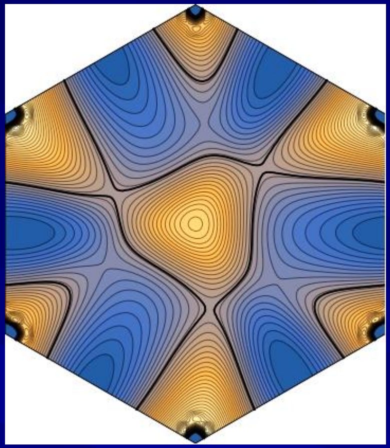
p-WAVE SUPERCONDUCTIVITY FROM VALLEY SYMMETRY BREAKING IN TWISTED TRILAYER GRAPHENE



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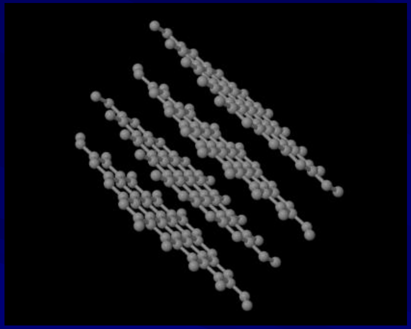
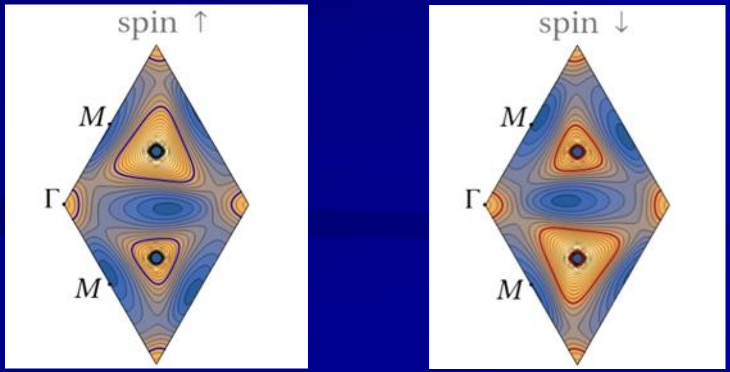
SUPERCONDUCTIVITY IN TWISTED TRILAYER GRAPHENE

Recently there have been consistent observations of superconductivity in twisted graphene trilayers, quadrilayers, pentalayers (in setups with alternating twist angle θ , $-\theta$, θ , $-\theta$ …), 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)
- J. M. Park *et al.*, Nature 595, 526 (2021)
- Y. Zhang *et al.*, arXiv:2112.09270
- J. M. Park *et al.*, arXiv:2112.10760

In the case of twisted trilayer graphene, 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



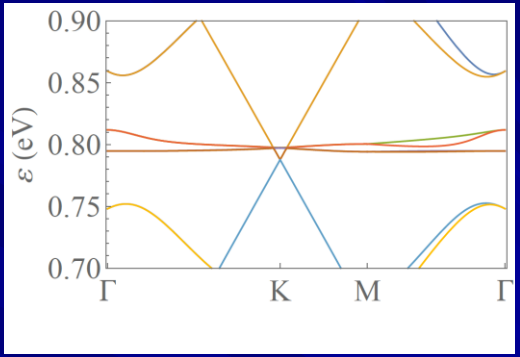
SUPERCONDUCTIVITY IN TWISTED TRILAYER GRAPHENE

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

$$H_0 = -\sum_{n=1}^{3} t_{\parallel}(\mathbf{r}_i - \mathbf{r}_j)\,(a^{+}_{n,i}a_{n,j} + \mathrm{h.c.}) - \sum_{n\neq m} t_{\perp}(\mathbf{r}_i - \mathbf{r}_j)\,(a^{+}_{n,i}a_{m,j} + \mathrm{h.c.})$$

In the case of twisted trilayer graphene with alternating twist angle, approximately flat bands are found for $\theta \approx 1.6°$ (taking also into account out-of-plane relaxation)



