Superconductivity in $\theta = 3.65°$ tWSe2

Mu-Yang Chen(陈沐阳)

International Center for Quantum Materials, Peking University

Advisor: Jiabin Yu（于家斌） B.A.Bernevig

Defense Advisor: Zhida Song(宋志达）

ICQM 国际量子材料科学中心 International Center for Quantum Materials

北京大學 PEKING UNIVERSITY

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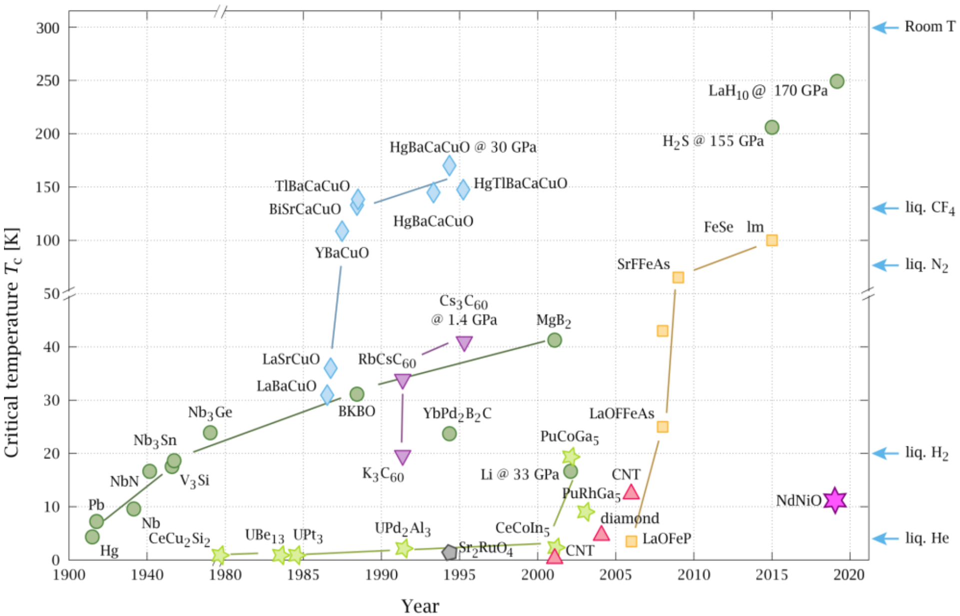
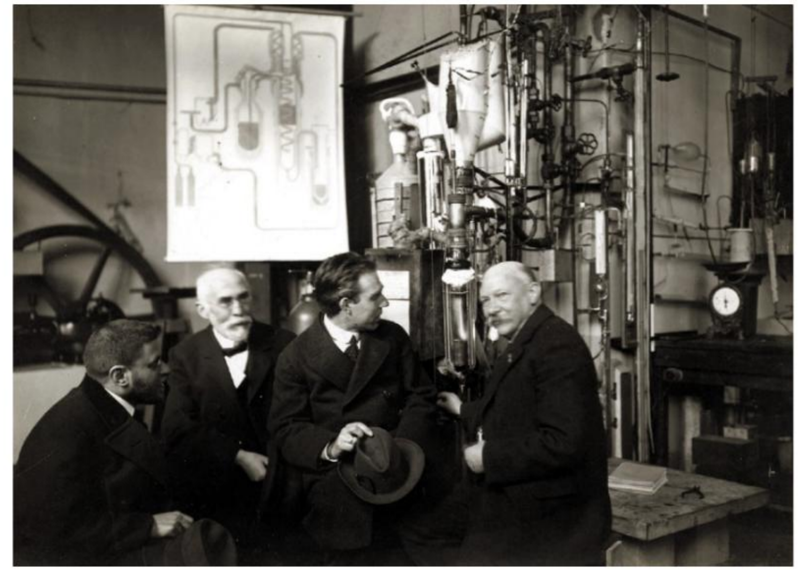
Introduction



