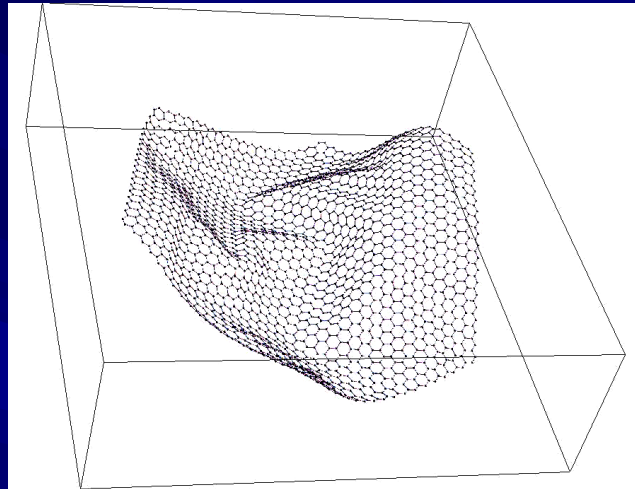


INTERPLAY OF ELECTRONIC EXCITATIONS AND FLEXURAL PHONONS IN GRAPHENE



J. González and P. San-José
Instituto de Estructura de la Materia, CSIC, Spain

(work in collaboration with F. Guinea)

Outline

- Stability of crystalline membranes
- Metallic crystalline membranes (graphene)
- Renormalization of elastic properties (self-consistent)
- Renormalization of elastic properties (scaling approach)
- Phase diagram of metallic membranes

RIPPLES AND OUT-OF-PLANE PHONONS IN GRAPHENE

- One of the most intriguing properties of graphene is its tendency to develop ripples, which are viewed as an imprint of the large fluctuations of the 2D material (A. Fasolino, J. H. Los and M. I. Katsnelson, *Nature Mat.* **6**, 858 (2007)).
- Ripples are supposed to have a significant impact on the electronic transport properties (M. I. Katsnelson and A. K. Geim, *Phil. Trans. Royal Soc. A* **366**, 195 (2008)).
- More generally, it has been shown that the scattering with flexural phonons may reduce the lifetime of electron quasiparticles in graphene (E. Mariani and F. von Oppen, *Phys. Rev. Lett.* **100**, 076801 (2008)).

What is the reverse effect of electrons on flexural phonons in graphene?

- There have been partial approaches in which the electron charge density is coupled to the flexural phonons (D. Gazit, *Phys. Rev. B* **79**, 113411 (2009), J. González and E. Perfetto, *New J. Phys.* **11**, 095015 (2009), D. Gazit, *Phys. Rev. B* **80**, 161406(R) (2009)).

STABILITY OF CRYSTALLINE MEMBRANES

(D. R. Nelson and L. Peliti, J. Physique **48**, 1085 (1987))

For a vector field of displacements of the membrane (u_1, u_2, h) , we have the strain tensor

$$u_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i + \partial_i h \partial_j h)$$

The free energy has bending and stretching terms

$$F = \underbrace{\frac{1}{2} \kappa \int d^2 x (\nabla^2 h)^2}_{\text{bending}} + \underbrace{\frac{1}{2} \int d^2 x (2\mu \text{Tr}(u_{ij}^2) + \lambda (\text{Tr } u_{ij})^2)}_{\text{stretching}}$$

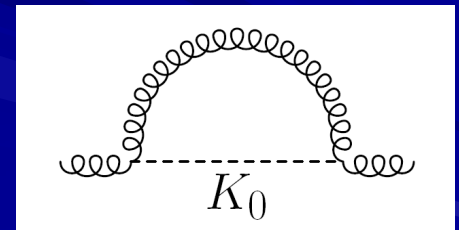
After integrating the in-plane phonon fields

$$F = \frac{1}{2} \kappa \int d^2 x (\nabla^2 h)^2 + \frac{1}{2} K_0 \int d^2 x \left(\frac{1}{2} P_{ij}^T \partial_i h \partial_j h \right)^2, \quad K_0 = \frac{4\mu(\mu + \lambda)}{2\mu + \lambda}$$

