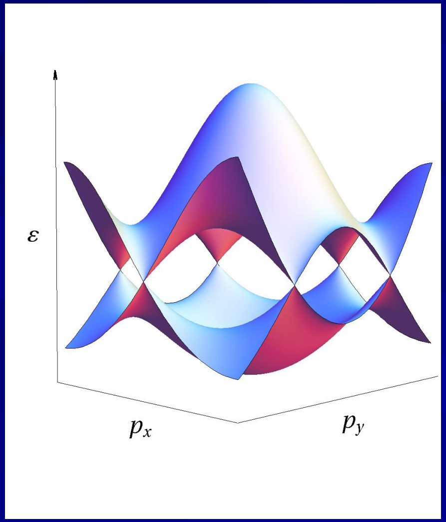
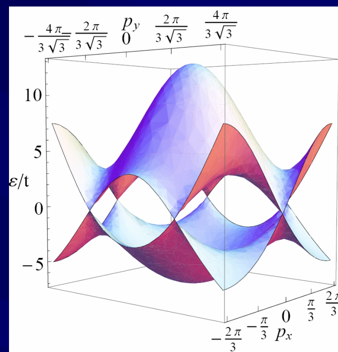
MAGNETIC AND KOHN-LUTTINGER INSTABILITIES NEAR A VAN HOVE SINGULARITY: MONOLAYER VERSUS TWISTED BILAYER GRAPHENE



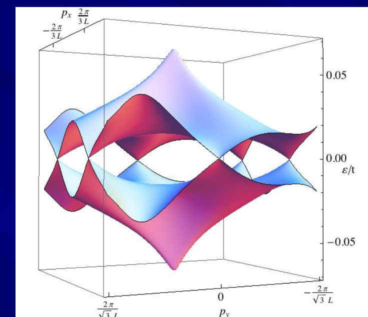
J. González
Instituto de Estructura de la Materia, CSIC, Spain

MAGNETIC AND KOHN-LUTTINGER INSTABILITIES

2D electron systems have saddle points in their momentum dispersion (Van Hove singularities in the spectrum) that offer the possibility of inducing large electronic correlations

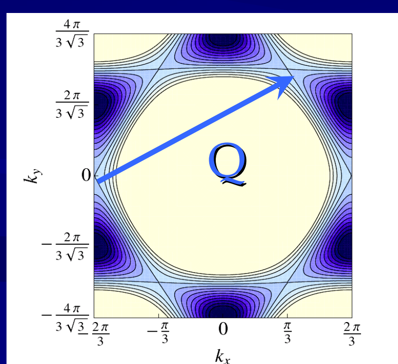


monolayer graphene



twisted graphene bilayer

The divergent density of states gives rise to large susceptibilities at certain momenta, depending on the parameters of the saddle point $\varepsilon(\mathbf{\delta k}) \approx -\alpha\, \delta k_x^2 + \beta\, \delta k_y^2$:



$$\chi_{\rm ph}(\mathbf{0},\omega) \approx \frac{1}{4\pi^2}\frac{1}{\sqrt{\alpha\beta}}\log\left(\frac{\Lambda_0}{|\omega|}\right)$$

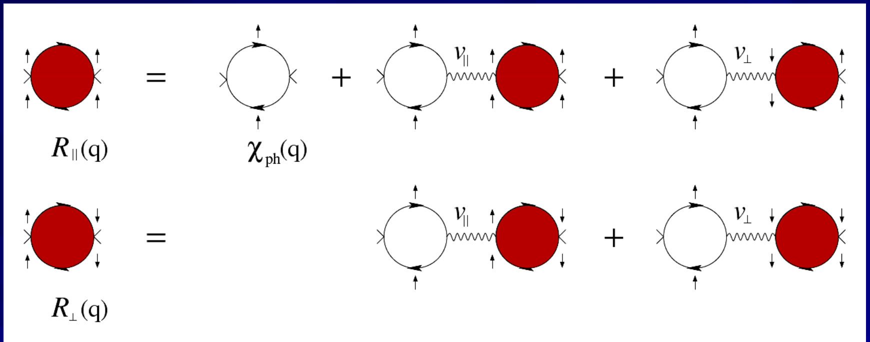
$$\chi_{\rm ph}(\mathbf{Q},\omega) \approx \frac{1}{2\sqrt{3}\pi^2}\frac{1}{\alpha+\beta}\log\left(\frac{(1+\sqrt{\beta/3\alpha})(1+\sqrt{3\beta/\alpha})}{(1-\sqrt{\beta/3\alpha})(1-\sqrt{3\beta/\alpha})}\right)\log\left(\frac{\Lambda_0}{|\omega|}\right)$$

$$\chi_{\rm pp}(\mathbf{0},\omega) \approx \frac{1}{4\pi^2}\frac{1}{\sqrt{\alpha\beta}}\log^2\left(\frac{\Lambda_0}{|\omega|}\right)$$