(a) Discovery of Superconductors

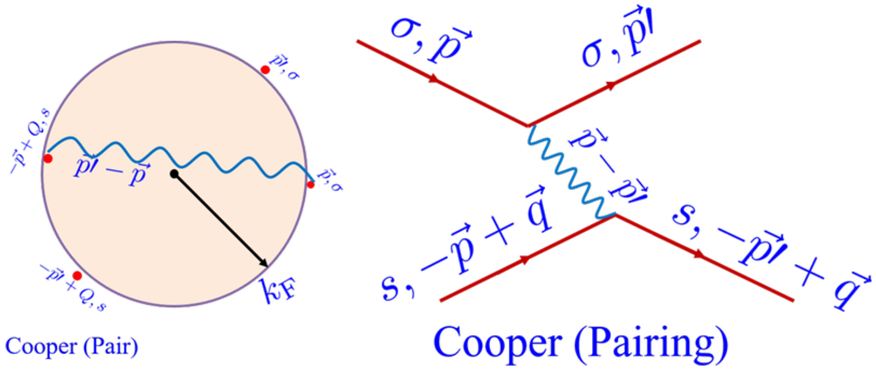


(b) P. Ehrenfest, H. Lorentz, N. Bohr and H.Onnes,Leiden (1919)

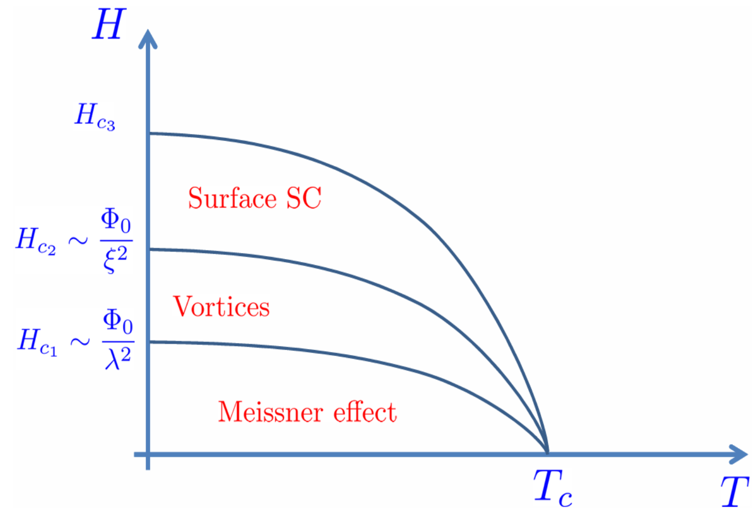
Superconductivity: Cornerstone of modern physics and technology