This is now an interacting theory, with important self-energy corrections

$$(\varepsilon(\mathbf{p}))^2 = \kappa_0 \mathbf{p}^4 + \Sigma(\mathbf{p})$$

$$\kappa \mathbf{p}^4 \approx \kappa_0 \mathbf{p}^4 + kT K_0 \mathbf{p}^4 \int \frac{d^2 q}{(2\pi)^2} \left(1 - \frac{(\mathbf{q} \cdot \mathbf{e}_p)^2}{\mathbf{q}^2} \right)^2 \frac{1}{\kappa(\mathbf{p} + \mathbf{q})^4}$$



The effective increase of the rigidity at long wavelengths stabilizes the membrane

$$\kappa_{\text{eff}}(\mathbf{p}) \sim \sqrt{kT K_0} \frac{1}{|\mathbf{p}|} \quad \Rightarrow \quad \langle \theta^2(x) \rangle \approx \langle (\nabla h)^2 \rangle = kT \int \frac{d^2 q}{(2\pi)^2} \frac{1}{\kappa_{\text{eff}}(\mathbf{q}) \mathbf{q}^2}$$

INTERACTION OF PHONONS WITH ELECTRONIC EXCITATIONS

It is also interesting to study the effect of the electronic excitations on flexural phonons, starting from the coupling to the charge density

$$S_{\text{e-ph}} = g \int dt d^2x \Psi^\dagger(\mathbf{r}) \Psi(\mathbf{r}) \text{Tr } u_{ij}$$

We can integrate first the electron degrees of freedom:

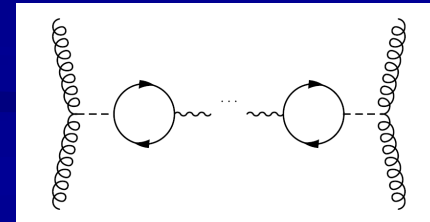
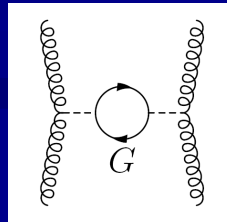
$$S_{\text{u-u}} = -\frac{1}{2} g^2 \int d\omega_q d^2q \chi(\mathbf{q}, \omega_q) (\text{Tr } u_{ij})(\text{Tr } u_{ij}) \quad , \quad \chi(\mathbf{q}, \omega_q) = -\frac{|\mathbf{q}|}{\sqrt{v_F^2 \mathbf{q}^2 - \omega_q^2}}$$

Integrating then the in-plane phonons as before, we get the action

$$S = \frac{1}{2} \int dt d^2r \left(-(\partial_i h)^2 + \kappa_0 (\nabla^2 h)^2 \right) + \frac{1}{2} \int dt d^2r d^2r' \left(\frac{1}{2} P_{ij}^T \partial_i h \partial_j h \right)_r K_{r,r'} \left(\frac{1}{2} P_{ij}^T \partial_i h \partial_j h \right)_{r'}$$

The interaction coupling is

$$K(\mathbf{q}) = 2\mu + \lambda - \underbrace{g^2 \frac{|\mathbf{q}|}{v_F}}_{\text{phonon self-energy}} - \underbrace{\frac{(\lambda - g^2 |\mathbf{q}| / v_F)^2}{2\mu + \lambda - g^2 |\mathbf{q}| / v_F}}_{\text{electron self-energy}}$$

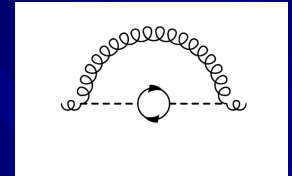
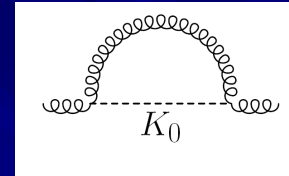


INTERACTION OF FLEXURAL PHONONS IN GRAPHENE

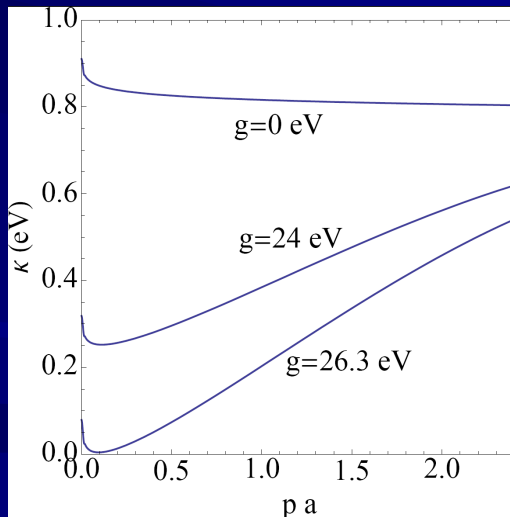
We compute the self-energy corrections at $T = 0$ with the effective interaction mediated by electronic excitations

