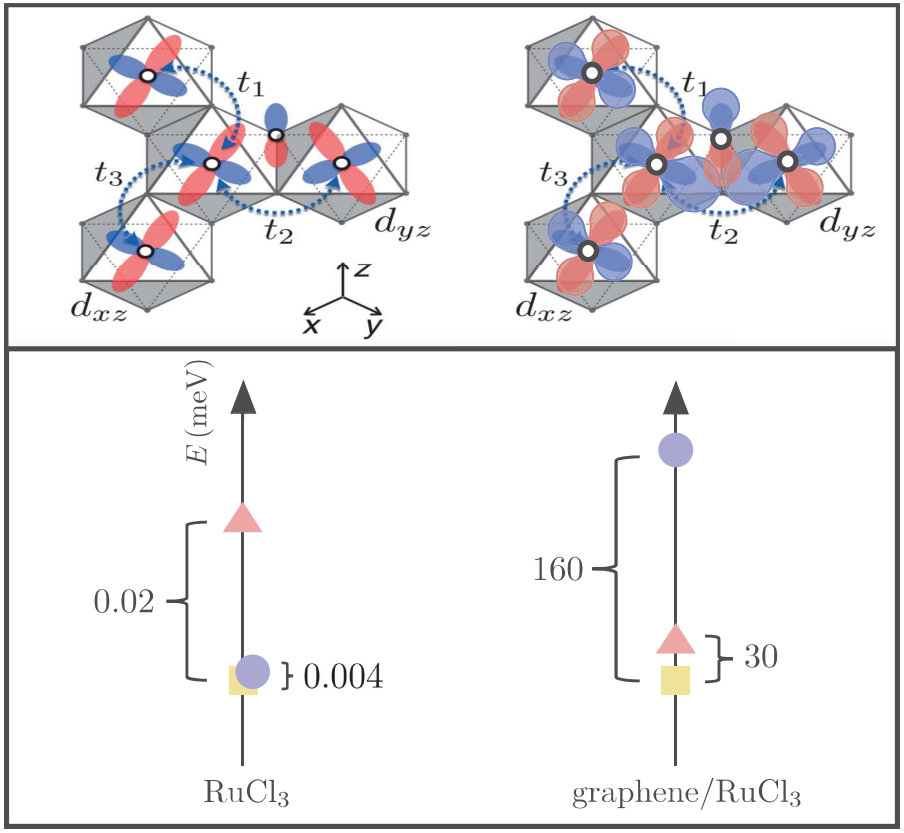




- Compute *ab initio* charge densities for each cluster averaged over $RuCl_3$ plane.
- Scale to atomic ratio of C/Ru=5.86, extrapolate doping for ideal heterostructure to construct MINT representation.

MINT: graphene on α-$RuCl_3$ (magnetism)

- δ changes orbital overlaps, hierarchy of magnetic states.
- Extract TB parameters via MLWO, obtain new J, K, Γ.



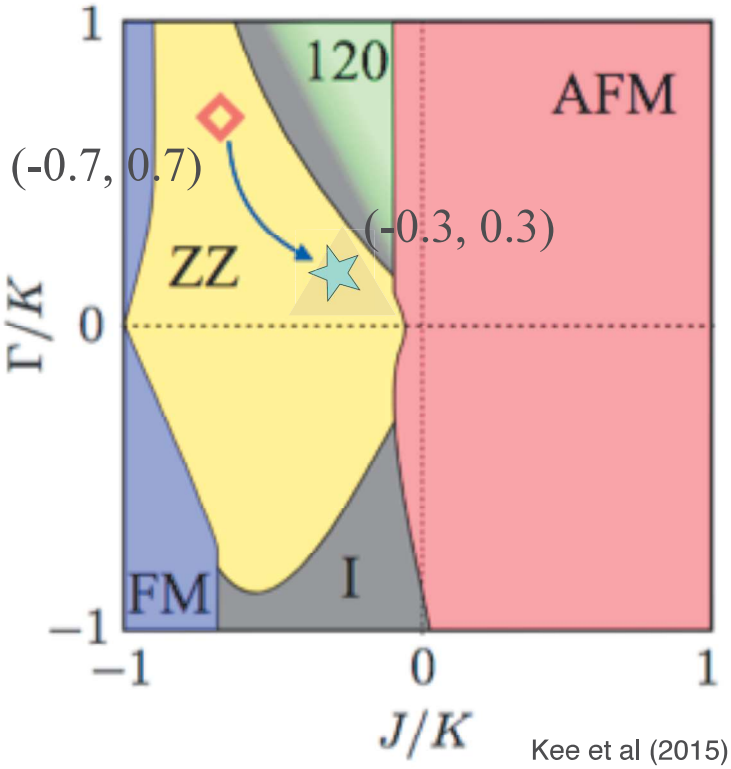
MINT: graphene on α-$RuCl_3$ (magnetism)

- δ changes orbital overlaps, hierarchy of magnetic states.

