CF-UM-UP

Universidade do Minho
Escola de Ciências

Strain in graphene and 2D materials

Bruno Amorim

Centre of Physics of the Universities of Minho and Porto, University of Minho

amorim.bac@gmail.com

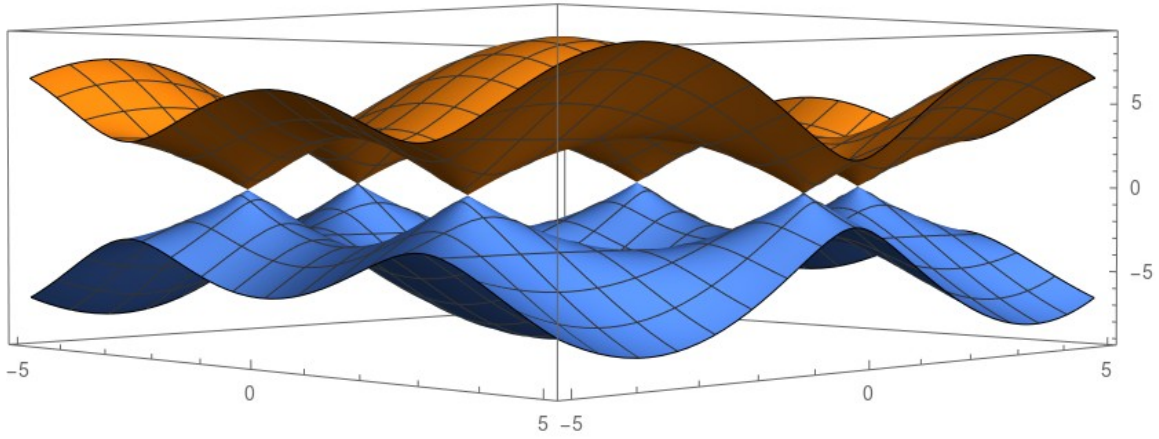
Overview

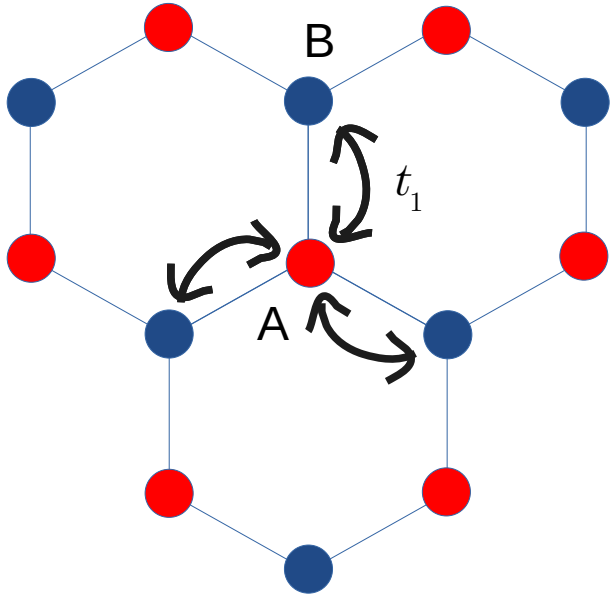
- Electron-lattice coupling in strained graphene
- Lattice dynamics in membranes

Electron-lattice coupling

Graphene NN tight-binding model for p_z orbitals:

$$H_0 = -t_1 \sum_{\mathbf{r},\mathbf{d}} c^{\dagger}_{\mathbf{r},A} c_{\mathbf{r}+\mathbf{d},B} + \text{h.c.}$$





Close to K points, $\mathbf{k} = \mathbf{K} + \mathbf{p}$:

$$H_0 \simeq v_F \sum_k \psi^{\dagger}_{\mathbf{p}} \boldsymbol{\sigma} \cdot \mathbf{p} \psi_{\mathbf{p}}$$

Strained graphene lattice

How can we model electrons in the presence of deformation?