$$D^{-1}(\mathbf{p}, \omega_p) = \omega_p^2 - \kappa_0 \mathbf{p}^4 - \Sigma(\mathbf{p})$$

$$\approx \omega_p^2 - \kappa_0 \mathbf{p}^4 - \mathbf{p}^4 \frac{1}{2} \int \frac{d^2 q}{(2\pi)^2} \frac{\sin^4(\theta) \mathbf{q}^2}{(\mathbf{p} - \mathbf{q})^4} \frac{K_0 - G_1 |\mathbf{p} - \mathbf{q}| - G_2 |\mathbf{p} - \mathbf{q}|^2}{\sqrt{\kappa}}$$



We can find a self-consistent solution for $\kappa(\mathbf{p})$:



- for $g = 0$, we find a hardening of the dispersion

$$\kappa(\mathbf{p}) \sim (\log(p_c / |\mathbf{p}|))^{2/3}$$

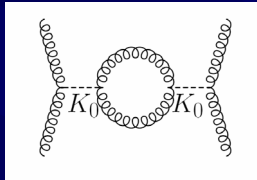
consistent with the analysis of Nelson and Peliti

- at large deformation potential $g > 20$ eV, there is an intermediate length scale where the rigidity is sensibly reduced
- beyond a critical g , $\kappa(\mathbf{p})$ is driven to negative values and the self-consistent solution does not exist

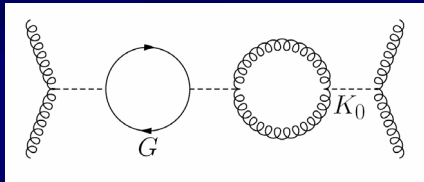
(P. San-José, J. G. and F. Guinea, arXiv:1003.3277)

INTERACTION OF FLEXURAL PHONONS IN GRAPHENE

When $\kappa(\mathbf{p})$ gets very small, there is also significant renormalization of the couplings through processes that depend logarithmically on the energy scale

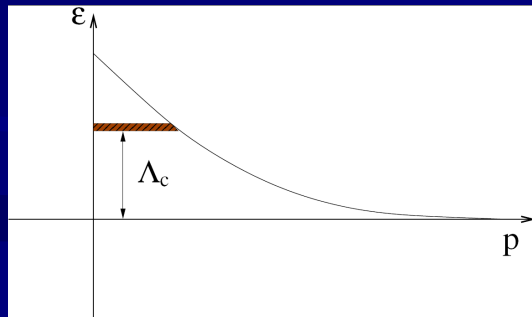


$$\sim K_0^2 \int d\omega d^2q \frac{q^4}{(\omega^2 - \varepsilon^2(\mathbf{q}))^2} \sim K_0^2 \int d^2q \frac{q^4}{\varepsilon(\mathbf{q})^3} \sim \frac{K_0^2}{\kappa^{3/2}} \int_0^{q_c} dq \frac{1}{|q|}$$



$$\sim \frac{K_0 G_n}{\kappa^{3/2}} \int_0^{q_c} dq \frac{1}{|q|}$$

Upon progressive integration of high-energy shells, we get the differential renormalization



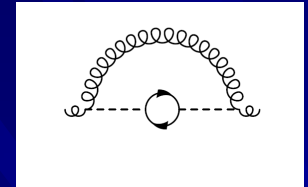
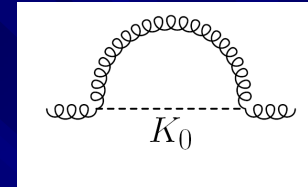
$$q \frac{\partial K_0}{\partial q} = \frac{3}{64\pi} \frac{K_0^2}{\kappa^{3/2}}$$

$$q \frac{\partial G_n}{\partial q} = nG + \frac{3}{32\pi} \frac{K_0 G_n}{\kappa^{3/2}} \quad \Rightarrow \quad G_n(q) = q^n \tilde{G}_n(q)$$