- Extract TB parameters via MLWO, obtain new J, K, Γ.

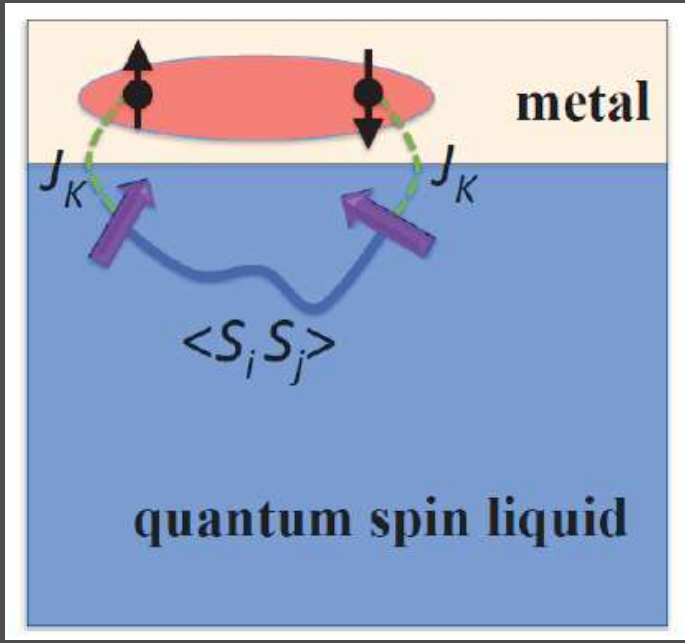
System has moved much closer to the origin!

Stay tuned on experiments:



Kee et al (2015)

TSC in Metal/Quantum Paramagnet Heterostructures



- Superconductor riding on QSL
- Selection Rule Dictated Intrinsic Topo SC for QSI.
- MINT for g/RuCl3: Doping!

Gerber, Arias, EAK, arXiv: https://arxiv.org/abs/1902.09550

Strategy III

Frustrated Systems with Strong Coupling

PHYSICAL REVIEW B **100**, 060506(R) (2019)

Rapid Communications

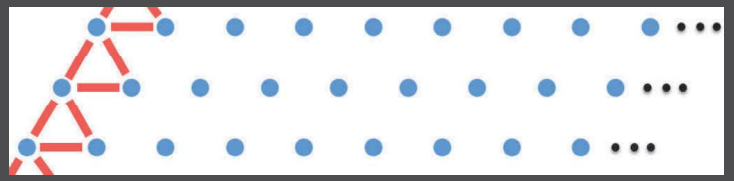
Density matrix renormalization group study of superconductivity in the triangular lattice Hubbard model

Jordan Venderley and Eun-Ah Kim

Department of Physics, Cornell University, Ithaca, New York 14850, USA

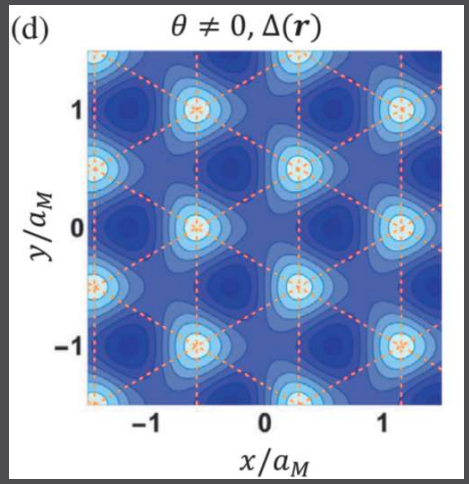
- Model:

$$H = -t \sum_{\langle i,j \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} - \mu \sum_{i\sigma} n_{i\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