$$\mathbf{r}_\alpha \rightarrow \vec{R}(\mathbf{r}_\alpha) = \mathbf{r}_\alpha + \vec{\xi}(\mathbf{r}_\alpha)$$

Assume hopping integrals depend on atomic separation:

$$H = -\sum_{\mathbf{r},\mathbf{r}'} t(\vec{R}(\mathbf{r}_A), \vec{R}(\mathbf{r}_B)) c^\dagger_{\mathbf{r},A} c_{\mathbf{r}',B} + \text{h.c.}$$

And approximate: $t(\vec{R}(\mathbf{r}_A), \vec{R}(\mathbf{r}_B)) \simeq t_1 + t_1' \Delta\ell(\mathbf{r}_A, \mathbf{r}'_B)$

Here $\Delta\ell(\mathbf{r}_A, \mathbf{r}'_B)$ is the change in the bond length

For smooth deformations: $\Delta\ell(\mathbf{r}_A, \mathbf{r}'_B) \simeq |\boldsymbol{\delta}| \hat{\delta}^i \hat{\delta}^j \varepsilon_{ij}$

Complete strain tensor:

$$\varepsilon_{ij} = \tfrac{1}{2}(\partial_i \xi_j + \partial_j \xi_i + \partial_i \vec{\xi} \cdot \partial_j \vec{\xi})$$

Electron-lattice coupling

Expanding the bond deformation in plane-waves:

$$\Delta\ell(\mathbf{r}_A,\mathbf{r}'_B)=\frac{1}{\sqrt{N}}\sum_{\mathbf{q}}e^{i\mathbf{q}\cdot(\mathbf{r}_A+\mathbf{r}'_B)/2}\Delta\ell(\mathbf{q};\boldsymbol{\delta}_{AB})$$

We obtain the electron-lattice coupling Hamiltonian

$$H_{\text{e-lat}}^{\text{NN-bond}}=\frac{1}{\sqrt{N}}\sum_{\mathbf{k},\mathbf{q}}\Psi^{\dagger}_{\mathbf{k}+\frac{\mathbf{q}}{2}}\boldsymbol{\Phi}^{\text{NN-bond}}_{\mathbf{k}+\frac{\mathbf{q}}{2},\mathbf{k}-\frac{\mathbf{q}}{2}}\Psi_{\mathbf{k}-\frac{\mathbf{q}}{2}}$$

Where:

$$\boldsymbol{\Phi}^{\text{NN-bond}}_{\mathbf{k}+\frac{\mathbf{q}}{2},\mathbf{k}-\frac{\mathbf{q}}{2}}=-t'_1\sum_{\boldsymbol{\delta}_1}\Delta\ell_{AB}\left(\mathbf{q};\boldsymbol{\delta}_1\right)\begin{bmatrix}0 & e^{i\mathbf{k}\cdot\boldsymbol{\delta}_1}\\ e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_1} & 0\end{bmatrix}$$

Electron-lattice coupling: Pseudo-vector potential

Writing $\Delta\ell(\mathbf{q};\boldsymbol{\delta}_1) = |\boldsymbol{\delta}_1|\hat{\delta}^i\hat{\delta}^j\varepsilon_{ij}(\mathbf{q})$, and approximating $\mathbf{k} \simeq \mathbf{K}$

$$\mathbf{\Phi}^{\text{NN-bond}}_{\mathbf{k}+\frac{\mathbf{q}}{2},\mathbf{k}-\frac{\mathbf{q}}{2}} \simeq -(-t_1')\frac{\sqrt{3}a_0}{4}\boldsymbol{\sigma}\cdot(\varepsilon_{xx}-\varepsilon_{yy},-2\varepsilon_{xy})$$

This is the celebrated elastic pseudo-vector potential term, which can be written as

$$\boldsymbol{H} \simeq v_F\boldsymbol{\sigma}\cdot\left(\mathbf{p}-\frac{\beta_1}{2a_{\text{cc}}}\mathbf{A}^{\text{el}}\right)$$