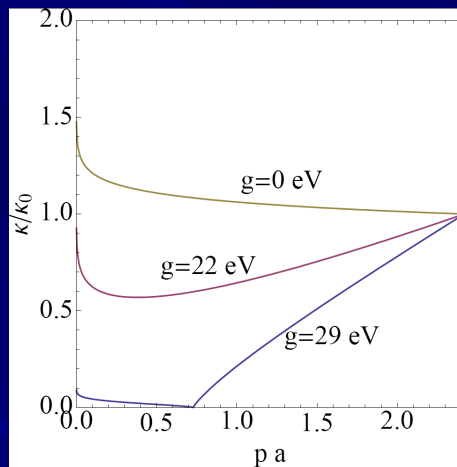
RENORMALIZATION OF FLEXURAL PHONONS

The rigidity κ has its own scaling equation

$$q \frac{\partial \kappa}{\partial q} = -\frac{3}{16\pi} \frac{K_0}{\sqrt{\kappa}} + \frac{3}{16\pi} \sum_n q^n \frac{\tilde{G}_n}{\sqrt{\kappa}}$$



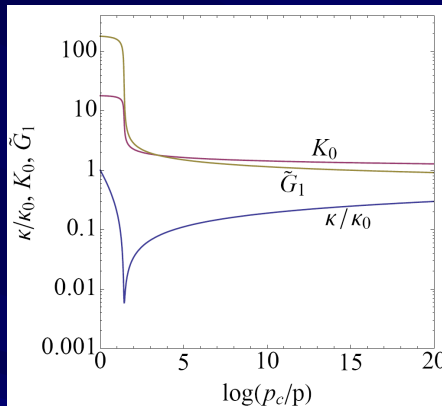
In this scaling approach we also get an effective dependence $\kappa(\mathbf{p})$:



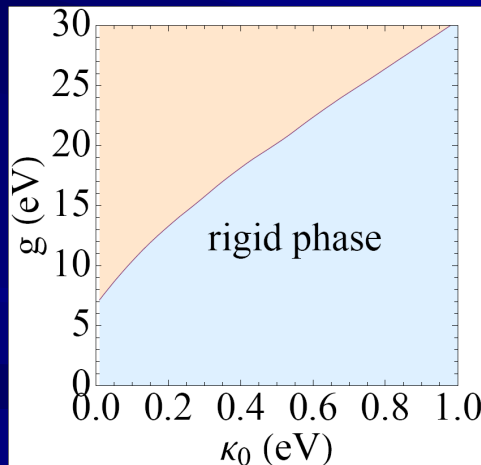
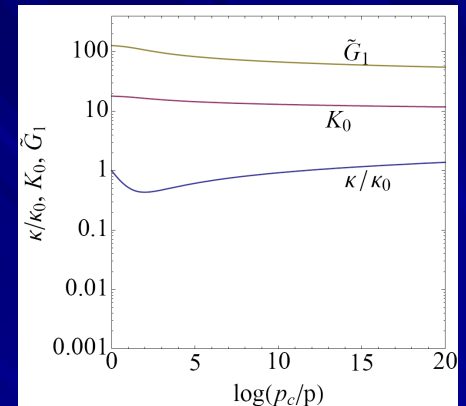
The behavior for $g = 0$ is consistent again with the analysis by Nelson and Peliti.

At large g , we find also a significant reduction of the bending rigidity, and now we can enter into the region that was forbidden before, finding a drastic softening of the dispersion.

RENORMALIZATION OF FLEXURAL PHONONS



We find that graphene has two different phases corresponding to mild and strong renormalization of the bending rigidity.



The boundary between the two phases can be characterized by looking for the values of the critical coupling beyond which the self-consistent solution for the phonon self-energy would lead to negative values of $\kappa(\mathbf{p})$.

In conclusion

- the combination of the self-consistent calculation of the phonon self-energy and renormalization group methods has allowed us to analyze the critical behavior of flexural phonons in graphene
- we find that graphene has a strongly renormalized phase where the effective bending rigidity becomes pinned at very small values below a certain momentum scale
- the phase with strong renormalization of the bending rigidity can be put in correspondence with the appearance of ripples in graphene, as very small values of κ imply a very large susceptibility for the development of a condensate (nonvanishing average value) of the flexural phonon field