(J. G, Phys. Rev. B **78**, 205431 (2008))

MAGNETIC AND KOHN-LUTTINGER INSTABILITIES

One of the possible instabilities in the system corresponds to the tendency to spin order. Taking formally the limit of large number N of fermion flavors, the dominant contributions to the response functions are given by the iteration in the exchange of electron-hole pairs:



The resolution of the self-consistent equations leads to the expressions

$$R_{\mathrm{charge}}(\mathbf{q},\omega) = \frac{2N\,\chi_{\mathrm{ph}}(\mathbf{q},\omega)}{1+N\left(v_{\parallel}(\mathbf{q})+v_{\perp}(\mathbf{q})\right)\chi_{\mathrm{ph}}(\mathbf{q},\omega)}$$

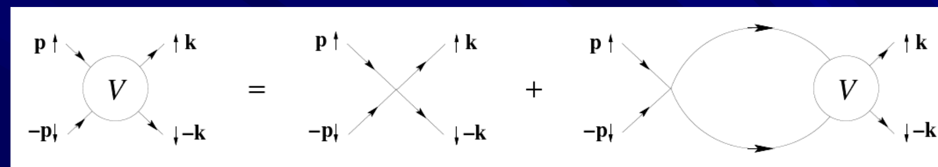
$$R_{\mathrm{spin}}(\mathbf{q},\omega) = \frac{2N\,\chi_{\mathrm{ph}}(\mathbf{q},\omega)}{1+N\left(v_{\parallel}(\mathbf{q})-v_{\perp}(\mathbf{q})\right)\chi_{\mathrm{ph}}(\mathbf{q},\omega)}$$

Under conditions such that $v_{\parallel}(\mathbf{q}) < v_{\perp}(\mathbf{q})$, we find an instability in the system at

$$\omega_c \approx \Lambda_0 \exp\left(-\frac{4\pi^2\sqrt{\alpha\beta}}{N\,(v_{\perp}-v_{\parallel})} \right)$$

MAGNETIC AND KOHN-LUTTINGER INSTABILITIES

We also have another potential instability in the Cooper-pair channel, for colliding particles with zero total momentum:



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

The self-consistent equation can be solved by reabsorbing the local density of states in the BCS vertex

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

and then expanding in a basis of the modes for the different irreducible representations γ of the point symmetry group

$$\hat{V}(\theta,\theta';\omega) = \sum_{\gamma,m,n} V^{(\gamma)}_{m,n}\ \Psi^{(\gamma)}_m(\theta)\,\Psi^{(\gamma)}_n(\theta')$$

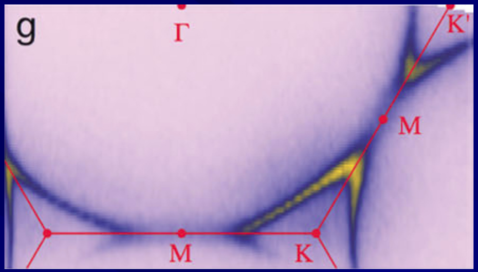
The different couplings admit a solution in terms of the initial condition $V_0^{(\gamma)}$:

$$V^{(\gamma)}(\omega) = \frac{V_0^{(\gamma)}}{1 + V_0^{(\gamma)}\log\left(\frac{\Lambda}{\omega}\right)}$$

(W. Kohn and J. M. Luttinger, PRL **15**, 524 (1965); M. Baranov, A. Chubukov and M. Kagan, IJMP B **6**, 2471 (1992))

MONOLAYER GRAPHENE

In the case of graphene, the dispersion around the saddle points in the conduction band has been already mapped

