

# High-temperature topological superconductivity in twisted double layer copper oxides

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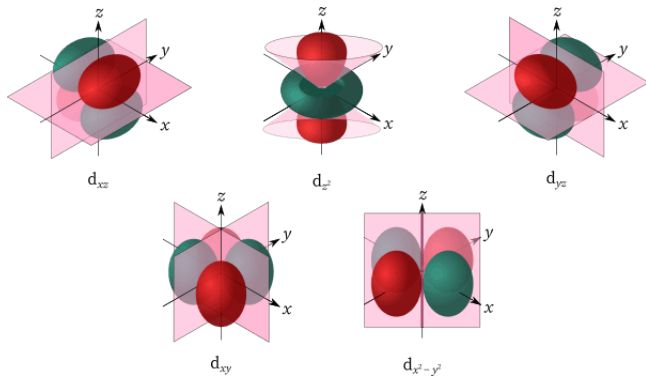
# Outline

- 1 Pairing Symmetry
- 2 Ginzburg Landau(GL) theory
- 3 Microscopic Theory
- 4 Lattice Model
- 5 Topological Phase
- 6 Experiment
- 7 Futher....

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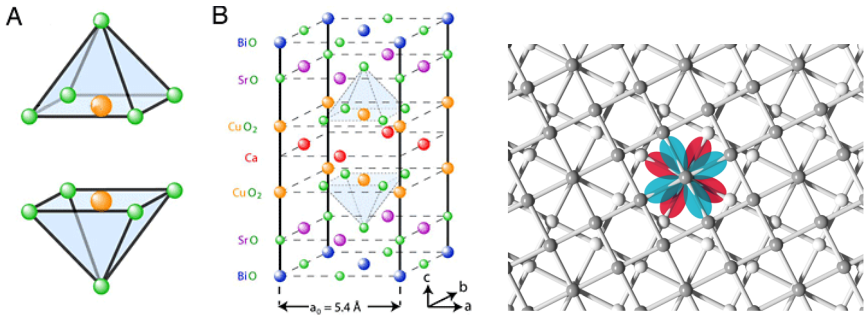
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# D-orbit of Hydrogen



$$\Delta(\mathbf{k}) = \Delta_0(\cos k_x - \cos k_y) \quad (1)$$

# Twisted double layer copper-oxygen square lattices<sup>1</sup>

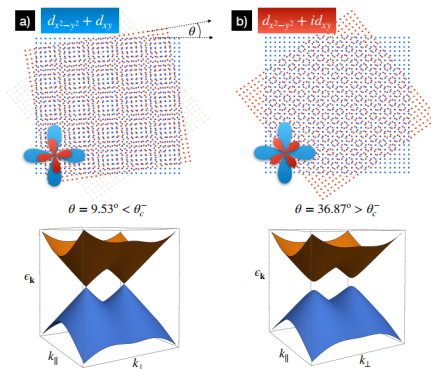


$$\Delta_{\mathbf{k}}^{\theta} = \Delta_0 \left[ \cos(2\theta)(\hat{k}_x^2 - \hat{k}_y^2) + \sin(2\theta)2\hat{k}_x\hat{k}_y \right] \quad (2)$$

The second term in Eq.(2) has the functional form of a  $d_{xy}$  order parameter.

<sup>1</sup>Nature, 575, 156

# Twisted double layer copper-oxygen square lattices



$T$ -breaking is evident because time reversal maps  $d + id'$  to  $d - id'$ .

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$$|\psi(\mathbf{r})|^2 = n_s(\mathbf{r}) \quad (3)$$

$$f_s = f_n + \alpha(T)n_s + \frac{1}{2}\beta(T)n_s^2 + \cdots \quad (4)$$

$$f_s = f_n + \alpha(T)|\psi(\mathbf{r})|^2 + \frac{1}{2}\beta(T)|\psi(\mathbf{r})|^4 \quad (5)$$



# GL Free Energy Density

$$\mathcal{F}[\psi_1, \psi_2] = f_0[\psi_1] + f_0[\psi_2] + A|\psi_1|^2|\psi_2|^2 + B(\psi_1\psi_2^* + c.c.) + C(\psi_1^2\psi_2^{*2} + c.c.) \quad (6)$$

where  $\psi_{a=1,2}$  are complex order parameters of two layers and

$f_0[\psi] = \alpha|\psi|^2 + \frac{1}{2}\beta|\psi|^4$  is the free energy of a monolayer.