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

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

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

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

SUPERCONDUCTIVITY IN TWISTED TRILAYER GRAPHENE

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

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

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

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

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

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

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

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

with the electron self-energy Σ

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

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

SUPERCONDUCTIVITY IN TWISTED TRILAYER GRAPHENE

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 patterns of symmetry breaking which arise in twisted trilayer graphene are:

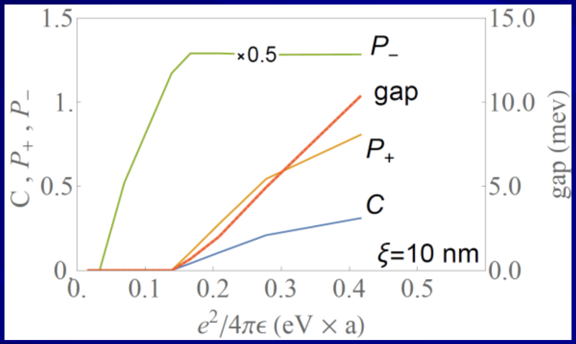
- chiral symmetry breaking characterized by staggered charge order in sublattices A and B

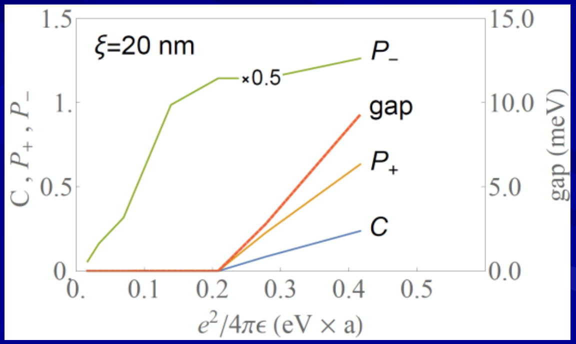
$$C^{(\sigma)} = \sum_{i\in A} h_{ii}^{(\sigma)} - \sum_{i\in B} h_{ii}^{(\sigma)}$$

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

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

2-hole doping





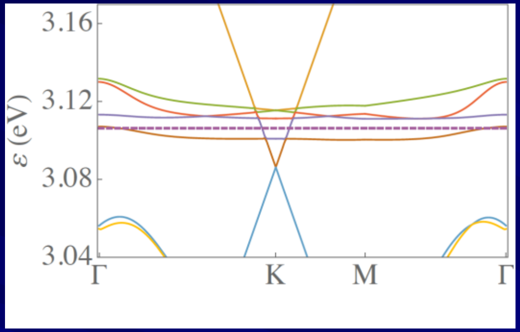
The dominant order parameter corresponds to valley symmetry breaking with $P_- \neq 0$

J. G. and T. Stauber, arXiv:2110.11294

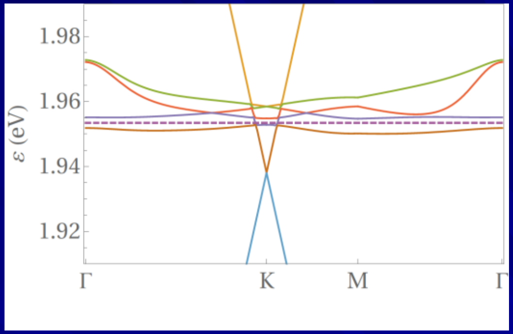
SUPERCONDUCTIVITY IN TWISTED TRILAYER GRAPHENE

The spontaneous breakdown of valley symmetry has important consequences, since at $\nu = -2$ it places the Fermi level between the first and the second valence band, where a sufficiently strong interaction can open a gap

$\epsilon = 24$

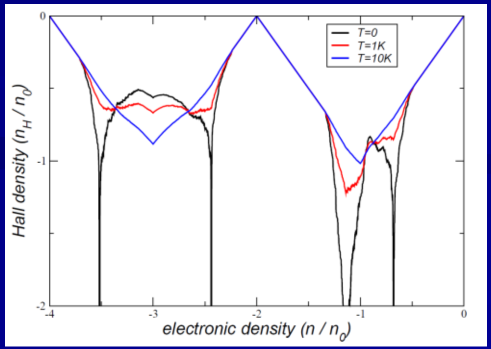


$\epsilon = 48$



The gap between the first two valence bands has an interesting experimental signature, which is the reset of the Hall density at $\nu = -2$.

