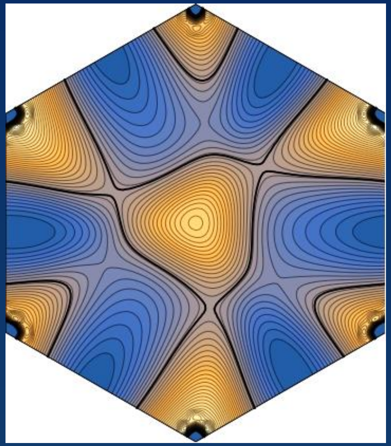
UNIVERSAL MECHANISM OF ISING SUPERCONDUCTIVITY IN TWISTED BILAYER, TRILAYER AND QUADRILAYER GRAPHENE



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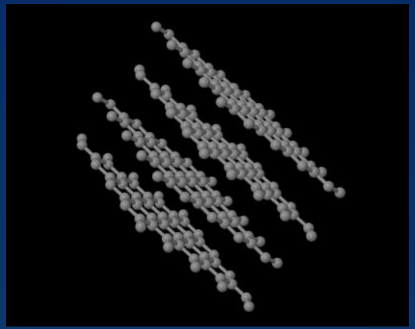
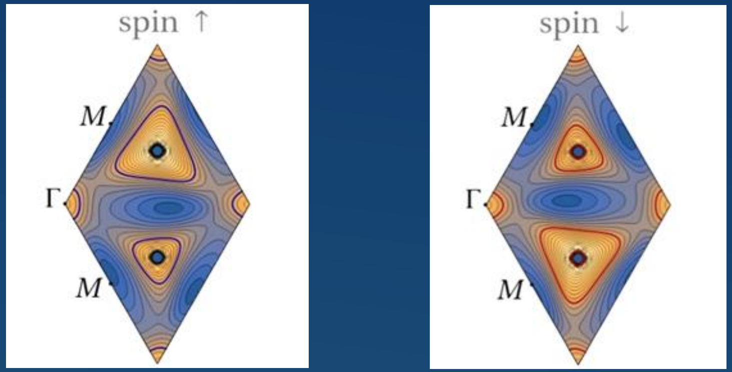
UNIVERSAL MECHANISM OF ISING SUPERCONDUCTIVITY

Recently there have been consistent observations of superconductivity in twisted graphene trilayers, quadrilayers, pentalayers (in setups with alternating twist angle $\theta, -\theta, \theta, -\theta \ldots$), specially in the hole-doped regime for filling fraction $\nu < -2$



- J. M. Park, Y. Cao, K. Watanabe, T. Taniguchi, and P. Jarillo-Herrero, Nature 590, 249 (2021)
- Z. Hao *et al.*, Science 371, 1133 (2021)
- Y. Cao *et al.*, Nature 595, 526 (2021)
- Y. Zhang *et al.*, Science 377, 1538 (2022)
- J. M. Park *et al.*, Nature Materials 21, 877 (2022)

In the twisted graphene multilayers, it can be shown that many of the experimental observations are the consequence of the spontaneous breakdown of the valley symmetry. This induces spin-valley locking, with important consequences for the superconductivity