If the two layers are physically identical, then the order parameter amplitudes must be the same and the most general solution (up to an overall phase) is

$$\psi_1 = \psi \quad \psi_2 = \psi e^{i\varphi} \quad (7)$$

$$\psi_a \rightarrow -\psi_a \quad \text{Under rotation } 90^\circ \quad (8)$$

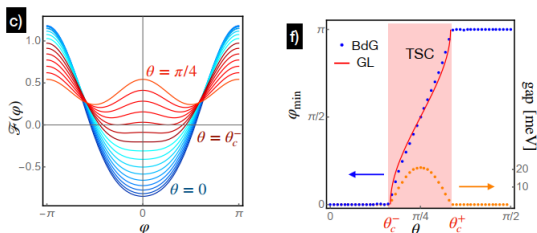
For the free energy (6) to remain invariant, the parameter  $B$  must also change sign

$$B = -B_0 \cos(2\theta) \quad (9)$$

# GL Free Energy Density

$$\mathcal{F}(\varphi) = \mathcal{F}_0 + 2B_0\psi^2 [-\cos(2\theta)\cos\varphi + \mathcal{K}\cos(2\varphi)] \quad (10)$$

where  $\mathcal{K} = C\psi^2/B_0$  and  $\mathcal{F}_0$  contains all terms independent of  $\varphi$ .



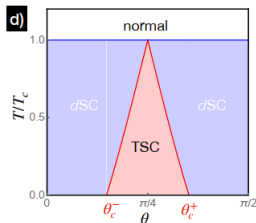
For  $\theta \neq 45^\circ$ , the free energy is minimized by

$$\varphi_{\min} = \arccos\left(\frac{\cos 2\theta}{4\mathcal{K}}\right) \quad (11)$$

Temperature dependence for the order parameter  $\psi(T) = \psi_0 \sqrt{1 - T/T_c}$ , we can obtain

$$\tilde{T}_c(\theta) = T_c \left(1 - \frac{|\cos 2\theta|}{4\mathcal{K}_0}\right) \quad \theta_c^- \leq \theta \leq \theta_c^+ \quad (12)$$

where  $\mathcal{K}_0 = C\psi_0^2/B_0$ .



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$$\begin{aligned} \mathcal{H} = & \sum_{\mathbf{k}\sigma a} \xi_{\mathbf{k}a} c_{\mathbf{k}\sigma a}^\dagger c_{\mathbf{k}\sigma a} + g \sum_{\mathbf{k}\sigma} (c_{\mathbf{k}\sigma 1}^\dagger c_{\mathbf{k}\sigma 2} + h.c) \\ & + \sum_{\mathbf{k}a} (\Delta_{\mathbf{k}a} c_{\mathbf{k}\uparrow a}^\dagger c_{-\mathbf{k}\downarrow a}^\dagger + h.c) - \sum_{\mathbf{k}a} \Delta_{\mathbf{k}a} \langle c_{\mathbf{k}\uparrow a}^\dagger c_{-\mathbf{k}\downarrow a}^\dagger \rangle \end{aligned} \quad (13)$$

$$\Delta_{\mathbf{k}a} = \sum_{\mathbf{p}} V_{\mathbf{k}\mathbf{p}}^{(a)} \langle c_{-\mathbf{p}\downarrow a} c_{\mathbf{p}\uparrow a} \rangle \quad (14)$$

where  $V_{\mathbf{k}\mathbf{p}}^{(a)}$  denotes the interaction matrix element in layer a.

$$V_{\mathbf{k}\mathbf{p}}^{(a)} = -2\mathcal{V} \cos(2\alpha_{\mathbf{k}}) \cos(2\alpha_{\mathbf{p}}) \quad (15)$$

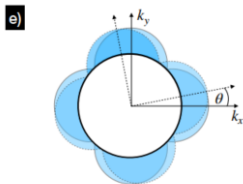
where  $\alpha_{\mathbf{k}}$  represents the polar angle of the vector  $\mathbf{k}$ .

