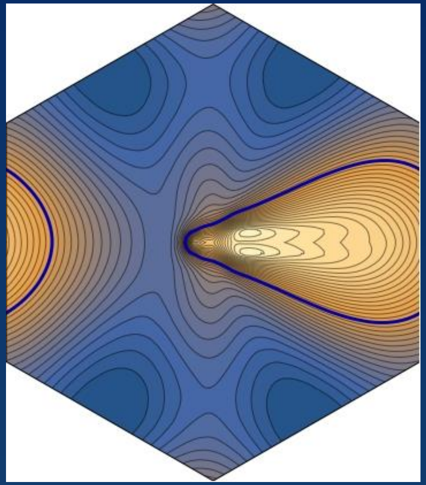
COMPETITION BETWEEN VALLEY SYMMETRY BREAKING AND INTERVALLEY COHERENCE (AND THEIR RESPECTIVE ROUTES TO KOHN-LUTTINGER SUPERCONDUCTIVITY) IN TWISTED BILAYER GRAPHENE



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VALLEY SYMMETRY BREAKING AND INTERVALLEY COHERENCE

We address the experimental signatures of different types of symmetry breaking in twisted bilayer graphene

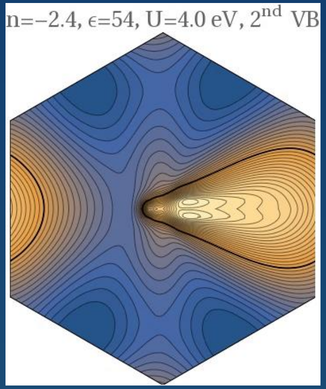
- nematicity

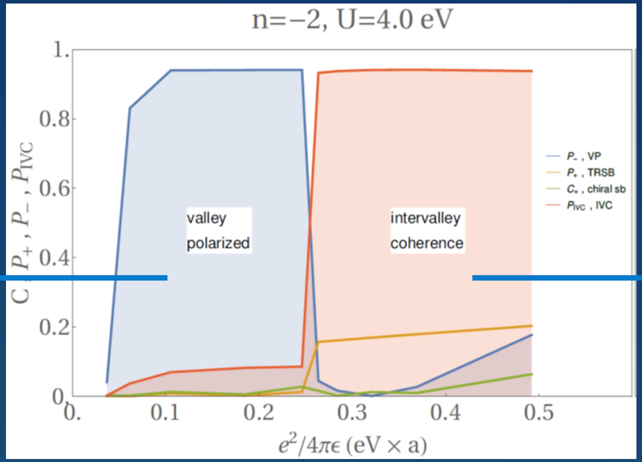
in measurements of the resistivity in superconducting samples by Y. Cao *et al.*, Science 372, 264 (2021)

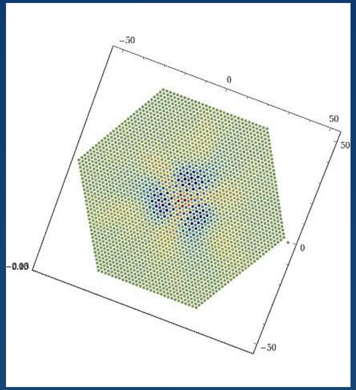
- Kekulé charge-density-wave order

in scanning tunneling microscopy experiments by K. P. Nuckolls *et al.*, Nature 620, 525 (2023)

We are going to see that it is possible to reconcile these different orders as they correspond to phases at different filling fractions and screening conditions in twisted bilayer graphene





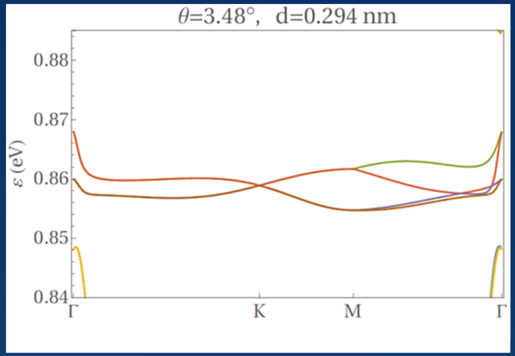


VALLEY SYMMETRY BREAKING AND INTERVALLEY COHERENCE

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

$$H_0 = -\sum_{n=1,2} t_{||}(\mathbf{r}_i - \mathbf{r}_j)\,(a^+_{n,i\sigma} a_{n,j\sigma} + \text{h.c.}) - \sum_{n\neq m} t_{\perp}(\mathbf{r}_i - \mathbf{r}_j)\,(a^+_{n,i\sigma} a_{m,j\sigma} + \text{h.c.})$$