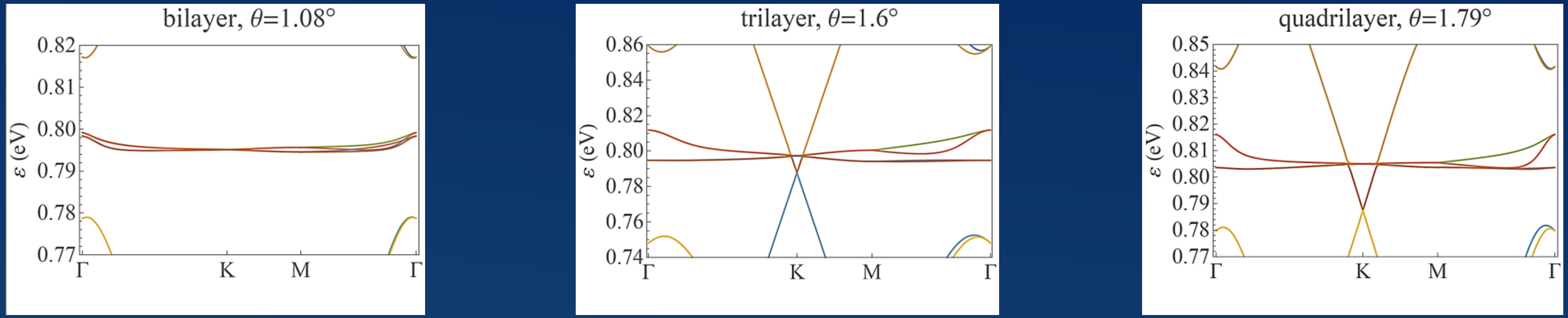


UNIVERSAL MECHANISM OF ISING SUPERCONDUCTIVITY

We study the dynamical symmetry breaking by means of a self-consistent Hartree-Fock approximation in real space, starting from a tight-binding approach.

The noninteracting Hamiltonian H_0 can be represented in the form

$$H_0 = -\sum_{n=1}^{N} t_{\parallel}(\mathbf{r}_i - \mathbf{r}_j)\,(a^{+}_{n,i}a_{n,j} + \mathrm{h.c.}) - \sum_{n \neq m} t_{\perp}(\mathbf{r}_i - \mathbf{r}_j)\,(a^{+}_{n,i}a_{m,j} + \mathrm{h.c.})$$



For the interacting part of the Hamiltonian H_{int}, we include both extended Coulomb (screened by metallic gates) and Hubbard contributions

$$H_{\mathrm{int}} = H_C + H_U$$

$$H_C = \frac{1}{2} \sum_{i,j,\sigma,\sigma'} a^{+}_{i\sigma}a_{i\sigma}\; v_C(\mathbf{r}_i - \mathbf{r}_j)\; a^{+}_{j\sigma'}a_{j\sigma'} \qquad v_C(\mathbf{r}) = \frac{e^2}{4\pi\varepsilon}\left(\frac{1}{r} - \frac{1}{\sqrt{r^2+\xi^2}}\right)$$

$$H_U = U \sum_{i} a^{+}_{i\uparrow}a_{i\uparrow}\; a^{+}_{i\downarrow}a_{i\downarrow}$$

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The Hartree-Fock approximation can be carried out in real space by assuming that, in the static limit, the full electron propagator G has a representation in terms of eigenvalues and eigenvectors

$$(G)_{i\sigma,j\sigma} = -\sum_a \frac{1}{\varepsilon_{a\sigma}} \phi_{a\sigma}(\mathbf{r}_i)\, \phi_{a\sigma}(\mathbf{r}_j)^*$$

The eigenvectors ϕ are obtained by solving self-consistently the Dyson equation

$$G^{-1} = G_0^{-1} - \Sigma$$

with the electron self-energy Σ made of Hartree and Fock terms

$$(\Sigma)_{i\sigma,j\sigma} = \mathbf{1}_{ij} \sum_{\substack{\text{filled} \\ \text{bands}}} \sum_{l\sigma'} v_{\sigma\sigma'}(\mathbf{r}_i - \mathbf{r}_l)\; \left|\phi_{a\sigma'}(\mathbf{r}_l)\right|^2$$

$$- v_{\sigma\sigma}(\mathbf{r}_i - \mathbf{r}_j) \sum_{\substack{\text{filled} \\ \text{bands}}} \phi_{a\sigma}(\mathbf{r}_i)\, \phi_{a\sigma}(\mathbf{r}_j)^*$$

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The condensation of different order parameters can be studied through the matrix elements h_{ij}

$$h_{ij}^{(\sigma)} = \sum_{\substack{\text{filled} \\ \text{bands}}} \phi_{a\sigma}(\mathbf{r}_i)\, \phi_{a\sigma}(\mathbf{r}_j)^*$$