# Microscopic Theory

Rotate the interaction in layer 2 by angle  $\theta$

$$V_{\mathbf{k}\mathbf{p}}^{(2)} = -2\mathcal{V} \cos(2\alpha_{\mathbf{k}} - 2\theta) \cos(2\alpha_{\mathbf{p}} - 2\theta) \quad (16)$$

Consider a circular Fermi surface generated by  $\xi_{\mathbf{k}a} = \hbar^2 k^2 / 2m - \mu$  that remains invariant under rotation



$$\mathcal{H} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger} h_{\mathbf{k}} \Psi_{\mathbf{k}} + E_0 \quad (17)$$

$$h_{\mathbf{k}} = \begin{bmatrix} \xi_{\mathbf{k}} & \Delta_{\mathbf{k}1} & g & 0 \\ \Delta_{\mathbf{k}1}^* & -\xi_{\mathbf{k}} & 0 & -g \\ g & 0 & \xi_{\mathbf{k}} & \Delta_{\mathbf{k}2} \\ 0 & -g & \Delta_{\mathbf{k}2}^* & -\xi_{\mathbf{k}} \end{bmatrix} \quad (18)$$

and  $E_0 = \sum_{\mathbf{k}} 2\xi_{\mathbf{k}} - \sum_{\mathbf{k}a} \Delta_{\mathbf{k}a} \langle c_{\mathbf{k}\uparrow a}^\dagger c_{-\mathbf{k}\downarrow a}^\dagger \rangle$ .

The free energy of the system can be calculated from the standard expression

$$\mathcal{F}_{\text{BdG}} = E_0 - 2k_B T \sum_{\mathbf{k}a} \ln [2 \cosh(E_{\mathbf{k}\alpha}/2k_B T)] \quad (19)$$

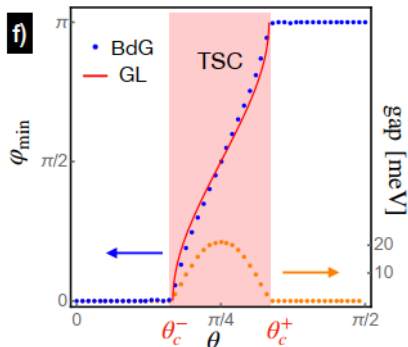
$$E_{\mathbf{k}\alpha} = \sqrt{(\Delta_{\mathbf{k}1}^2 + \Delta_{\mathbf{k}2}^2)/2 + \xi_{\mathbf{k}}^2 + g^2 + (-)^\alpha D_{\mathbf{k}}}$$

$$D_{\mathbf{k}}^2 = (D_{\mathbf{k}1}^2 - D_{\mathbf{k}2}^2)^2/4 + g^2(\Delta_{\mathbf{k}1}^2 + \Delta_{\mathbf{k}2}^2 + 4\xi_{\mathbf{k}}^2) - 2g^2\Delta_{\mathbf{k}1}\Delta_{\mathbf{k}2}\cos\varphi \quad (20)$$

# Microscopic Theory

$$\Delta_{\mathbf{k}1} = \psi \cos(2\alpha_{\mathbf{k}}) \quad \Delta_{\mathbf{k}2} = \psi \cos(2\alpha_{\mathbf{k}} - 2\theta) \quad (21)$$

$$\mathcal{F}(\varphi) = \mathcal{F}_0 + 2B_0\psi^2 [-\cos(2\theta)\cos\varphi + \mathcal{K}\cos(2\varphi)] \quad (22)$$