Introduction

(a) Cooper Pairing



(b) Phase Diagram

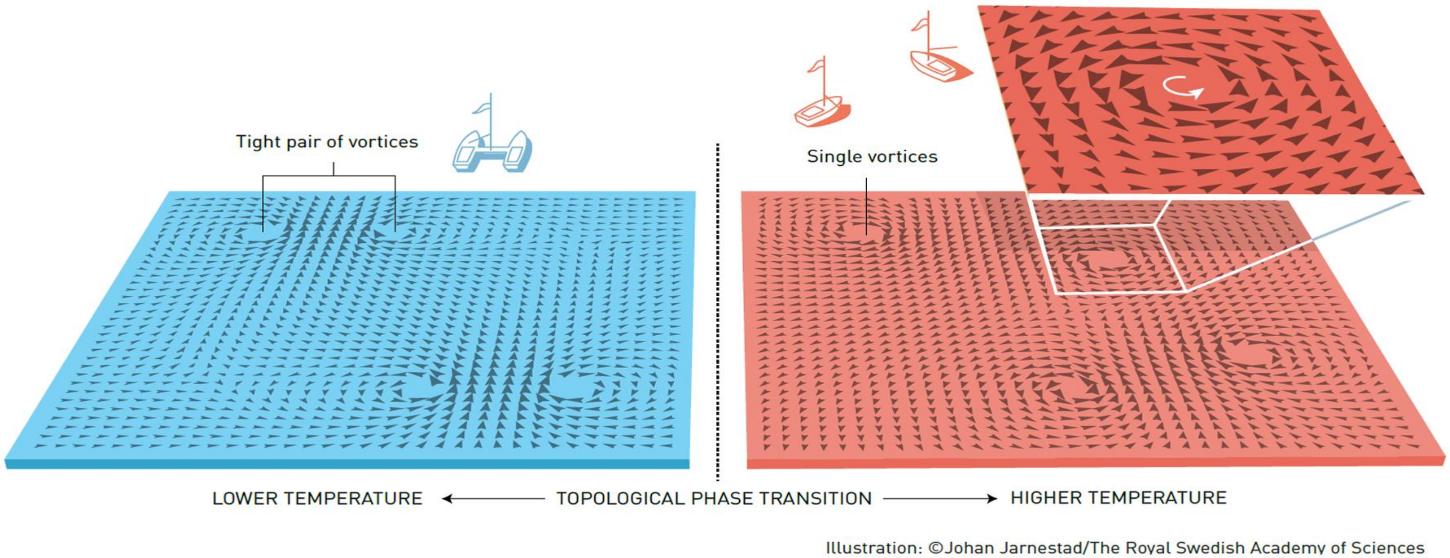


$$H = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} n_{\mathbf{k},\sigma} - \frac{g}{\Omega} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \psi^{\dagger}_{\mathbf{k+q},\uparrow} \psi^{\dagger}_{-\mathbf{k}\downarrow} \psi_{-\mathbf{k}'+\mathbf{q}\downarrow} \psi_{\mathbf{k}'\uparrow}$$

$$T_c = C\omega_D e^{-\frac{1}{gN(\epsilon_F)}}$$

BCS Superconductors: Large DOS/Debye frequency, long range ordered

Introduction



$$H = -\kappa \sum_{\langle i,j \rangle} cos(\phi_i - \phi_j) \approx E_0 + \frac{\kappa}{2} \int d^2x (\nabla \phi(\mathbf{r}))^2$$

$$\oint \nabla \phi(\boldsymbol{r}) \cdot d\boldsymbol{r} = 2\pi n, n \in \mathbb{Z}$$

$$\Downarrow$$

$$T_{KT} = \frac{\pi}{2} \kappa$$

BKT Superconductors: Topological defects, quasi long range ordered

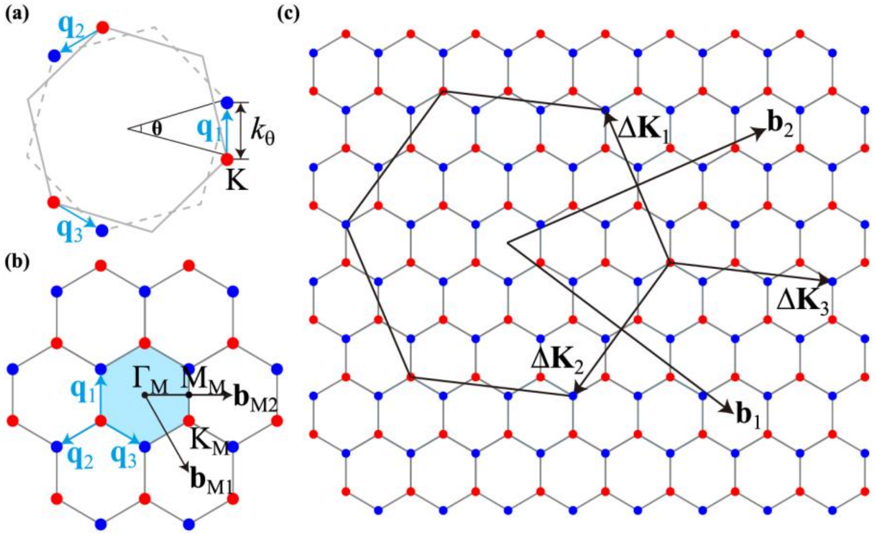
Model

$$\left[h^{\mathrm{bl}}_{\mathrm{AA}}\left(\mathbf{k},\mathbf{k}'\right)\right]_{s_1 l; s_2(-l)} = \sum_{\substack{\mathbf{q},\mathbf{G}\\ \mathbf{G}',\mathbf{G}''}} \frac{t^{\mathrm{AA}}_{s_1 s_2}\left(\mathbf{q}+\mathbf{G}\right)}{\Omega_{tot}} \delta_{\mathbf{q}+\mathbf{G}-\mathbf{k}',\mathcal{R}_{\theta,-l}\mathbf{G}'} \delta_{\mathbf{k}-\mathbf{q}-\mathbf{G},\mathcal{R}_{\theta,l}\mathbf{G}''}$$