Where $\beta_1 = -\frac{d\log t_1}{d\log\ell}$ and the elastic pseudo-vector potential is:

$$\mathbf{A}^{\text{el}} = (\varepsilon_{xx}-\varepsilon_{yy},-2\varepsilon_{xy})$$

This can give origin to elastic pseudo-magnetic fields:

$$B_z^{\text{el}} = \partial_x A_y^{\text{el}} - \partial_y A_x^{\text{el}}$$

Psedo magnetic fields of ~300 T [N. Levy et al, Science 329, 544-547 (2010)]

Beyond the pseudo-vector potential: symmetry

For small and smooth deformations we have the possible electron-lattice couplings (formed with $\mathbf{p}$, $\boldsymbol{\sigma}$, ε_{ij} and $\mathbf{A}^{\mathrm{el}}$):

Coupling	Interpretation
$\boldsymbol{H}_1 = \mathrm{tr}(\varepsilon)\boldsymbol{\sigma}_0$	Deformation potential
$\boldsymbol{H}_2 = \boldsymbol{\sigma} \cdot \mathbf{A}^{\mathrm{el}}$	Pseudo-vector potential
$\boldsymbol{H}_3 = \mathbf{p} \cdot \mathbf{A}^{\mathrm{el}}\boldsymbol{\sigma}_0$	Dirac cone tilt
$\boldsymbol{H}_4 = \mathrm{tr}(\boldsymbol{\varepsilon})\boldsymbol{\sigma} \cdot \mathbf{p}$	Isotropic Fermi velocity correction
$\boldsymbol{H}_5 = \varepsilon_{ij}\sigma^i p^j$	Anisotropic Fermi velocity correction
$\boldsymbol{H}_6 = B_z^{\mathrm{el}}\sigma_z$	Pseudo-Zeeman term

[J. Mañes et al, Phys. Rev. B 88, 155405 (2013)]

Beyond the pseudo-vector potential: generalized model

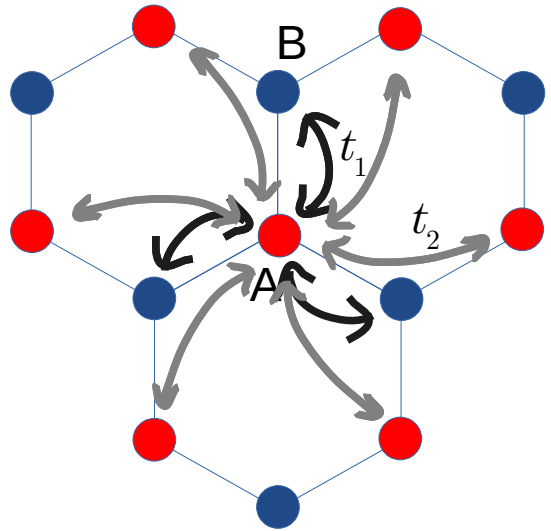
The simple nearest-neighbour tight-binding model for graphene does not generate all the allowed terms.

Generalized model:
Nearest-Neighbours + Next-Nearest-Neighbours + Rigid-ion potential

$$H = -\sum_{\langle \mathbf{r},\mathbf{r}'\rangle} t_1\left(\vec{R}(\mathbf{r}_A),\vec{R}(\mathbf{r}'_B)\right) c^\dagger_{\mathbf{r},A} c_{\mathbf{r}',B} + \text{h.c.}$$

$$- \sum_{\langle\langle \mathbf{r},\mathbf{r}'\rangle\rangle} t_2\left(\vec{R}(\mathbf{r}_A),\vec{R}(\mathbf{r}'_A)\right) c^\dagger_{\mathbf{r},A} c_{\mathbf{r}',A} + (A \leftrightarrow B)$$

$$+ \sum_{\mathbf{r}} V(\mathbf{r}_A) c^\dagger_{\mathbf{r},A} c_{\mathbf{r},A} + (A \leftrightarrow B)$$



Rigid-ion potential:

$$V(\mathbf{r}_A) = \sum_{\langle \mathbf{r}'_B\rangle} V(\mathbf{r}_A - \mathbf{r}'_B)$$