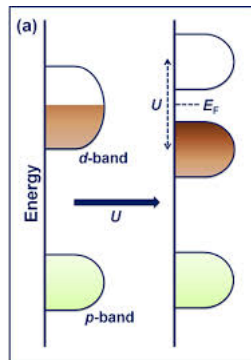
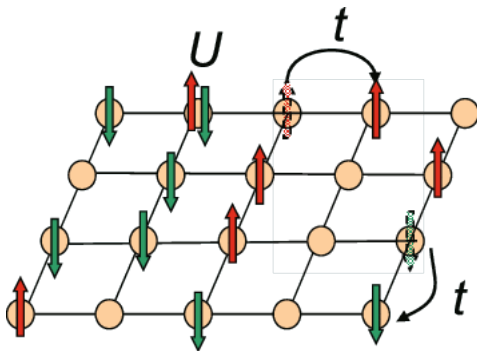




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# Hubbard Model



$$H = \sum_{ij,\sigma} t_{ij} C_{i\sigma}^\dagger C_{j\sigma} + U \sum_{i\sigma} n_{i\sigma} n_{i\bar{\sigma}} \quad n_{i\sigma} = C_{i\sigma}^\dagger C_{i\sigma} \quad (23)$$

# Hubbard Model

$$H = - \sum_{ij,\sigma a} t_{ij} c_{i\sigma a}^\dagger c_{j\sigma a} - \mu \sum_{i\sigma a} n_{i\sigma a} + \sum_{ij,a} V_{ij} n_{ia} n_{ja} - \sum_{ij\sigma} g_{ij} c_{i\sigma 1}^\dagger c_{j\sigma 2} \quad (24)$$

Mean field approximation

$$c_i c_j = \langle c_i c_j \rangle + (c_i c_j - \langle c_i c_j \rangle) \quad (25)$$

$$H = -t \sum_{\langle ij \rangle \sigma a} c_{i\sigma a}^\dagger c_{j\sigma a} - t' \sum_{\langle\langle ij \rangle\rangle \sigma a} c_{i\sigma a}^\dagger c_{j\sigma a} - \mu \sum_{i\sigma a} n_{i\sigma a} \\ + \sum_{\langle ij \rangle a} (\Delta_{ij,a} c_{i\uparrow a}^\dagger c_{j\downarrow a}^\dagger + h.c.) - \sum_{ij\sigma} g_{ij} c_{i\sigma 1}^\dagger c_{j\sigma 2} \quad (26)$$

$$\Delta_{ij,a} = V \langle c_{i\uparrow a} c_{j\downarrow a} \rangle \quad (27)$$

# Hubbard-Stratonovich Transformation<sup>2</sup>

$$S[\psi, \bar{\psi}] = \sum_p \bar{\psi}_{p\sigma} \left( -i\omega_n + \frac{p^2}{2m} - \mu \right) \psi_{p\sigma} + \frac{T}{2L^3} \sum_{pp'q} \bar{\psi}_{p+q\sigma} \bar{\psi}_{p'-q\sigma'} V(\mathbf{q}) \psi_{p'\sigma'} \psi_{p\sigma} \quad (28)$$

$$1 \equiv \int D\phi \exp \left[ -\frac{e^2 \beta}{2L^d} \sum_q \phi_q V^{-1}(\mathbf{q}) \phi_{-q} \right] \quad (29)$$

Employing the variable shift  $\phi_q \rightarrow \phi_q + ie^{-1}V(q)\rho_q/\beta$ , where  $\rho_q \equiv \sum_p \bar{\psi}_{p\sigma} \psi_{p+q\sigma}$ ,  $q = (\omega_m, \mathbf{q})$ .

$$1 = \int D\phi \exp \left[ \frac{1}{L^d} \sum_q \left( -\frac{e^2 \beta}{2} \phi_q V^{-1}(q) \phi_{-q} + ie \rho_q \phi_{-q} + \frac{1}{2\beta} \rho_q V(\mathbf{q}) \rho_{-q} \right) \right] \quad (30)$$

<sup>2</sup>Condensed Matter Field Theory(Alexander Altland,Ben Simons)