$$= \sum_{\mathbf{G}',\mathbf{G}''} \frac{t^{\mathrm{AA}}_{s_1 s_2}\left(\mathbf{k}'+\mathcal{R}_{\theta,-l}\mathbf{G}'\right)}{\Omega_{tot}} \delta_{\mathbf{k}-\mathbf{k}',\mathcal{R}_{\theta,l}\mathbf{G}''+\mathcal{R}_{\theta,-l}\mathbf{G}'},$$

$$\left[h^{\mathrm{bl}}_{\mathrm{AB}}\left(\mathbf{k},\mathbf{k}'\right)\right]_{s_1 l; s_2(-l)} = \sum_{\substack{\mathbf{q},\mathbf{G}\\ \mathbf{G}',\mathbf{G}''}} \frac{t^{\mathrm{AB}}_{s_1 s_2}\left(\mathbf{q}+\mathbf{G}\right)}{\Omega_{tot}} \delta_{\mathbf{q}+\mathbf{G}-\mathbf{k}',-l\mathcal{R}_{\theta,-l}\mathbf{G}'} \delta_{\mathbf{k}-\mathbf{q}-\mathbf{G},l\mathcal{R}_{\theta,l}\mathbf{G}''}$$

$$= \sum_{\mathbf{G}',\mathbf{G}''} \frac{t^{\mathrm{AB}}_{s_1 s_2}\left(\mathbf{k}'-l\mathcal{R}_{\theta,-l}\mathbf{G}'\right)}{\Omega_{tot}} \delta_{\mathbf{k}-\mathbf{k}',l\mathcal{R}_{\theta,l}\mathbf{G}''-l\mathcal{R}_{\theta,-l}\mathbf{G}'}$$



Moiré Superlattice*

Continuum Model:

1. **Commonly used approach: two-center approximation**
2. **Another approach: symmetry-guided modeling** **More Intuitional!!**