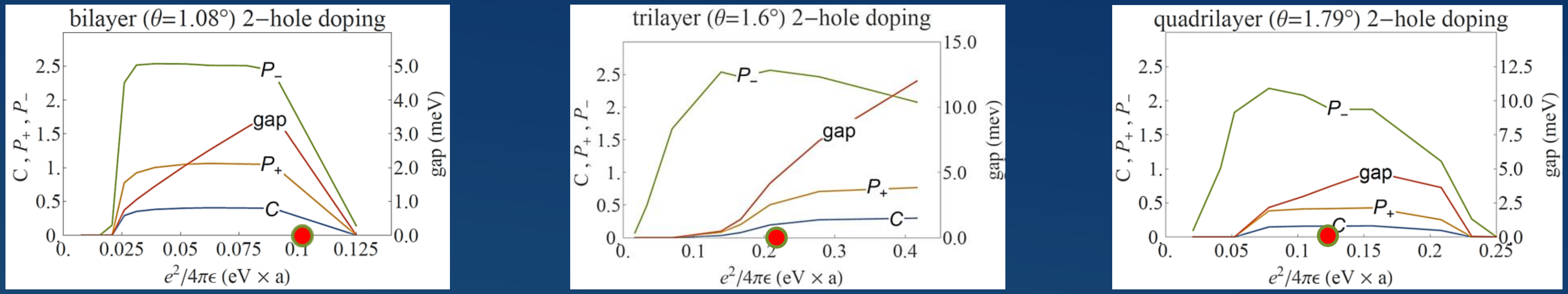
The relevant patterns of symmetry breaking are:

- chiral symmetry breaking characterized by staggered charge order in sublattices A and B

$$C^{(\sigma)} = \sum_{i \in A} h_{ii}^{(\sigma)} - \sum_{i \in B} h_{ii}^{(\sigma)}$$

- time-reversal symmetry breaking with currents circulating along nearest neighbors i_1, i_2, i_3 of each site

$$P_{\pm}^{(\sigma)} = \mathrm{Im}\left(\sum_{i \in A} (h_{i_1 i_2}^{(\sigma)} h_{i_2 i_3}^{(\sigma)} h_{i_3 i_1}^{(\sigma)})^{1/3} \pm \sum_{i \in B} (h_{i_1 i_2}^{(\sigma)} h_{i_2 i_3}^{(\sigma)} h_{i_3 i_1}^{(\sigma)})^{1/3} \right)$$



J. G. and T. Stauber, arXiv:2110.11294 (to appear Nature Commun.), arXiv:2303.00583

In a wide range of couplings, the dominant order parameter corresponds to valley symmetry breaking with $P_- \neq 0$, until a valley-coherent phase takes over in the strong coupling limit.

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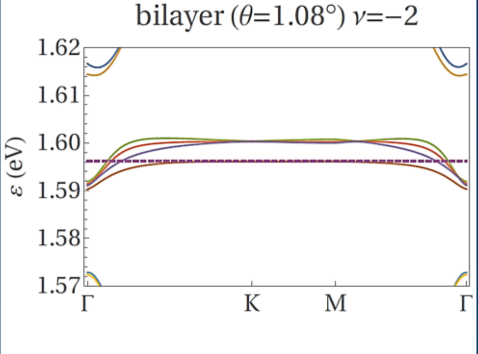
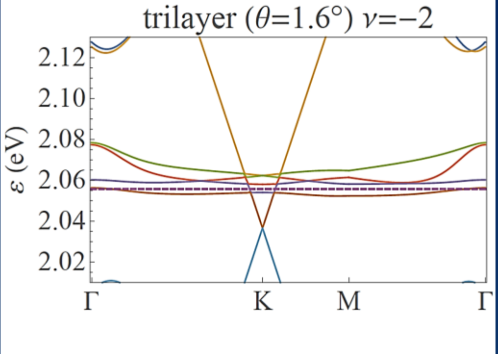
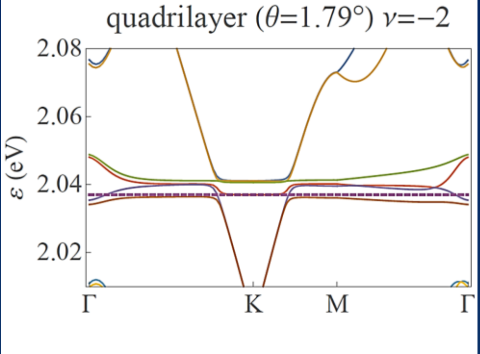
The spontaneous breakdown of valley symmetry has important consequences, since at $\nu = -2$ it places the Fermi level at the Dirac nodes of the lower valley, where a sufficiently strong interaction can open a gap between the Dirac cones