# Hubbard-Stratonovich Transformation

The field integral

$$\mathcal{Z} = \int D\phi \int D(\bar{\psi}_\sigma, \psi_\sigma) e^{-S[\phi, \bar{\psi}_\sigma, \psi_\sigma]} \quad (31)$$

$$S[\phi, \bar{\psi}_\sigma, \psi_\sigma] = \frac{\beta}{8\pi L^d} \sum_q \phi_q \mathbf{q}^2 \phi_{-q} + \sum_{pp'} \bar{\psi}_{p\sigma} \left[ (-i\omega + \frac{\mathbf{p}}{2m} - \mu) \delta_{pp'} + \frac{ie}{L^d} \phi_{p'-p} \right] \psi_{p'\sigma} \quad (32)$$

# Hubbard-Stratonovich Transformation

After decoupling the attractive pairing potential in the Cooper channel with the Hubbard-Stratonovich transformation we obtain the action corresponding to the Hamiltonian (26)

$$S = \sum_{\mathbf{k}n} \Psi_{\mathbf{k}n}^\dagger [-i\omega_n + h_{\mathbf{k}}] \Psi_{\mathbf{k}n} + \frac{\beta\mathcal{N}}{V} \sum_{i,j \in u.c.a} \Delta_{ij,a} \Delta_{ij,a}^* \quad (33)$$

The effective action for  $\Delta_{ij,a}$  can be determined by integrating out fermionic degrees of freedom

$$S_{\text{eff}} = - \sum_{\mathbf{k}n} \text{Tr} \log [-\mathcal{G}(\mathbf{k}, i\omega)^{-1}] + \frac{\beta\mathcal{N}}{V} \sum_{i,j \in u.c.a} \Delta_{ij,a} \Delta_{ij,a}^* \quad (34)$$

where  $\mathcal{G}(\mathbf{k}, i\omega_n) = -(-i\omega_n + h_{\mathbf{k}})^{-1}$

# Hubbard-Stratonovich Transformation

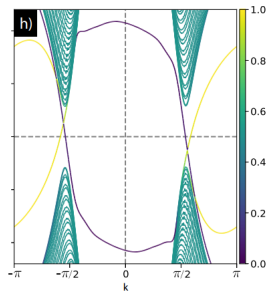
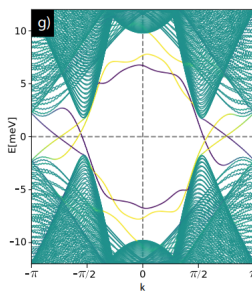
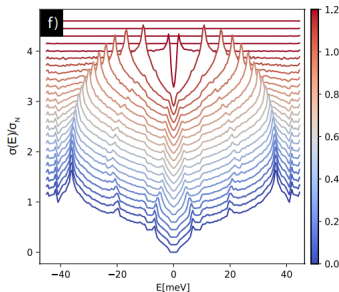
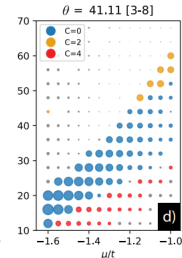
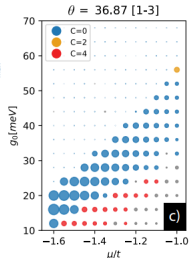
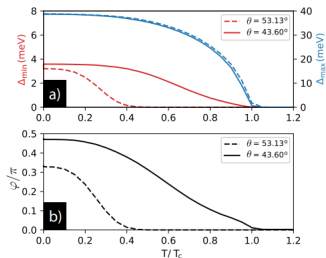
Calculate the saddle point condition for this effective action

$\partial S_{\text{eff}}/\partial \delta_{ij,a}^* = 0$ , employ the identity  $\partial_{\Delta}(\text{Tr} \log A) = \text{Tr} [\partial_{\Delta} A A^{-1}]$ . After performing the Matsubara sum

$$\Delta_{ij,a} = -\frac{V}{\mathcal{N}} \sum_{\mathbf{k}} \text{Tr} \left[ \frac{\partial h_{\mathbf{k}}}{\partial \Delta_{ij,a}^*} U_{\mathbf{k}} n_F(E_{\mathbf{k}}) U_{\mathbf{k}}^{\dagger} \right] \quad (35)$$

where  $U_{\mathbf{k}}^{\dagger} h_{\mathbf{k}} U_{\mathbf{k}} = E_{\mathbf{k}}$  and  $n_F(E_{\mathbf{k}})$  is Fermi function.