Model

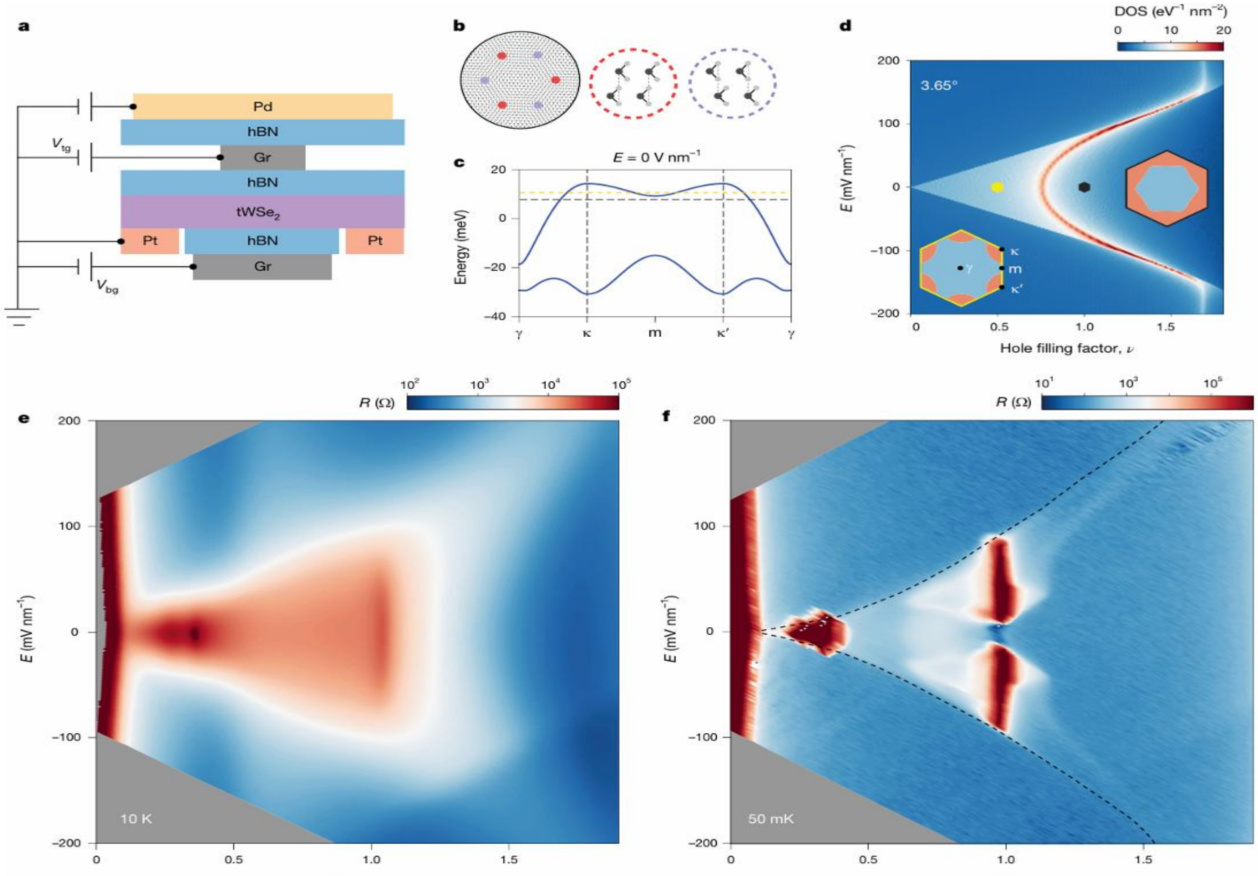
$$h_{K,\mathbf{QQ}'}^{AA}(\mathbf{k}) = -\,\delta_{\mathbf{QQ}'}\frac{\hbar^2(\mathbf{k}-\mathbf{Q})^2}{2m*} + \sum_{l}\sum_{m_1m_2n_1n_2}\sum_{\mathbf{G}_M}\delta_{\mathbf{Q},\mathbf{Q}'+\mathbf{G}_M}V_{l,\mathbf{G}_M}^{m_1m_2n_1n_2}(k-Q)_z^{m_1}(k-Q)_{z*}^{m_2}(k-Q')_z^{n_1}(k-Q')_{z*}^{n_2} + \sum_{m_1m_2n_1n_2}\sum_{\mathbf{G}_M}\sum_{l}\delta_{\mathbf{Q},\mathbf{Q}'+\mathbf{G}_M+\mathbf{q}_1}w_{l-l,\mathbf{G}_M}^{m_1m_2n_1n_2}(k-Q)_z^{m_1}(k-Q)_{z*}^{m_2}(k-Q')_z^{n_1}(k-Q')_{z*}^{n_2}$$

$$h_{ij}(\mathbf{k}) = \sum_{\alpha=1}^{d}\lambda_\alpha h_{\alpha;ij}(\mathbf{k}) \qquad C_0(\{\lambda_\alpha\}) = \sum_{\mathbf{k}\in\mathcal{M}}\mathrm{Tr}\left[\left(h(\mathbf{k}) - h^{\mathrm{DFT}}(\mathbf{k})\right)^2\right]$$

DFT Model:

1. **The model is based on ab-initio calculations***
2. **Linear extraction: higher precision and no need for fitting**