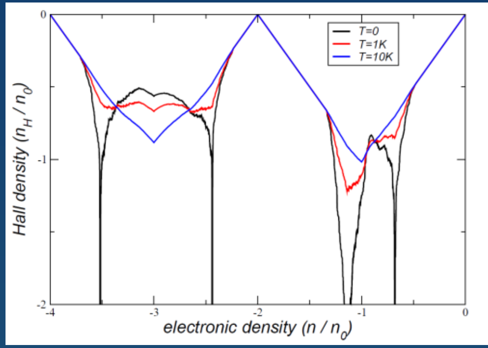






The gap opened at the Dirac nodes of the lower valley has an interesting experimental signature, which is the reset of the Hall density at $\nu = -2$.

In the case of twisted trilayer graphene, our estimates from the self-consistent Hartree-Fock approach lead to good agreement with the experimental observations of the Hall density



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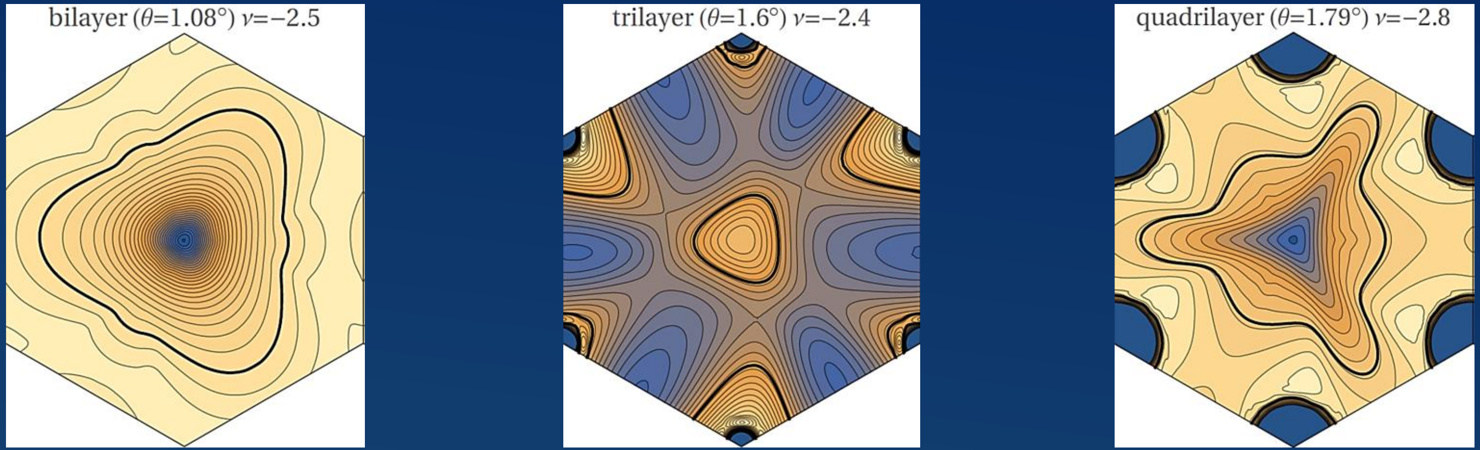
The other important consequence of valley symmetry breaking is the reduction of symmetry from C_6 to C_3, since this latter group is the one operating in a single graphene valley.