# Hubbard Model





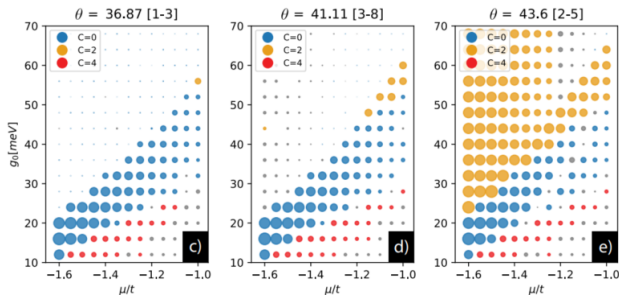
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# Chern Number

$$C = \frac{1}{2\pi} \int_{BZ} \Omega(\mathbf{k}) d^2k \quad (36)$$

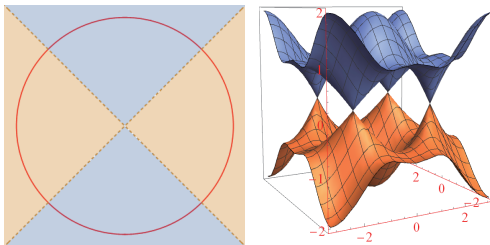
$$\Omega(\mathbf{k}) = \sum_{m \neq n} \frac{\langle n | \nabla_{\mathbf{k}} h_{\mathbf{k}} | m \rangle \times \langle m | \nabla_{\mathbf{k}} h_{\mathbf{k}} | n \rangle}{(E_m - E_n)^2} \quad (37)$$



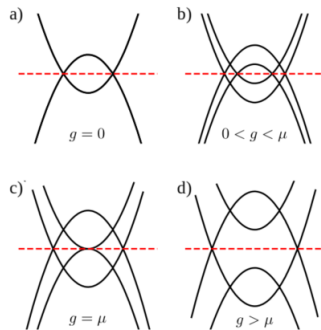
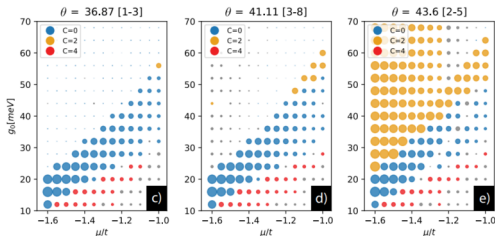
# *d*-wave Superconductor

$$H = \sum_{\mathbf{k}\sigma} \epsilon(\mathbf{k}) d_{\mathbf{k}\sigma}^\dagger d_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} \Delta(\mathbf{k}) (d_{\mathbf{k}\uparrow}^\dagger d_{-\mathbf{k}\downarrow}^\dagger + h.c) \quad (38)$$

where  $\epsilon(\mathbf{k}) = -2t(\cos k_x + \cos k_y) - \mu$ ,  $\Delta(\mathbf{k}) = \Delta_0(\cos k_x - \cos k_y)$



# Chern Number

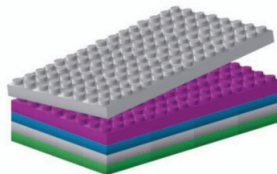
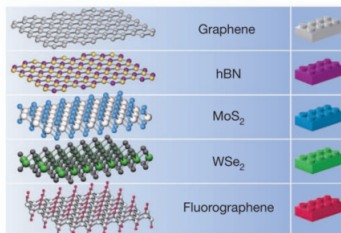
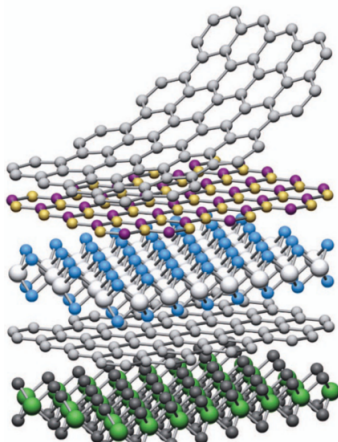


If the interlayer coupling  $g$  is strong enough to push one of the bands above the Fermi level, half of the Dirac cones disappear, leaving four Dirac cones behind.