Experiment

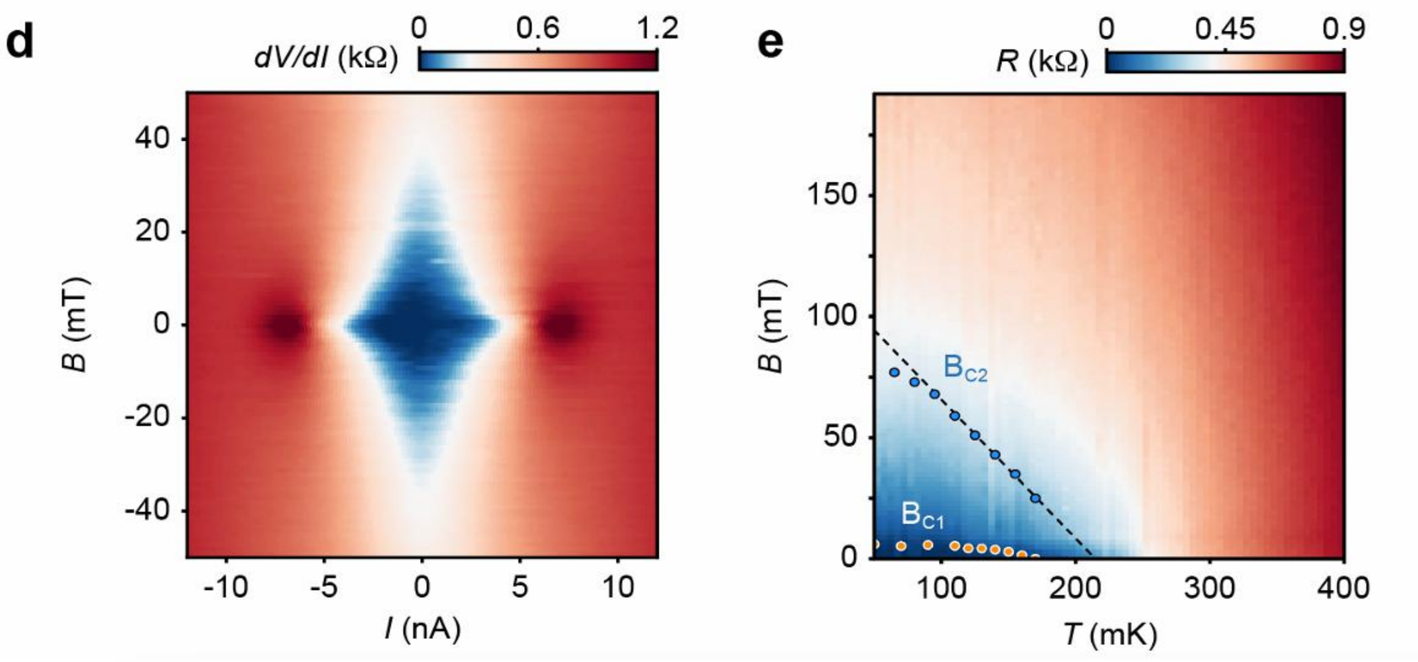


- Longitudinal resistance R at 10K and 50mK
  - Superconducting states appear only at low displacement fields hole filling $\nu = 1$
  - Critical temperature T_c~220mK, 1%-2% of T_F
  - IVC-ordered insulating states

Experiment

Superconductivity in tWSe2*

- Superconductivity at $\nu = 1$ and low displacement field
  - $R \sim \frac{B}{B_{C2}}$ between two critical perpendicular magnetic fields(50mK)
  - G-L result $B_{C2} = \frac{\Phi_0}{2\pi\xi^2}(1 - \frac{T}{T_P})$ fits well