We can observe the reduction of symmetry in the plot of the second valence band in the Brillouin zone, for twisted bilayer, trilayer and quadrilayer graphene



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There is then an increase in the anisotropy of the bands, with the consequent amplification of the modulations of the *e-e* scattering along the Fermi line. This makes the system very prone to a Kohn-Luttinger (superconducting) instability.

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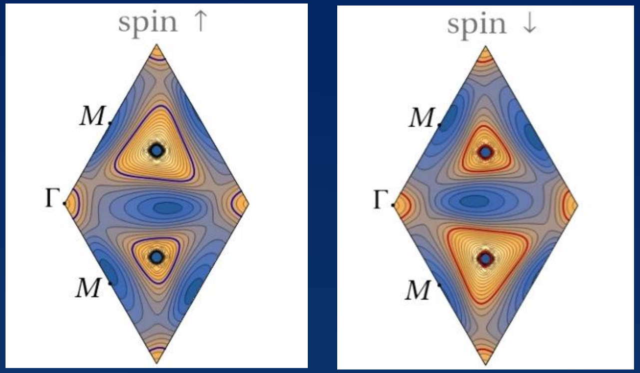
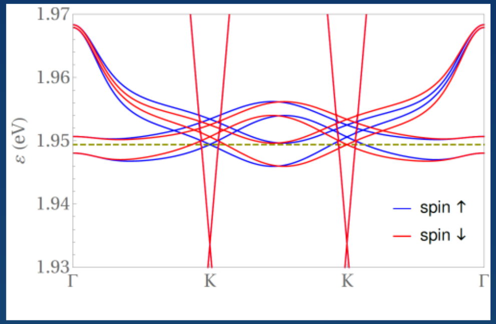


The self-consistent Hartree-Fock approach leads actually to a solution where the two spin projections have opposite sign of the valley polarization (i.e. with the exchange of the two valleys)

There is then spin-valley locking in the twisted multilayers, which opens the possibility of having Ising superconductivity, with the pairing of electrons arranged so that each spin projection is attached to a different valley.



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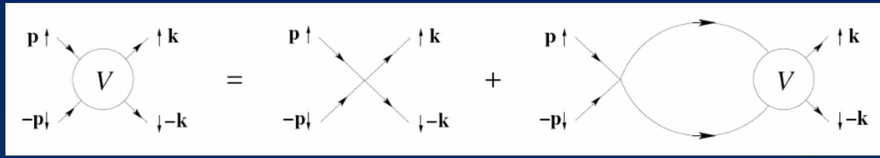
This spin-valley locking represents a strong enhancement of the small bare spin-orbit coupling, leading to spins pointing in the out-of-plane direction, and lending protection to the superconductivity against in-plane magnetic fields.

UNIVERSAL MECHANISM OF ISING SUPERCONDUCTIVITY

When we have a highly anisotropic Fermi surface, electronic instabilities may arise. Focusing on superconductivity, we have to look at the divergences in the Cooper-pair (BCS) channel



$$V(\theta,\theta';\omega) = V_0(\theta,\theta') - \frac{1}{(2\pi)^2}\int_0^{\Lambda} d\varepsilon \int_0^{2\pi} d\theta'' \frac{\partial k_\perp}{\partial \varepsilon}\frac{\partial k_\parallel}{\partial \theta''} V_0(\theta,\theta'') \frac{1}{\varepsilon - \frac{\omega}{2}} V(\theta'',\theta';\omega)$$