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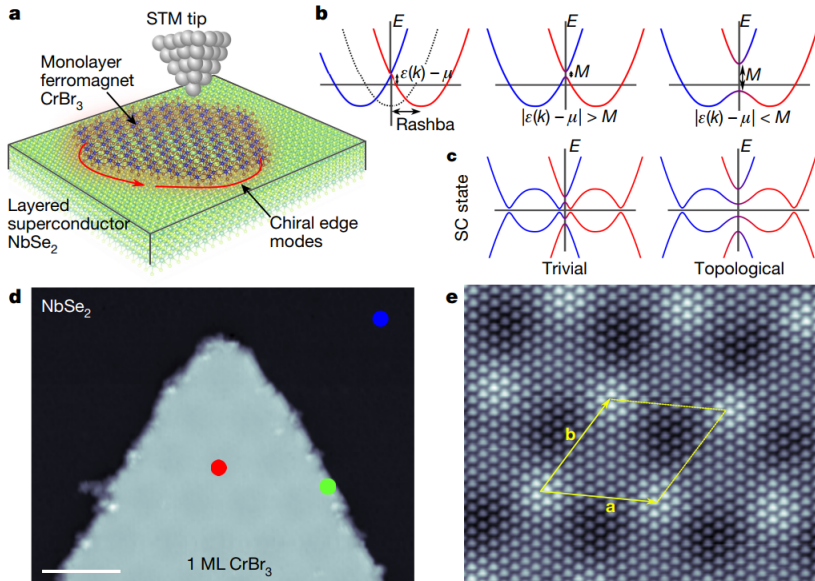
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# Van der Waals heterostructures<sup>3</sup>

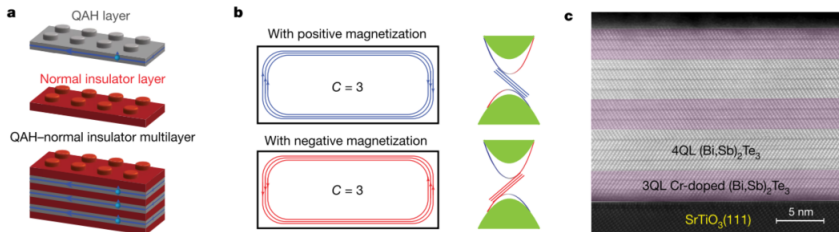


<sup>3</sup>Nature, 499, 419-425 (2013)

# Topological superconductivity<sup>4</sup>



# Quantum anomalous Hall insulators<sup>5</sup>



**Fig. 1 | The high-CQAH effect in magnetic-undoped topological insulator multilayer structures.** **a**, Schematics of the high- $C$  QAH insulator in  $C=1$  QAH-normal insulator multilayer structures. The blue arrows illustrate the chiral edge channels of the QAH insulators. **b**, Schematics of the high- $C$  QAH effect.

We take a  $C=3$  QAH insulator as an example. Three chiral edge channels are shown in real space (left) and momentum space (right) for positive (top) and negative (bottom) magnetization. **c**, Cross-sectional STEM image of the  $m=0$  multilayer structure grown on a  $\text{SrTiO}_3$  substrate.

<sup>5</sup>Nature,588,419-423(2020)



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# Twisted

- arXiv:2012.07860v1 (Magic angles and current-induced topology in twisted nodal superconductors)
- arXiv:2012.03986v1 (Chiral  $p$ -wave superconductivity in a twisted array of proximitized quantum wires)