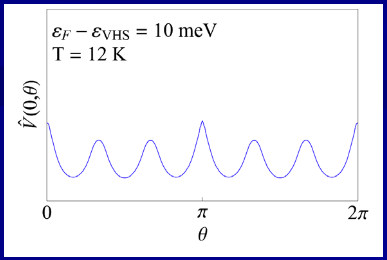


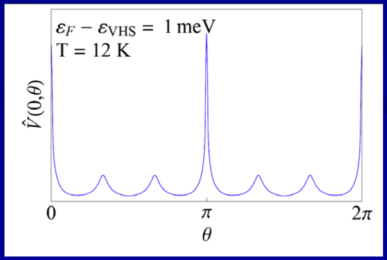
J. L. McChesney *et al.*,
Phys. Rev. Lett. **104**, 136803 (2010)

The BCS vertex can be expanded in the modes for the different irreducible representations $\{\cos(6n\theta)\}$, $\{\sin(6n\theta)\}$, $\{\cos((6n+3)\theta)\}$, $\{\sin((6n+3)\theta)\}$, $n \in \mathbb{Z}$, and $\{\cos(m\theta), \sin(m\theta)\}$, $m \neq 3p$:

$$\hat{V}(\theta,\theta') = V_{0,0} + \sqrt{2}V_{0,6}\left(\cos(6\theta)+\cos(6\theta')\right) + V_{2,2}\left(\cos(2\theta)\cos(2\theta')+\sin(2\theta)\sin(2\theta')\right)$$
$$+ V_{2,4}\left(\cos(2\theta)\cos(4\theta')-\sin(2\theta)\sin(4\theta')+\theta\leftrightarrow\theta'\right) + V_{3,3}\left(\sin(3\theta)\sin(3\theta')\right) + V'_{3,3}\left(\cos(3\theta)\cos(3\theta')\right) + \ldots$$

For nested Fermi lines the dominant negative coupling is found in a *d*-wave channel (J. G., Phys. Rev. B **78**, 205431 (2008); R. Nandkishore, L. Levitov and A. Chubukov, Nature Phys. **8**, 158 (2012)), but here the extended character of the saddle points leads to dominant negative values of $V_{3,3}$





$$\hat{V}(\pi/6,\pi/6) - \hat{V}(\pi/2,-\pi/2) \approx 4\hat{V}_{3,3} < 0$$

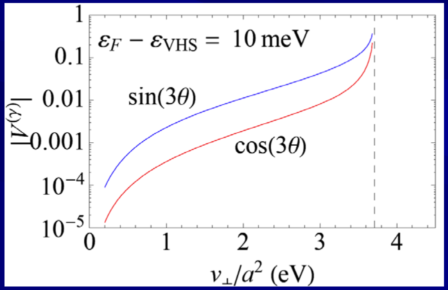
MONOLAYER GRAPHENE

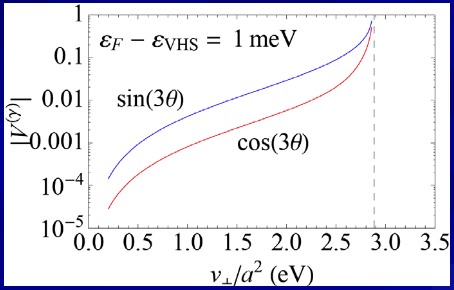
The strong screening effects from the divergent density of states at the Van Hove singularity lead to an effective Hubbard interaction $v_\perp$, and the bare BCS vertex can be expressed in the RPA as

$$\widehat{V}_0(\theta,\theta') = F(\theta)F(\theta')\left(v_\perp + \frac{v_\perp^2 \chi_{\rm ph}(\mathbf{k}+\mathbf{k}')}{1 - v_\perp \chi_{\rm ph}(\mathbf{k}+\mathbf{k}')} + \frac{v_\perp^3 \chi_{\rm ph}^2(\mathbf{k}-\mathbf{k}')}{1 - v_\perp^2 \chi_{\rm ph}^2(\mathbf{k}-\mathbf{k}')}\right) \qquad F(\theta) = \sqrt{\frac{1}{2\pi}\frac{\partial k_\perp(\theta)}{\partial \varepsilon}\frac{\partial k_\parallel(\theta)}{\partial \theta}}$$

$$V_{m,n}^{(\gamma)} = \frac{1}{(2\pi)^2}\int_0^{2\pi} d\theta \int_0^{2\pi} d\theta' \widehat{V}(\theta,\theta')\Psi_m^{(\gamma)}(\theta)\Psi_n^{(\gamma)}(\theta')$$