The self-consistent equation of the BCS vertex can be simplified by reabsorbing the density of states

$$\hat{V}(\theta,\theta';\omega) = \sqrt{\frac{1}{2\pi}\frac{\partial k_\perp(\theta)}{\partial \varepsilon}\frac{\partial k_\parallel(\theta)}{\partial \theta}}\sqrt{\frac{1}{2\pi}\frac{\partial k_\perp(\theta')}{\partial \varepsilon}\frac{\partial k_\parallel(\theta')}{\partial \theta'}}V(\theta,\theta';\omega)$$

Taking the derivative with respect to the cutoff Λ, we arrive at

$$\Lambda \frac{\partial}{\partial \Lambda}\hat{V}(\theta,\theta') = \frac{1}{2\pi}\int_0^{2\pi} d\theta'' \, \hat{V}(\theta,\theta'')\hat{V}(\theta'',\theta')$$

This equation has a divergent flow when any of the harmonics has a coefficient $\hat{V}_n < 0$, with

$$\hat{V}_n(\omega) \approx \frac{\hat{V}_n(\Lambda)}{1 + \hat{V}_n(\Lambda)\, \log\left(\frac{\Lambda}{\omega}\right)}$$

which leads to the signature of the pairing instability in the low-energy limit $\omega \to 0$.

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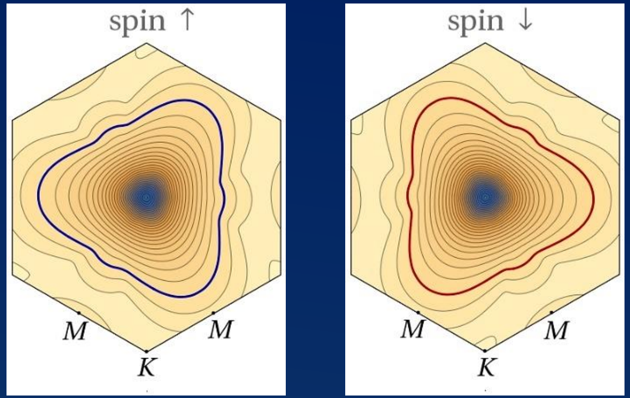
In twisted graphene multilayers, we may have a pairing instability as the scattering of the electrons in a Cooper pair has a very strong modulation along the anisotropic Fermi line



bilayer

The bare BCS vertex at the high-energy cutoff can be expressed as a sum of particle-hole contributions (in terms of the particle-hole susceptibility χ_q)

$$V_0(\phi,\phi') = v_{\boldsymbol{k}-\boldsymbol{k}'} + \frac{v_{\boldsymbol{Q}}^2\,\widetilde{\chi}_{\boldsymbol{k}+\boldsymbol{k}'}}{1 - v_{\boldsymbol{Q}}\,\widetilde{\chi}_{\boldsymbol{k}+\boldsymbol{k}'}}\,,$$

The expansion of $\hat{V}_0(\theta,\theta')$ can be grouped in terms of irreducible representations of C_{3v} ,
$A_1 \to \{\cos(3n\theta)\}$, $A_2 \to \{\sin(3n\theta)\}$, $E \to \{\cos(m\theta), \sin(m\theta)\}$ $(m \neq 3n)$

The solution of the scaling equation

$$\hat{V}_n(\omega) \approx \frac{\hat{V}_n(\Lambda)}{1 + \hat{V}_n(\Lambda)\,\log\left(\frac{\Lambda}{\omega}\right)}$$

leads to a pairing instability at the energy scale

$$\omega_c = \Lambda \exp\left(-1/\left|\hat{V}_n(\Lambda)\right|\right)$$

which is consistent with a critical temperature of ~ 1 K.