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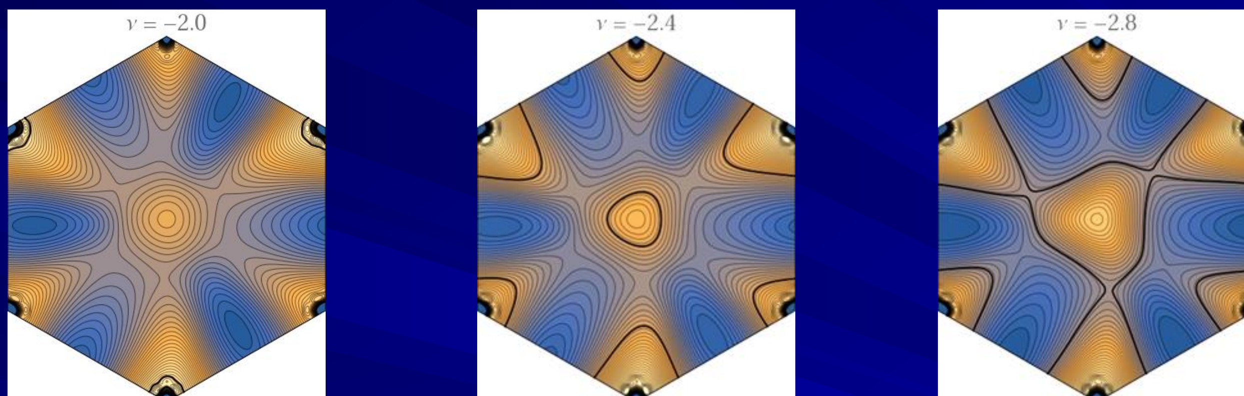
The other important consequence of valley symmetry breaking is the reduction of symmetry from C_6 to C_3, since this latter group is the one operating in a single graphene valley.

We can observe the reduction of symmetry in the plot of the second valence band in the Brillouin zone, for different values of the filling fraction



$\epsilon = 48$

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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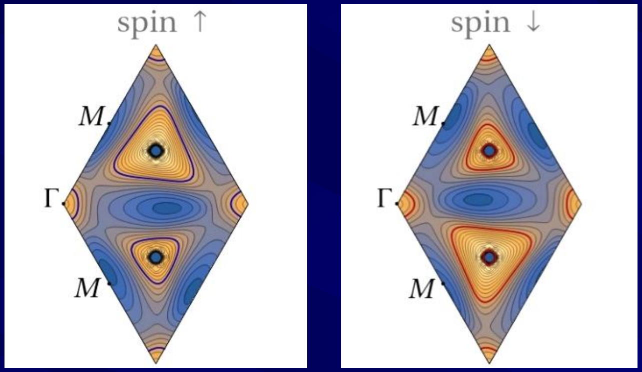


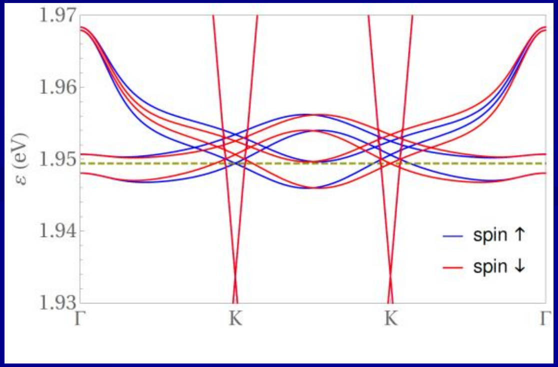
The self-consistent Hartree-Fock approach leads actually to a solution where the two spin projections have opposite sign of the valley symmetry breaking (i.e. with exchange of the two valleys)

There is then spin-valley locking in twisted trilayer graphene, which opens the possibility of having a (so-called) Ising superconductivity. The pairing of electrons takes place with each spin projection attached to a different valley of the trilayer.