In order to achieve an exact implementation of the method, we are going to induce flat bands by applying hydrostatic pressure, which increases the value of the magic angle



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

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

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

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

VALLEY SYMMETRY BREAKING AND INTERVALLEY COHERENCE

The noninteracting Hamiltonian H_0 can be written in terms of the eigenvalues and eigenvectors of the large tight-binding matrix

$$(H_0)_{i\sigma,j\sigma} = \sum_a \varepsilon^{(0)}_{a\sigma}\, \varphi^{(0)}_{a\sigma}(\mathbf{r}_i)\, \varphi^{(0)}_{a\sigma}(\mathbf{r}_j)^*$$

The noninteracting electron propagator G_0 becomes the inverse of H_0 in the zero-frequency (static) limit

$$(G_0)_{i\sigma,j\sigma} = -\sum_a \frac{1}{\varepsilon^{(0)}_{a\sigma}}\, \varphi^{(0)}_{a\sigma}(\mathbf{r}_i)\, \varphi^{(0)}_{a\sigma}(\mathbf{r}_j)^*$$

The Hartree-Fock approximation proceeds by assuming that the full electron propagator G has a similar representation

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

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

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

with the electron self-energy

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

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

VALLEY SYMMETRY BREAKING AND INTERVALLEY COHERENCE

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

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

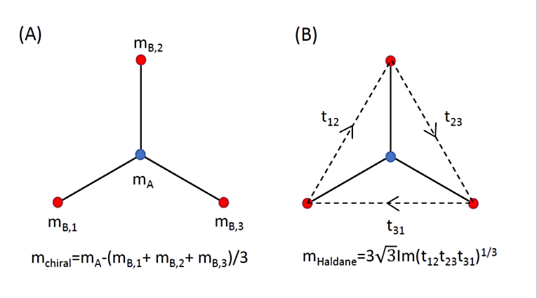
The relevant patterns of symmetry breaking are:

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

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

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

$$P_{\pm}^{(\sigma)} = \sum_{i\in A} \mathrm{Im}\,(t_{i_1 i_2}^{(\sigma)} + t_{i_2 i_3}^{(\sigma)} + t_{i_3 i_1}^{(\sigma)}) \;\pm\; \sum_{i\in B} \mathrm{Im}\,(t_{i_1 i_2}^{(\sigma)} + t_{i_2 i_3}^{(\sigma)} + t_{i_3 i_1}^{(\sigma)})$$



We have to add also the order parameters for intervalley coherence, with currents circulating along the hexagons of the carbon lattice

$$P_{\mathrm{IVC}}^{(\sigma)} = \sum_{\hexagon} \mathrm{Im}\,(t_{i_1 i_2}^{(\sigma)} + t_{i_2 i_3}^{(\sigma)} + t_{i_3 i_4}^{(\sigma)} + t_{i_4 i_5}^{(\sigma)} + t_{i_5 i_6}^{(\sigma)} + t_{i_6 i_1}^{(\sigma)})$$