Eigenvalue λ	harmonics	Irr. Rep.
4.25	1	
2.14 2.09	$\{\cos(\phi), \sin(\phi)\}$	E
−0.43 −0.40	$\{\cos(7\phi), \sin(7\phi),$ $\cos(8\phi), \sin(8\phi)\}$	E
−0.36	$\cos(6\phi)$	A_1
0.33	$\cos(3\phi)$	A_1
0.26 0.21	$\{\cos(2\phi), \sin(2\phi),$ $\cos(5\phi), \sin(5\phi)\}$	E

J. G. and T. Stauber, arXiv:2303.00583

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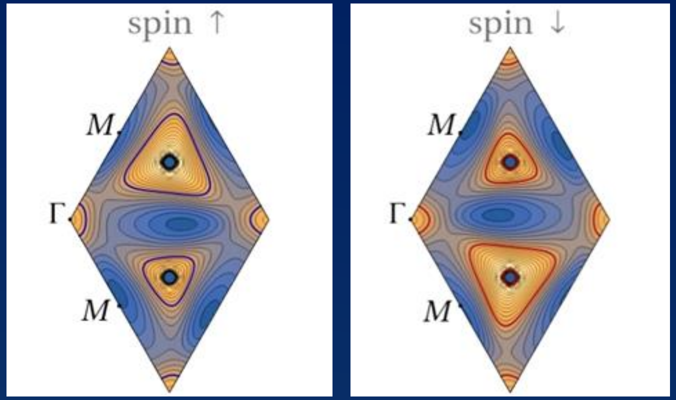

trilayer

The bare BCS vertex at the high-energy cutoff can be expressed as a sum of particle-hole contributions (in terms of the particle-hole susceptibility χ_q)

$$V_0(\phi,\phi') = v_{\boldsymbol{k}-\boldsymbol{k}'} + \frac{v_{\boldsymbol{Q}}^2\,\widetilde{\chi}_{\boldsymbol{k}+\boldsymbol{k}'}}{1 - v_{\boldsymbol{Q}}\,\widetilde{\chi}_{\boldsymbol{k}+\boldsymbol{k}'}} ,$$

The expansion of $\hat{V}_0(\theta,\theta')$ can be grouped in terms of irreducible representations of C_{3v} ,
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The solution of the scaling equation

$$\hat{V}_n(\omega) \approx \frac{\hat{V}_n(\Lambda)}{1 + \hat{V}_n(\Lambda)\,\log\left(\frac{\Lambda}{\omega}\right)}$$

leads to a pairing instability at the energy scale

$$\omega_c = \Lambda \exp\left(-1/\left|\hat{V}_n(\Lambda)\right|\right)$$

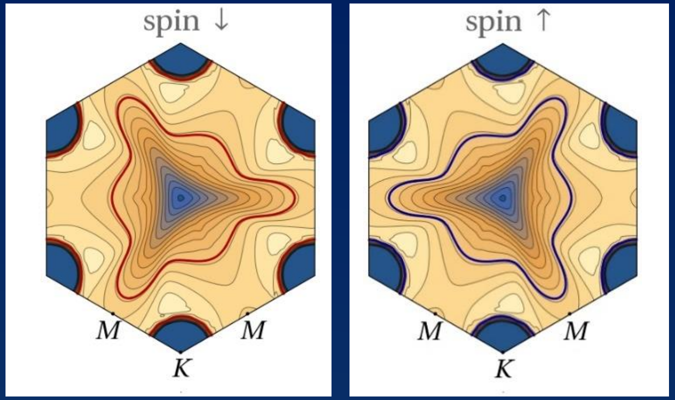
which is consistent with a critical temperature of ~ 1 K.

Eigenvalue λ	harmonics	Irr. Rep.
2.66	1	
1.80 1.80	$\{\cos(\phi), \sin(\phi)\}$	E
0.65	$\cos(3\phi)$	A_1
0.42 0.42	$\{\cos(4\phi), \sin(4\phi)\}$	E
−0.37 −0.37	$\{\cos(4\phi), \sin(4\phi)\}$	E
−0.37	$\sin(3\phi)$	A_2