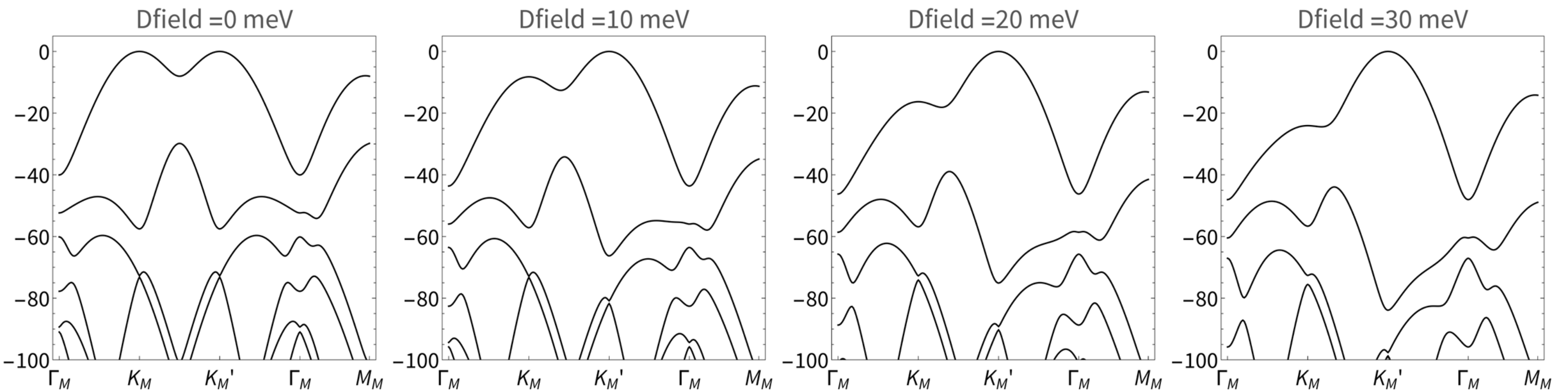
Result

$$V(\mathbf{q}) = \pi\xi^2 U_\xi \frac{\tanh(\xi|\mathbf{q}|/2)}{\xi|\mathbf{q}|/2}, \quad V(\mathbf{r}) = U_\xi \sum_{n=-\infty}^{\infty} \frac{(-1)^n}{\sqrt{(\mathbf{r}/\xi)^2 + n^2}}$$

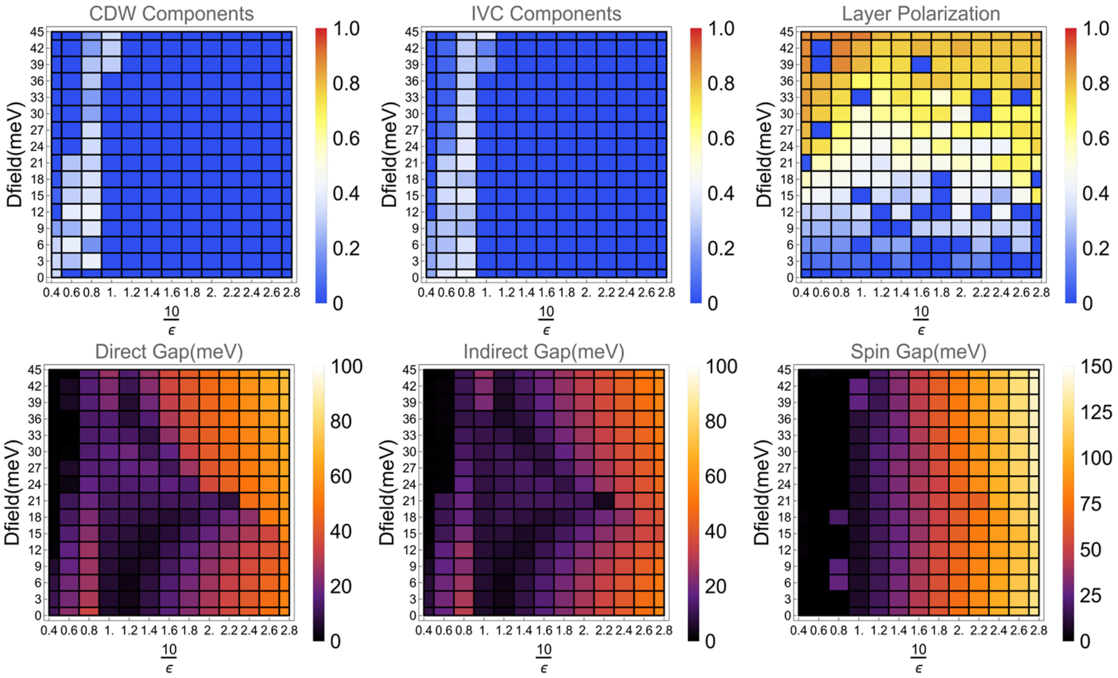
$$H_h = \sum_{\mathbf{k},n\le N_b,\eta} \tilde{\gamma}^\dagger_{\mathbf{k},n,\eta}\tilde{\gamma}_{\mathbf{k},n,\eta}(-E^\eta_n(\mathbf{k}))$$
$$+ \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\sum_{\eta\eta'}\sum_{mm'n'n\le N_b} V^{\eta\eta'}_{mm'n'n}(\mathbf{k},\mathbf{k}',\mathbf{q})\tilde{\gamma}^\dagger_{\mathbf{k}+\mathbf{q},m,\eta}\tilde{\gamma}^\dagger_{\mathbf{k}'-\mathbf{q},m',\eta'}\tilde{\gamma}_{\mathbf{k}',n',\eta'}\tilde{\gamma}_{\mathbf{k},n,\eta}$$