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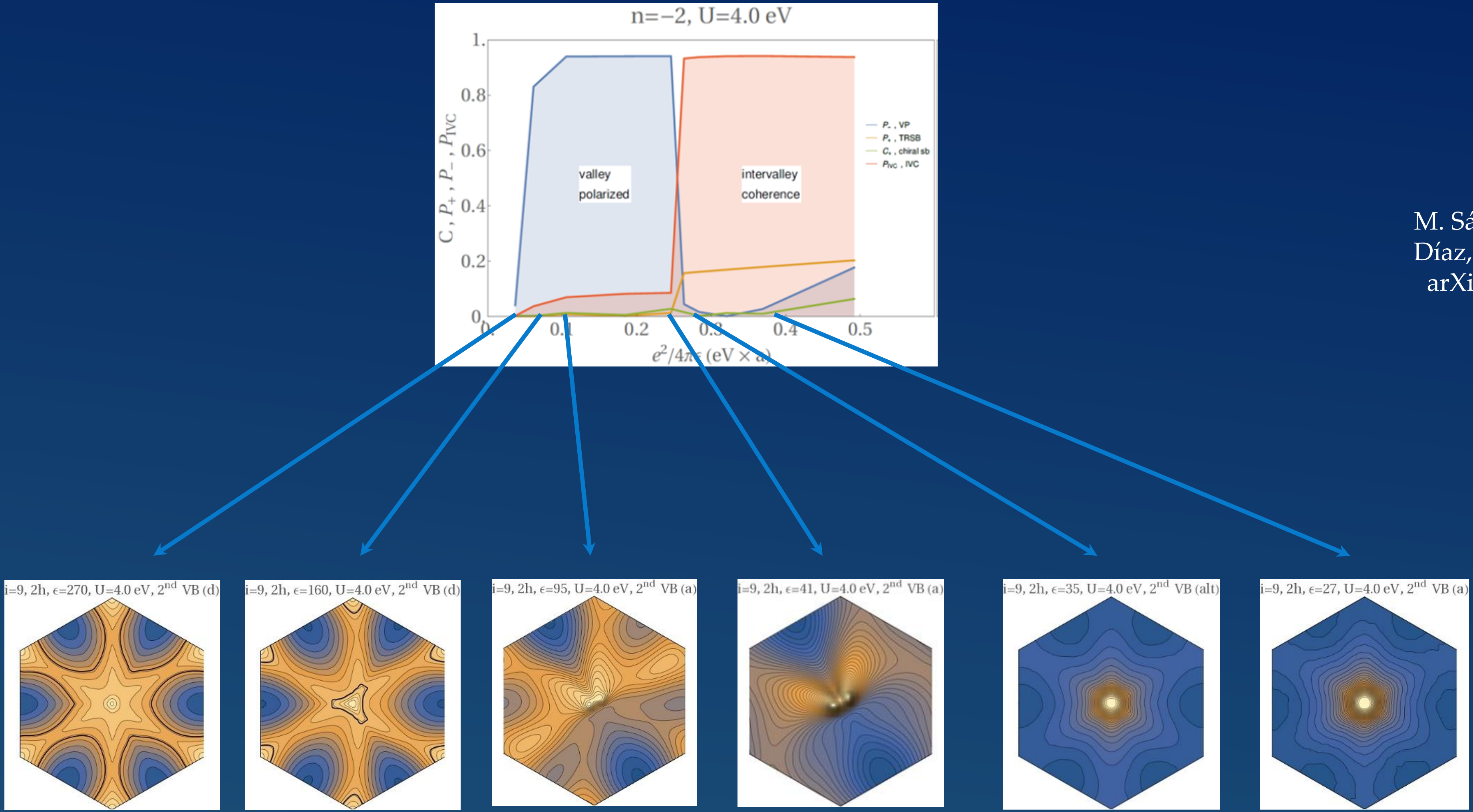
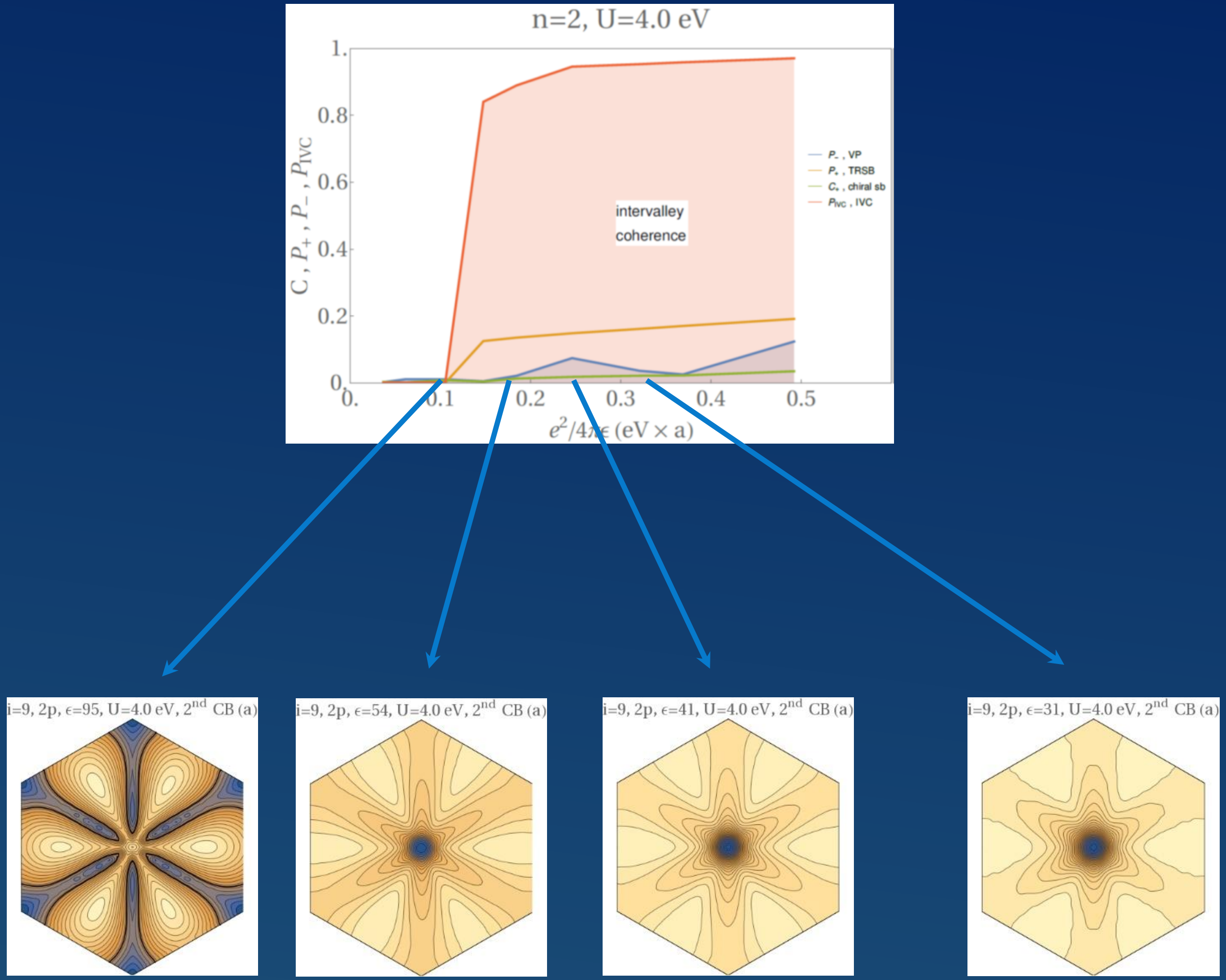
Looking at the phase diagram for filling fraction $n = -2$, we find several transitions between phases with different symmetry as the screening of the long-range Coulomb interaction is reduced