The extended character of the Van Hove singularity leads to a divergence of the negative BCS couplings at the point of the singularity that the bare vertex has in the RPA:





J. L. McChesney *et al.*, PRL **104**, 136803 (2010); J. G., PRB **88**, 125434 (2013)

This means that the pairing instability is triggered in the *f*-wave channel at

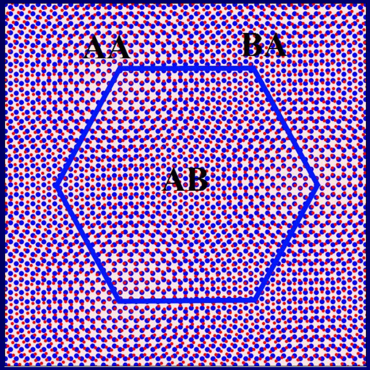
$$k_B T_c \approx \Lambda_0 \exp\left(-\frac{1}{|V^{(\gamma)}|}\right)$$

before a magnetic instability can take place at vanishing momentum.

(reminiscent of the *f*-wave pairing found in the honeycomb lattice by M. Kiesel *et al.*, PRB **86**, 020507 (2012))

TWISTED GRAPHENE BILAYER

In the case of the twisted graphene bilayers, we have low-energy saddle points in a reduced Brillouin zone, arising from the superlattice of the bilayer

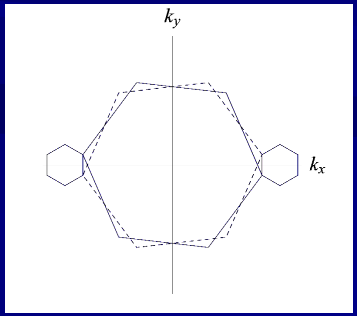


commensurate lattices at twist angles

$$\theta = \arccos\left(\frac{1}{2}\frac{n^2+m^2+4mn}{n^2+m^2+mn}\right)$$

We have commensurate lattices labeled by a pair of integers (n,m) , with a sequence $(n,n+1)$ of superlattices with increasing period $L_n = (3n^2 + 3n + 1)^{1/2}$

The electronic spectrum can be obtained by taking into account the hybridization of the Dirac cones split by the relative rotation of the two carbon layers

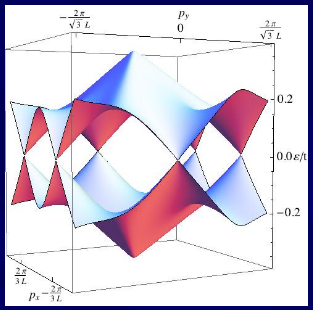


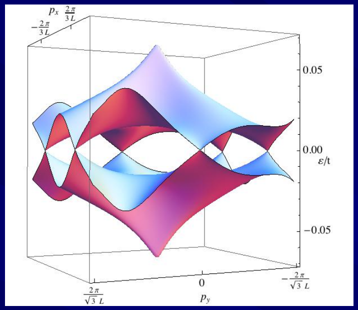
$$H = v_F\begin{pmatrix} 0 & -i(\partial_x - i\partial_y) + i\Delta K/2 & V_{AA'}(\mathbf{r}) & V_{AB'}(\mathbf{r}) \\ -i(\partial_x + i\partial_y) - i\Delta K/2 & 0 & V_{BA'}(\mathbf{r}) & V_{BB'}(\mathbf{r}) \\ V^*_{AA'}(\mathbf{r}) & V^*_{BA'}(\mathbf{r}) & 0 & -i(\partial_x - i\partial_y) - i\Delta K/2 \\ V^*_{AB'}(\mathbf{r}) & V^*_{BB'}(\mathbf{r}) & -i(\partial_x + i\partial_y) + i\Delta K/2 & 0 \end{pmatrix}$$

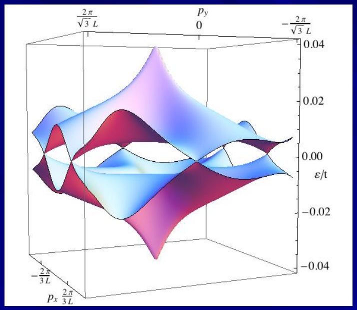
TWISTED GRAPHENE BILAYER

The dispersion of the lowest subband shows saddle points midway each pair of Dirac cones,