This protects the superconductivity against magnetic fields, since there is a gap between the bands for the two spin projections at each valley

$\nu = -2.4$

$\epsilon = 48$



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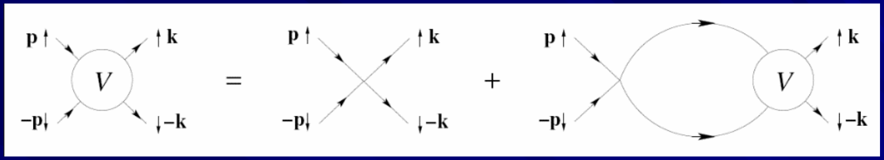
SUPERCONDUCTIVITY IN TWISTED TRILAYER GRAPHENE

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

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

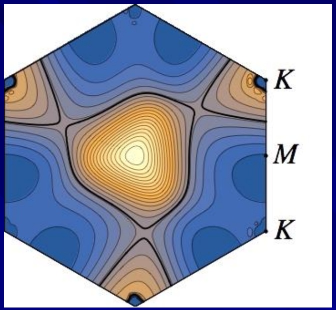
This equation has a divergent flow when any of the harmonics has a coefficient $\hat{V}_n < 0$, with

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

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

SUPERCONDUCTIVITY IN TWISTED TRILAYER GRAPHENE

In twisted trilayer graphene, 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



$\nu = -2.4$

$\epsilon = 24$

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)

$$V_0(\phi, \phi') = U + \frac{U^2 \chi_{\boldsymbol{k}+\boldsymbol{k}'}}{1 - U\chi_{\boldsymbol{k}+\boldsymbol{k}'}} + \frac{U^3 \chi^2_{\boldsymbol{k}-\boldsymbol{k}'}}{1 - U^2 \chi^2_{\boldsymbol{k}-\boldsymbol{k}'}}$$

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

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.
0.75 0.73	$\{\cos(2\phi), \sin(2\phi)\}$	E
0.35 0.32	$\{\cos(4\phi), \sin(4\phi)\}$	E
-0.23 -0.22	$\{\cos(\phi), \sin(\phi)\}$	E
0.21	$\cos(6\phi)$	A_1
0.17	$\sin(6\phi)$	A_2
-0.15	$\cos(3\phi)$	A_1

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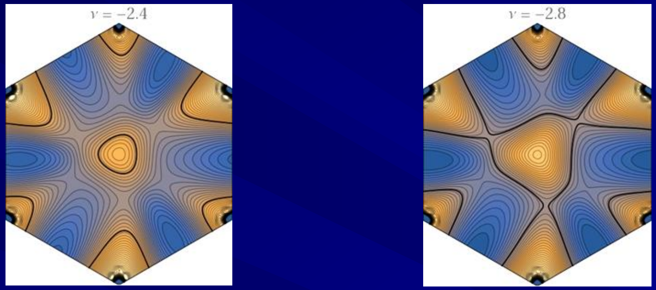
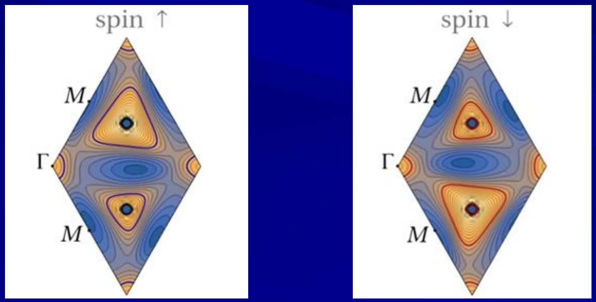
SUPERCONDUCTIVITY IN TWISTED TRILAYER GRAPHENE

In conclusion,

- we have seen that the valley symmetry is spontaneously broken in twisted trilayer graphene, in the hole-doped regime relevant for superconductivity



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



- 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 instability at a critical temperature consistent with the experimental observations