M. Sánchez-Sánchez, I. Díaz, J. G. and T. Stauber, arXiv:2403.03140

VALLEY SYMMETRY BREAKING AND INTERVALLEY COHERENCE

The dominant order parameter in the electron-doped regime at $n = 2$ corresponds to intervalley coherence, with the lowest conduction bands displaying C_6 symmetry



M. Sánchez-Sánchez, I. Díaz, J. G. and T. Stauber, arXiv:2403.03140

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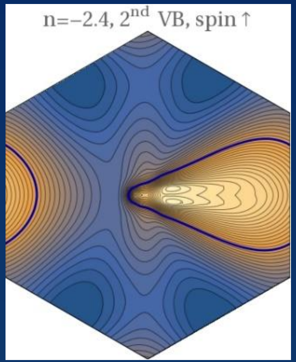
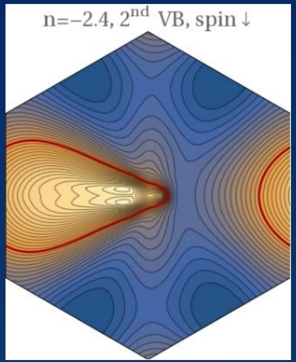
The nematicity of the hole-doped regime has an immediate effect on the superconductivity, since it comes from a valley polarized state with a Fermi line which is non-centrosymmetric

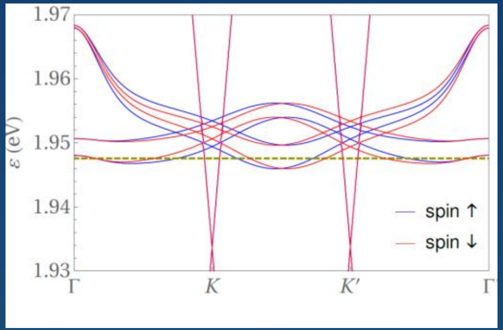




The self-consistent Hartree-Fock approach leads actually to a solution where the two spin projections have opposite sign of the valley polarization (i.e. with the exchange of the two valleys)

There is then spin-valley locking, 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.

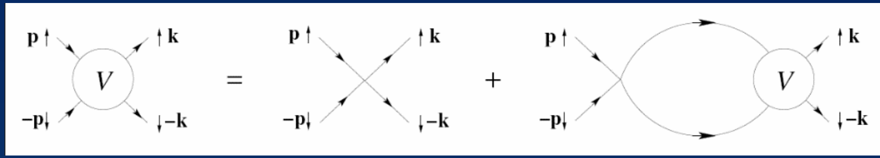
The same phenomenon has been found in twisted trilayer graphene, where the spin-valley locking leads to a strong enhancement of the small bare spin-orbit coupling, lending protection to the superconductivity against in-plane magnetic fields.