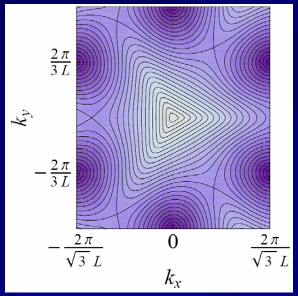
$n = 10$ $n = 22$ $n = 25$

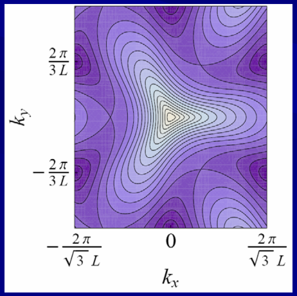


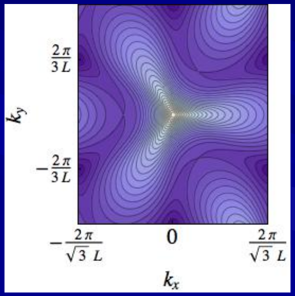




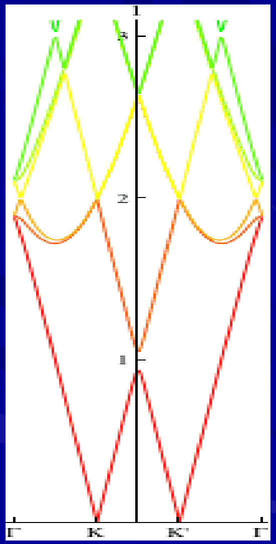
The shape of the dispersion deviates progressively from C_{6v} symmetry as the period L of the superlattice increases







$n = 10$ $n = 22$ $n = 25$



and the lowest subband gets narrower, being almost flat at a sequence of "magic" twist angles

(R. Bistritzer and A. H. MacDonald, PNAS **108**, 12233 (2011); P. San-José, J. G. and F. Guinea, PRL **108**, 216802 (2012))

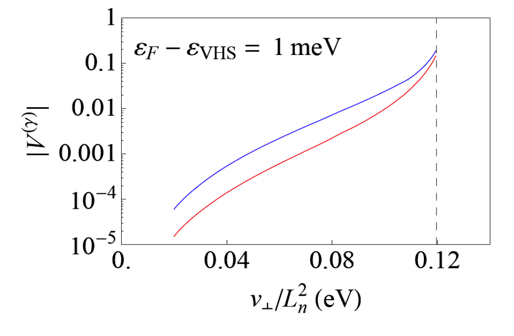
TWISTED GRAPHENE BILAYER

The BCS couplings can be obtained again from the projection of the BCS vertex in the channels corresponding to the different representations of the symmetry group

$$\widehat{V}_0(\theta,\theta') = F(\theta)F(\theta')\left(v_\perp + \frac{v_\perp^2 \chi_{\rm ph}(\mathbf{k}+\mathbf{k}')}{1 - v_\perp \chi_{\rm ph}(\mathbf{k}+\mathbf{k}')} + \frac{v_\perp^3 \chi_{\rm ph}^2(\mathbf{k}-\mathbf{k}')}{1 - v_\perp^2 \chi_{\rm ph}^2(\mathbf{k}-\mathbf{k}')}\right) \qquad F(\theta) = \sqrt{\frac{1}{2\pi}\frac{\partial k_\perp(\theta)}{\partial \varepsilon}\frac{\partial k_\parallel(\theta)}{\partial \theta}}$$

$$V_{m,n}^{(\gamma)} = \frac{1}{(2\pi)^2}\int_0^{2\pi} d\theta \int_0^{2\pi} d\theta' \widehat{V}(\theta,\theta')\Psi_m^{(\gamma)}(\theta)\Psi_n^{(\gamma)}(\theta')$$

In this case the absence of extended saddle points in the dispersion leads to BCS couplings that do not grow large near the point of the magnetic instability



For a twisted bilayer with $n = 10$ and $L_n^2 \approx 340\, a_0^2$, we can estimate $v_\perp / L_n^2 \approx 10\,\text{eV}/340 \sim 0.03\,\text{eV}$, which corresponds to very small BCS couplings near the Van Hove singularity.