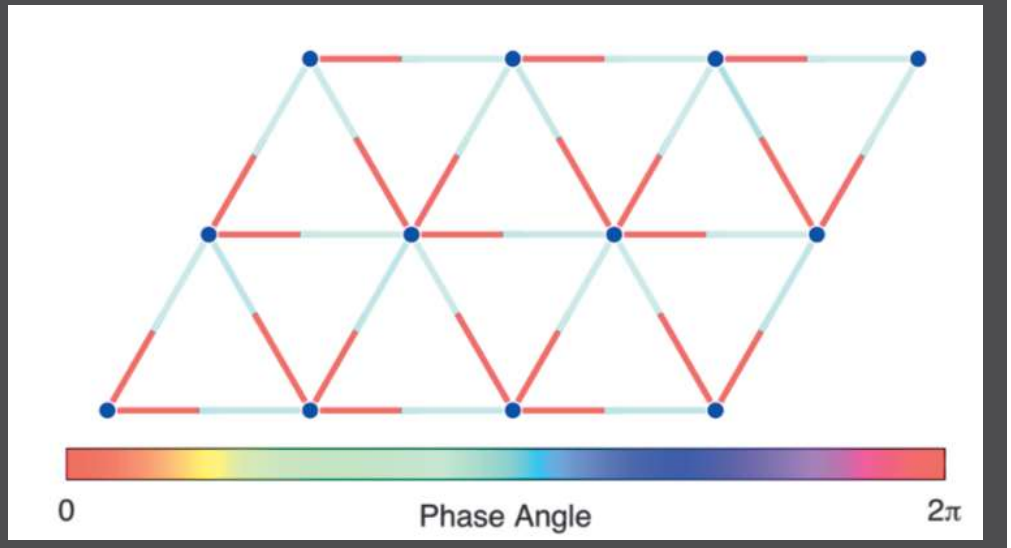
- Materialization?
  Twisted hetero-TMD

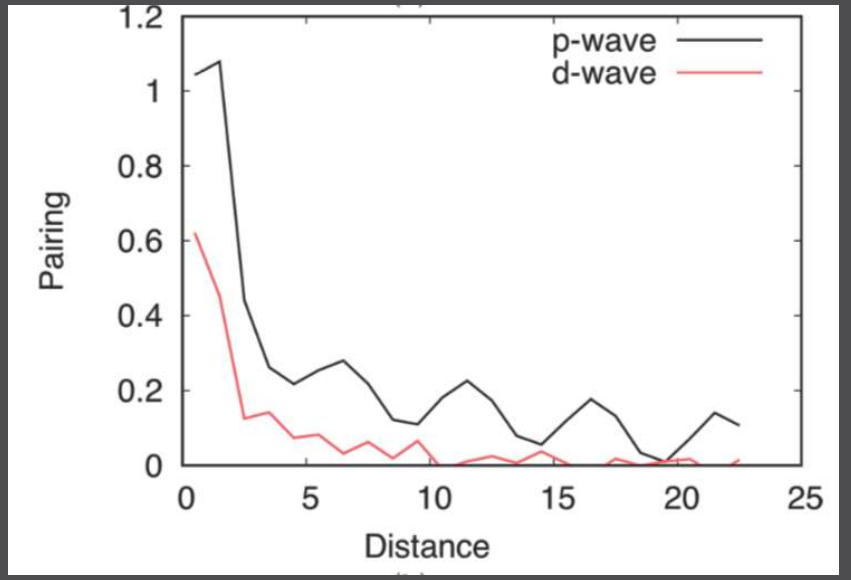
Wu, MacDonald et al, PRL 121, 026402 (2018)



Pairing Response to Random Edge Pair Field

$$\Delta_{ij}^{\text{singlet}} = \langle c_{i\uparrow}^{\dagger} c_{j\downarrow}^{\dagger} - c_{i\downarrow}^{\dagger} c_{j\uparrow}^{\dagger} \rangle,$$
$$\Delta_{ij}^{\text{triplet}} = \langle c_{i\uparrow}^{\dagger} c_{j\downarrow}^{\dagger} + c_{i\downarrow}^{\dagger} c_{j\uparrow}^{\dagger} \rangle.$$





Designing 2D topological SC's

- Spin-valley locking: hole-doped TMD,
  Hsu et al, Nat. Comm 8, 14985 (2017)
- Quantum Paramagent Heterostructure:
  She et al, npj Quantum Materials, 2, 64 (2017)
  Gerber et al, arXiv: 1902.09550
- Correlated Triangular Lattice: e.g., hetero TMD bilayer
  Venderley & Kim, PRB 100, 060506 (R)(2019)