J. G. and T. Stauber, Nature Commun. 14, 2746 (2023)

VALLEY SYMMETRY BREAKING AND INTERVALLEY COHERENCE

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

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

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

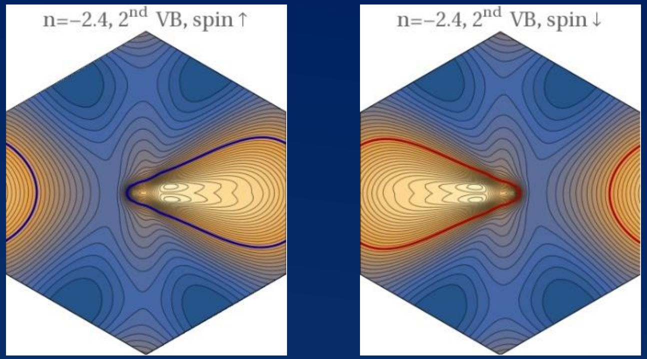
$$\Lambda \frac{\partial}{\partial \Lambda} \hat{V}(\theta,\theta') = \frac{1}{2\pi}\int_0^{2\pi} d\theta''\, \hat{V}(\theta,\theta'')\, \hat{V}(\theta'',\theta')$$

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 $\omega \to 0$.

VALLEY SYMMETRY BREAKING AND INTERVALLEY COHERENCE



In the region of nematicity, a pairing instability may arise from the strong modulation along the Fermi line of the scattering of the electrons in a Cooper pair

The bare BCS vertex at the high-energy cutoff Λ can be expressed in the RPA as an iteration of the particle-hole susceptibility χ_q

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

From the expansion of $\hat{V}_0(\theta,\theta')$ in harmonics $\cos(n\theta), \sin(n\theta)$, we may look for channels of attraction characterized by coefficients $\hat{V}_n < 0$.

Then, the solution of the scaling equation

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

has a singularity 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.
2.12	1	
0.51	$\sin(\phi)$	A''
0.38	$\cos(\phi)$	A'
−0.19	$\sin(4\phi)$	A''
0.18	$\sin(2\phi)$	A''
−0.12	$\cos(6\phi)$	A'

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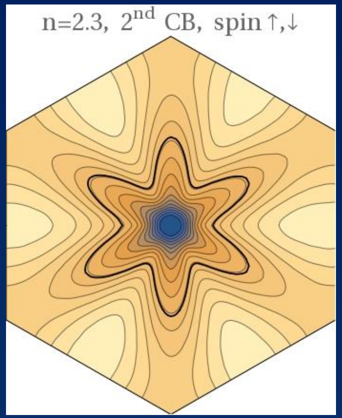
VALLEY SYMMETRY BREAKING AND INTERVALLEY COHERENCE



In the electron-doped regime, the electrons in the Cooper pair share the same centrosymmetric Fermi line, also with a strong modulation of the electron scattering

The bare BCS vertex at the high-energy cutoff Λ can be expressed again in the RPA as an iteration of the particle-hole susceptibility χ_q

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

From the expansion of $\hat{V}_0(\theta,\theta')$ in irreducible representations of the C_{6v} group, we may look for channels of attraction with coefficients $\hat{V}_n < 0$.

Then, the solution of the scaling equation

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

has a singularity 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.
3.47	1	
0.89 0.82	$\{\cos(\phi), \sin(\phi)\}$	E_2
0.30 0.29	$\{\cos(2\phi), \sin(2\phi)\}$	E_1
0.18	$\sin(3\phi)$	B_2
−0.17	$\cos(3\phi)$	B_1

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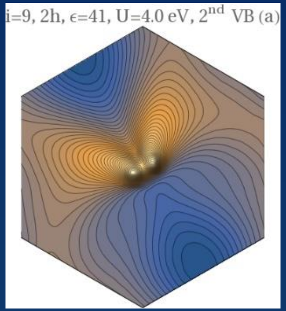
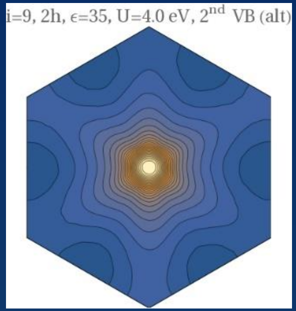
VALLEY SYMMETRY BREAKING AND INTERVALLEY COHERENCE

In conclusion,

- ➢ we have found that twisted bilayer graphene may have phases with nematicity and Kekulé order, but excluding each other as they correspond to different ranges in the screening of the Coulomb interaction





- ➢ nematicity is only present in the hole-doped regime, which means that there the (Ising) superconductivity must have different properties compared to the conventional superconductivity in the electron-doped regime