Band	Ch
1	1
2	1
3	-1

Apply band projection to the hole Hamiltonian



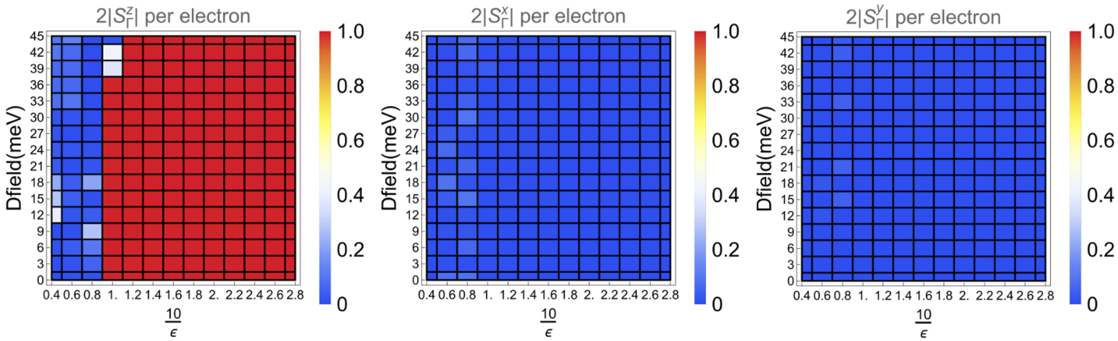
Result



Phase Diagram:

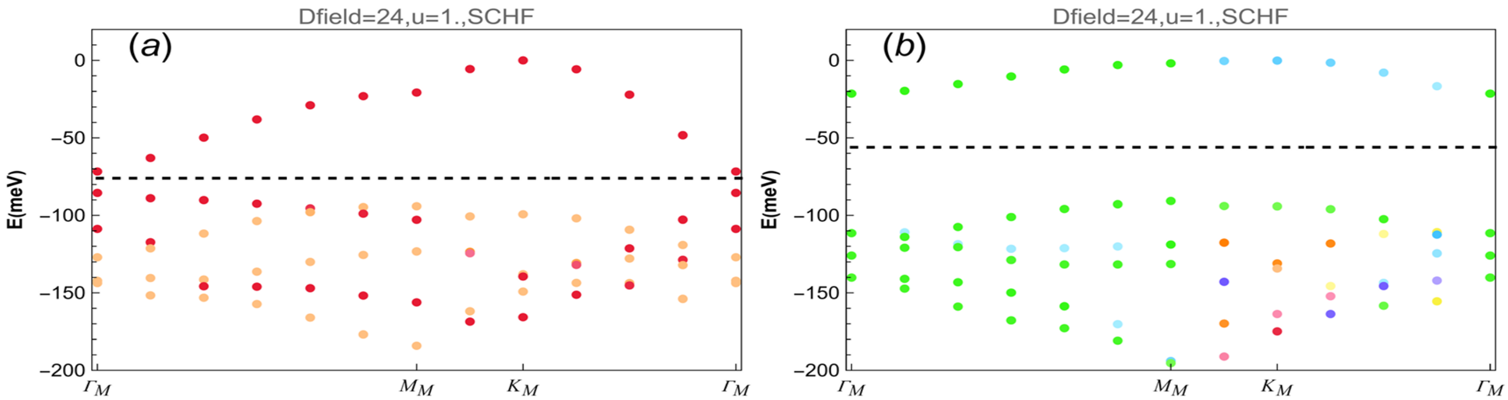
1. **Translational symmetry breaking: CDW, IVC order, IKS order**
2. **Observation of IVC-ordered correlated insulators**

Result



Phase Diagram:

1. **Weak interaction: translational symmetry breaking**
2. **Strong interaction: U(1) symmetry breaking → Valley polarized states**



Benchmark: 2BPV Hartree-Fock band structures

Conclusion and Outlook

1. A general method to construct continuum models from DFT date was introduced.
2. Numerical simulation of $3.65°$ tWSe2 aligned well with the experiment.
3. Mechanisms behind the unconventional superconductivity: spin fluctuation?

Thank you for your attention!