J. G. and T. Stauber, arXiv:2110.11294 (to appear Nature Commun.)

UNIVERSAL MECHANISM OF ISING SUPERCONDUCTIVITY

In twisted graphene multilayers, we may have a pairing instability as the scattering of the electrons in a Cooper pair has a very strong modulation along the anisotropic Fermi line



quadrilayer

The bare BCS vertex at the high-energy cutoff can be expressed as a sum of particle-hole contributions (in terms of the particle-hole susceptibility χ_q)

$$V_0(\phi,\phi') = v_{\boldsymbol{k}-\boldsymbol{k}'} + \frac{v_{\boldsymbol{Q}}^2\,\widetilde{\chi}_{\boldsymbol{k}+\boldsymbol{k}'}}{1 - v_{\boldsymbol{Q}}\,\widetilde{\chi}_{\boldsymbol{k}+\boldsymbol{k}'}} ,$$

The expansion of $\hat{V}_0(\theta,\theta')$ can be grouped in terms of irreducible representations of C_{3v} ,
$A_1 \rightarrow \{\cos(3n\theta)\}$, $A_2 \rightarrow \{\sin(3n\theta)\}$, $E \rightarrow \{\cos(m\theta), \sin(m\theta)\}$ $(m \neq 3n)$

The solution of the scaling equation

$$\hat{V}_n(\omega) \approx \frac{\hat{V}_n(\Lambda)}{1 + \hat{V}_n(\Lambda)\,\log\left(\frac{\Lambda}{\omega}\right)}$$

leads to a pairing instability at the energy scale

$$\omega_c = \Lambda \exp\left(-1/\left|\hat{V}_n(\Lambda)\right|\right)$$

which is consistent with a critical temperature of ~ 1 K.

Eigenvalue λ	harmonics	Irr. Rep.
3.54	1	
1.40 1.39	$\{\cos(\phi), \sin(\phi),$ $\cos(2\phi), \sin(2\phi)\}$	E
0.37	$\cos(3\phi)$	A_1
−0.31 −0.30	$\{\cos(5\phi), \sin(5\phi),$ $\cos(7\phi), \sin(7\phi)\}$	E
−0.30	$\cos(6\phi)$	A_1
0.27	$\sin(6\phi)$	A_2

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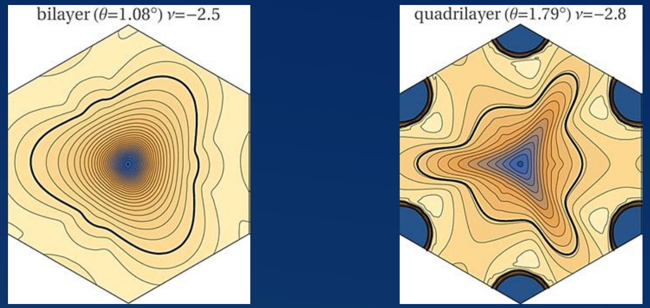
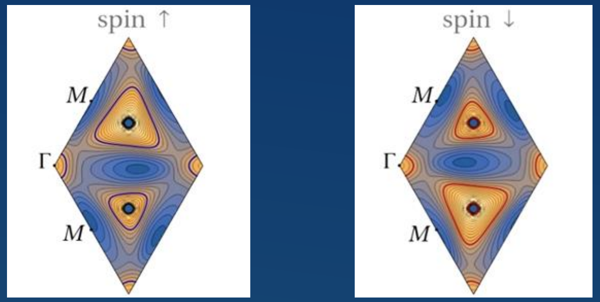
UNIVERSAL MECHANISM OF ISING SUPERCONDUCTIVITY

In conclusion,

- we have seen that the valley symmetry is spontaneously broken in twisted graphene multilayers, with the consequent breakdown of the rotational C_6 symmetry



- the breakdown of valley symmetry leads to spin-valley locking, by which the two spin projections are energetically favored at opposite valleys



(twisted trilayer graphene)

- the anisotropy in the dispersion of the second valence band gives rise to a strong modulation of the *e-e* scattering along the Fermi line, promoting a Kohn-Luttinger (pairing) instability at a critical temperature consistent with the experimental observations