[J. Mañes et al, Phys. Rev. B 88, 155405 (2013)]

Beyond the pseudo-vector potential: generalized model

To lowest order in the bond-length change and expanding in plane-waves, one gets:

$$H_{\text{e-lat}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k},\mathbf{q}} \Psi^{\dagger}_{\mathbf{k}+\frac{\mathbf{q}}{2}} \mathbf{\Phi}^{\text{e-lat}}_{\mathbf{k}+\frac{\mathbf{q}}{2},\mathbf{k}-\frac{\mathbf{q}}{2}} \Psi_{\mathbf{k}-\frac{\mathbf{q}}{2}}$$

where $\mathbf{\Phi}^{\text{e-lat}}_{\mathbf{k}+\frac{\mathbf{q}}{2},\mathbf{k}-\frac{\mathbf{q}}{2}} = \mathbf{\Phi}^{\text{NN-bond}}_{\mathbf{k}+\frac{\mathbf{q}}{2},\mathbf{k}-\frac{\mathbf{q}}{2}} + \mathbf{\Phi}^{\text{NNN-bond}}_{\mathbf{k}+\frac{\mathbf{q}}{2},\mathbf{k}-\frac{\mathbf{q}}{2}} + \mathbf{\Phi}^{\text{rigid-ion}}_{\mathbf{k}+\frac{\mathbf{q}}{2},\mathbf{k}-\frac{\mathbf{q}}{2}}$

$$\mathbf{\Phi}^{\text{NN-bond}}_{\mathbf{k}+\frac{\mathbf{q}}{2},\mathbf{k}-\frac{\mathbf{q}}{2}} = -t'_1 \sum_{\boldsymbol{\delta}_1} \Delta\ell_{AB}\left(\mathbf{q};\boldsymbol{\delta}_1\right) \begin{bmatrix} 0 & e^{i\mathbf{k}\cdot\boldsymbol{\delta}_1} \\ e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_1} & 0 \end{bmatrix}$$

$$\mathbf{\Phi}^{\text{NNN-bond}}_{\mathbf{k}+\frac{\mathbf{q}}{2},\mathbf{k}-\frac{\mathbf{q}}{2}} = -t'_2 \sum_{\boldsymbol{\delta}_2} \begin{bmatrix} \Delta\ell_{AA}\left(\mathbf{q};\boldsymbol{\delta}_2\right) e^{i\boldsymbol{\delta}_2\cdot\mathbf{k}} & 0 \\ 0 & \sum_{\boldsymbol{\delta}_2} \Delta\ell_{BB}\left(\mathbf{q};\boldsymbol{\delta}_2\right) e^{i\boldsymbol{\delta}_2\cdot\mathbf{k}} \end{bmatrix}$$

$$\mathbf{\Phi}^{\text{rigid-ion}}_{\mathbf{k}+\frac{\mathbf{q}}{2},\mathbf{k}-\frac{\mathbf{q}}{2}} = V' \sum_{\boldsymbol{\delta}_1} \Delta\ell_{AB}\left(\mathbf{q};\boldsymbol{\delta}_1\right) \begin{bmatrix} e^{i\boldsymbol{\delta}_1\cdot\frac{\mathbf{q}}{2}} & 0 \\ 0 & e^{-i\boldsymbol{\delta}_1\cdot\frac{\mathbf{q}}{2}} \end{bmatrix}$$

Beyond the pseudo-vector potential: generalized model

Writing the bond-length change in terms of the strain tensor, expanding to lowest order in the phonon, $\mathbf{q}$, and electron momenta, $\mathbf{k} = \mathbf{K} + \mathbf{p}$, we obtain:

Coupling	Coupling constant		
	NN-bond	NNN-bond	Rigid-ion
$\boldsymbol{H}_1 = \mathrm{tr}(\varepsilon)\boldsymbol{\sigma}_0$		$t_2' \frac{3a_0}{2}$	$V' \frac{\sqrt{3}a_0}{2}$
$\boldsymbol{H}_2 = \boldsymbol{\sigma} \cdot \mathbf{A}^{\mathrm{el}}$	$-t_1' \frac{\sqrt{3}a_0}{4}$		
$\boldsymbol{H}_3 = \mathbf{p} \cdot \mathbf{A}^{\mathrm{el}} \boldsymbol{\sigma}_0$		$-t_2' \frac{3\sqrt{3}a_0}{4}$	
$\boldsymbol{H}_4 = \mathrm{tr}(\boldsymbol{\varepsilon})\boldsymbol{\sigma} \cdot \mathbf{p}$	$t_1' \frac{a_0^2}{8}$		
$\boldsymbol{H}_5 = \varepsilon_{ij}\sigma^i p^j$	$t_1' \frac{a_0^2}{4}$		
$\boldsymbol{H}_6 = B_z^{\mathrm{el}} \sigma_z$			$V' \frac{a_0^2}{8}$

Dirac equation in curved space

An alternative approach is to consider the Dirac equation in curved space:

[F. Juan et al, PRL 108, 227205 (2012)]

$$H_D = -iv_F \int d^2\mathbf{x}\sqrt{g}\psi^\dagger(\mathbf{x})\sigma^a e_a^i \left(\partial_i + \Omega_i\right)\psi(\mathbf{x})$$

Where $g = \det(g_{ij})$, e_i^a are frame fields defined such that

$$g_{ij} = e_i^a e_{aj}$$

And the (pseudo-)spin connection is given by

$$\Omega_i = -\frac{1}{4}\sigma_a\sigma_b e_j^a g^{jk}\left[\partial_i e_k^b - \Gamma_{ik}^l e_l^b\right]$$

With the usual Cristoffel symbols

$$\Gamma_{ij}^k = \frac{1}{2}g^{kl}\left(g_{ik,j} + g_{jk,i} - g_{ij,k}\right)$$

Since $g_{ij} = \delta_{ij} + 2\varepsilon_{ij}$, we can choose to lowest order in the strain

$$e_i^a \simeq \delta_i^a + \delta^{aj}\varepsilon_{ij}$$

Dirac equation in curved space

To lowest order in the strain and after an integration by parts, one gets:

$$
\begin{aligned}
H_D \simeq & -iv_F \int d^2\mathbf{x}\psi^\dagger(\mathbf{x})\boldsymbol{\sigma}\cdot\boldsymbol{\partial}\psi(\mathbf{x}) \\
& -iv_F \int d^2\mathbf{x}\mathrm{tr}(\boldsymbol{\varepsilon})\psi^\dagger(\mathbf{x})\sigma_i \overleftrightarrow{\partial}_j \psi(\mathbf{x}) \\
& +iv_F \int d^2\mathbf{x}\psi^\dagger(\mathbf{x}) \left[\varepsilon_{ij}\sigma_i \overleftrightarrow{\partial}_j\right] \psi(\mathbf{x})
\end{aligned}
$$

[F. Juan et al, PRL 108, 227205 (2012)]

Dirac equation in curved space vs TB model

Coupling	Coupling constant			
	NN-bond	NNN-bond	Rigid-ion	Curved Dirac
$\boldsymbol{H}_1 = \mathrm{tr}(\varepsilon)\boldsymbol{\sigma}_0$		$t_2' \frac{3a_0}{2}$	$V' \frac{\sqrt{3}a_0}{2}$	
$\boldsymbol{H}_2 = \boldsymbol{\sigma} \cdot \mathbf{A}^{\mathrm{el}}$	$-t_1' \frac{\sqrt{3}a_0}{4}$			
$\boldsymbol{H}_3 = \mathbf{p} \cdot \mathbf{A}^{\mathrm{el}} \boldsymbol{\sigma}_0$		$-t_2' \frac{3\sqrt{3}a_0}{4}$		
$\boldsymbol{H}_4 = \mathrm{tr}(\boldsymbol{\varepsilon})\boldsymbol{\sigma} \cdot \mathbf{p}$	$t_1' \frac{a_0^2}{8}$			$\frac{\sqrt{3}a_0 t_1}{2}$
$\boldsymbol{H}_5 = \varepsilon_{ij}\sigma^i p^j$	$t_1' \frac{a_0^2}{4}$			$-\frac{\sqrt{3}a_0 t_1}{2}$
$\boldsymbol{H}_6 = B_z^{\mathrm{el}} \sigma_z$			$V' \frac{a_0^2}{8}$	