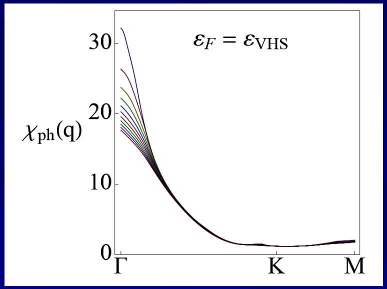
TWISTED GRAPHENE BILAYER

The spin response function

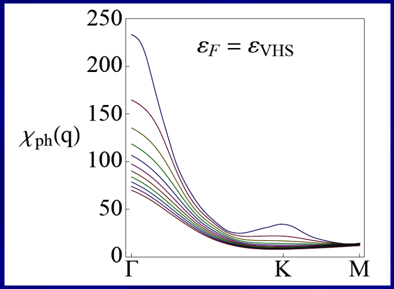
$$R_{\text{spin}}(\mathbf{q},\omega) = \frac{2N\,\chi_{\text{ph}}(\mathbf{q},\omega)}{1 + N\big(v_{\|}(\mathbf{q}) - v_{\perp}(\mathbf{q})\big)\chi_{\text{ph}}(\mathbf{q},\omega)}$$

may still diverge for doping levels close to the Van Hove singularity, since the susceptibility $\chi(\mathbf{0},\omega)$ grows large in the limit of low temperature, as shown in the figures (for $k_B T = 0.1$, 0.5, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5 and 5.0 meV) :

$n = 10$

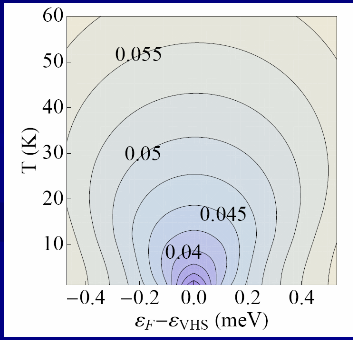


$n = 22$

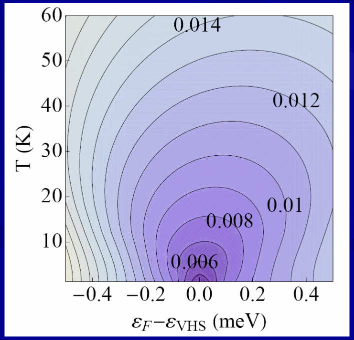


Sufficiently close to the singularity, for a given T there is some critical value of the coupling at which the response function R_{spin} blows up, as shown in the contour plots for $v_{\perp}/L_n^2$ (in eV) :

$n = 10$



$n = 22$



(J. G, Phys. Rev. B 88, 125434 (2013))

estimated couplings: $v_{\perp}/L_n^2 \sim 0.03$ eV $\quad v_{\perp}/L_n^2 \sim 0.007$ eV

MAGNETIC AND KOHN-LUTTINGER INSTABILITIES

We may think of different imperfections that can weaken the Van Hove singularity:

- Vacancies or voids. They give rise to features preferentially close to the Dirac point.
- Substitutional impurities. The effects of disorder are enhanced by the nesting of the Fermi line, and the Van Hove singularity is attenuated by logarithmic corrections,

$$n(\Lambda) \approx n^{(0)}(\Lambda)\left(1-\frac{1}{2\pi\, t\tau_\pi}\log\left(\frac{1}{4\tau_\pi|\varepsilon|}\right)+\ldots\right)$$

  where τ_π is the relaxation time in the impurity scattering.
  However, in clean graphene samples where the mean free path is above the micron scale, we have $t\tau_\pi \sim 10^4$

- Ripples. They can act as an intrinsic source of scattering, modulating the hopping in the graphene lattice. This may induce a splitting of the Van Hove singularity by an energy

$$\Delta\varepsilon \sim t\,(a_{C-C}/R)^2$$

  R being the radius of curvature of the ripples.

  However, R is typically above the scale of 10 nm, giving rise to a splitting of the order of ~ 0.1 meV , which is ineffective to attenuate the strength of the singularity.

In conclusion

- we have seen that a Van Hove singularity may induce in general spin and pairing instabilities, with different strengths depending on the particular geometry of the saddle points
- in the case of the Van Hove singularity in the conduction band of graphene, the extended character of the saddle points leads to a dominant pairing instability, that arises in a channel with *f*-wave symmetry
- twisted graphene bilayers have Van Hove singularities at much lower energy but the reduced symmetry of the dispersion precludes the development of any significant pairing instability, while a spin instability is favored instead by the trend towards narrow lowest subbands