Lattice dynamics

Lattice dynamics in graphene and other membranes

The potential energy of a membrane contains two parts:

$$U_{\text{elastic}} = U_{\text{stretch}} + U_{\text{bend}}$$

where

$$U_{\text{stretch}} = \frac{1}{2}\int d^2\mathbf{x} c^{ijkl}\varepsilon_{ij}\varepsilon_{kl}$$

$$U_{\text{bend}} = \frac{1}{2}\int d^2\mathbf{x}\kappa\left(\partial^2 h\right)^2$$

with the elastic constants tensor $c^{ijkl} = \lambda\delta^{ij}\delta^{kl} + \mu\left(\delta^{ik}\delta^{jl} + \delta^{il}\delta^{jk}\right)$
and κ the bending rigidity

Acoustic phonon modes in membranes

From the stretching energy we obtain the dispersion relation for the **Longitudinal** and **Transverse** acoustic phonon modes:

$$\omega_{L,\mathbf{q}} = \sqrt{\frac{\lambda + 2\mu}{\rho}}\,|\mathbf{q}|$$

$$\omega_{T,\mathbf{q}} = \sqrt{\frac{\mu}{\rho}}\,|\mathbf{q}|$$

The stretching energy describes the restoring for out-of-plane or **Flexural** phonons

$$\omega_{F,\mathbf{q}} = \sqrt{\frac{\kappa}{\rho}}\,|\mathbf{q}|^2$$

In-plane/Flexural anharmonic coupling

Out-of-plane motion also leads to stretching of the membrane. This gives origin to an anharmonic coupling between in-plane and out-of-plane motion

$$U_{\text{stretch}} = \frac{1}{2}\int d^2\mathbf{x} c^{ijkl}\varepsilon_{ij}\varepsilon_{kl}$$

Stretching depends on the full strain tensor

$$\begin{aligned}\varepsilon_{ij} &= \frac{1}{2}\left(\partial_i u_j + \partial_j u_i + \partial_i \vec{u}\cdot\partial_j\vec{u}\right)\\ &\simeq \frac{1}{2}\left(\partial_i u_j + \partial_j u_i + \partial_i h\partial_j h\right) = \gamma_{ij}\end{aligned}$$

Von Kármán energy for thin plates:

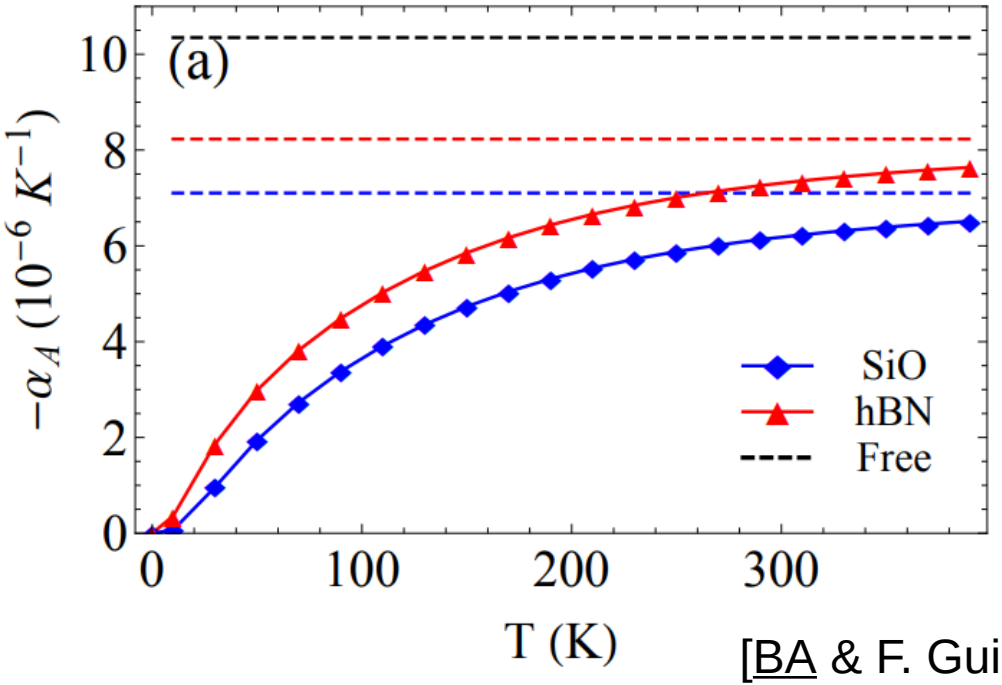
$$U_{\text{elastic}} = U_{\text{phonons}} + \frac{1}{2}\int d^2\mathbf{x} c^{ijkl}\left(\partial_i u_j\right)\left(\partial_k h\partial_l h\right) + \frac{1}{8}\int d^2\mathbf{x} c^{ijkl}\left(\partial_i h\partial_j h\right)\left(\partial_k h\partial_l h\right)$$

In-plane thermal contraction

Upon heating a membrane contracts due to the activation of out-of-plane motion.

Membrane effects:

$$\alpha_A = -\frac{1}{2}\frac{\partial}{\partial T}\langle \partial_i h \partial_i h \rangle$$



If out-of-plane motion is quenched by substrate, thermal contraction is reduced

[BA & F. Guinea, PRB 88, 115418 (2013)]

Strong anharmonic effects

At a classical level, integrating out the in-plane phonons, one obtains an effective action for the flexural motion

$$U_{eff}[h] = \frac{\kappa}{2}\int d^2\mathbf{x}\left(\partial^2 h\right)^2 + \frac{Y_{2D}}{8}\int d^2\mathbf{x}\left(P^T_{ij}\partial_i h\partial_j h\right)^2$$

At lowest order in the interaction

$$\langle h_{\mathbf{q}} h_{-\mathbf{q}}\rangle = \frac{k_B T}{\kappa\left|\mathbf{q}\right|^4 + \Sigma_{\mathbf{q}}} \qquad \Sigma_{\mathbf{q}} = \frac{3Y_{2D}k_B T}{16\pi\kappa}\left|\mathbf{q}\right|^2$$

Perturbation theory breaks down for

$$q < q_* = \sqrt{\frac{3k_B T Y_{2D}}{16\pi\kappa^2}}$$

[Nelson & Peliti, J. Phys. Paris 48, 1085 (1987)]

Anomalous elasticity

The breakdown of perturbation theory requires the use of non-perturbative techniques

In general one obtains

$$\langle h_{\mathbf{q}} h_{-\mathbf{q}} \rangle \sim |\mathbf{q}|^{-4+\eta_h}$$

$$\left\langle u^i_{\mathbf{q}} u^j_{-\mathbf{q}} \right\rangle \sim |\mathbf{q}|^{-2-\eta_u}$$

where $\eta_u + 2\eta_h = 2$

Self-consistent Screening approximation gives

$$\eta_h \simeq 0.821$$

[Le Doussal & Radzihovsky, PRL 69, 1209 (1992)]

Conclusions

- Strain gives origin to rich physics in graphene
- The same ideas can be applied to other 2D materials
- Lattice anharmonic effects in crystalline membranes play an important role

“Novel effects of strains in graphene and other two dimensional materials”
B. Amorim, A. Cortijo, F. de Juan, A.G. Grushin, F. Guinea, A. Gutiérrez-Rubio, H. Ochoa, V. Parente, R. Roldán, P. San-Jose, J. Schiefele, M.Sturla, M.A.H. Vozmediano
Physics Reports 617, 1-54 (2016)

Thank you for your attention