Radboud Universiteit

Statistical physics and geometry of two dimensional materials in classical and quantum cases

Mikhail Katsnelson

with Achille Mauri

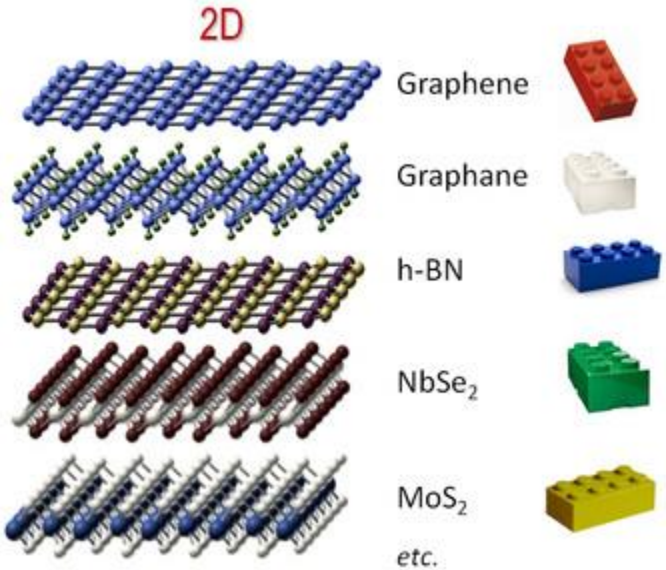
Earlier works with Jan Los and Annalisa Fasolino

Outline

1. Examples of two-dimensional materials
2. Nonexistence of 2D crystals at finite temperatures
3. Elasticity theory of membranes
4. Thermally induced ripples
5. Field theory approach: RG and epsilon-expansion
6. Scaling without conformal symmetry
7. Quantum case: Problem of thermal expansion

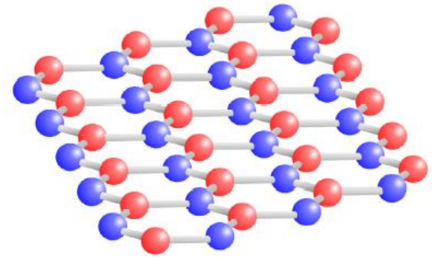
Zoo of 2D materials

Plenty of 2D materials starting from graphene



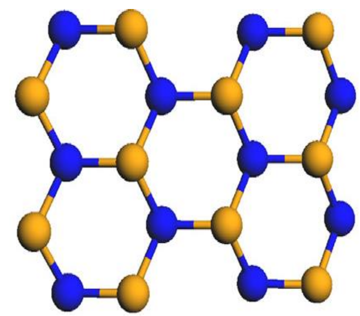
Semimetals (graphene), semiconductors, metals, superconductors, broad-gap insulators…

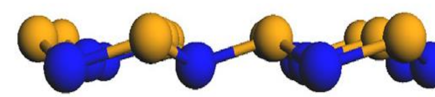
Graphene



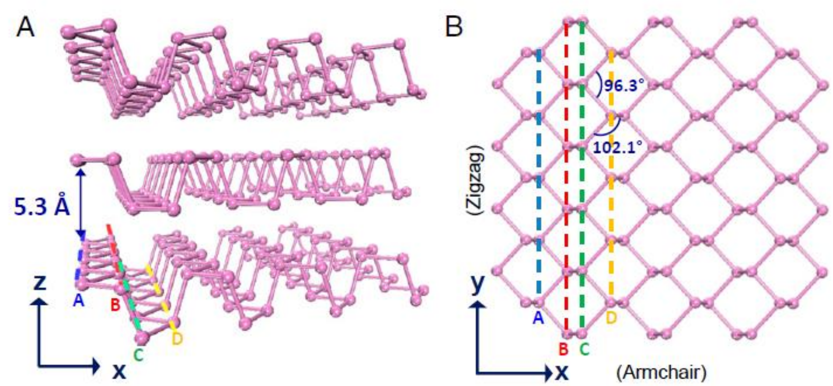
Silicene, germanene

Buckling



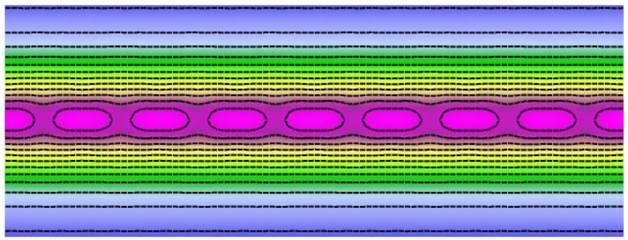


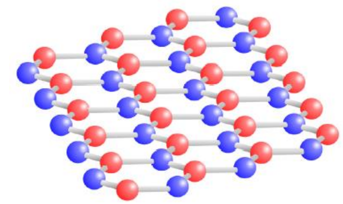
Phosphorene (monolayer of black phosphorus)



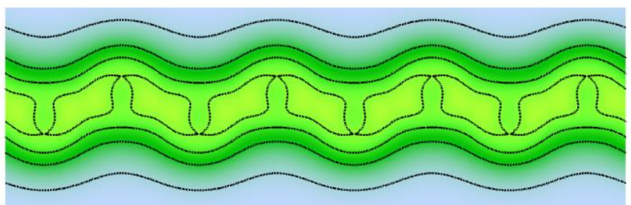
Flat at T=0: graphene vs silicene/germanene

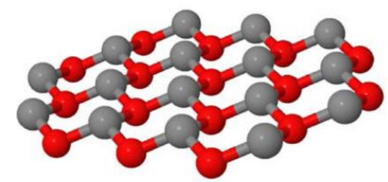
charge density, DFT, courtesy of A. Rudenko



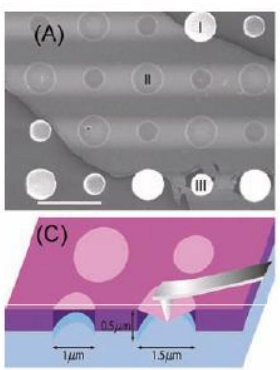


graphene
flat, sp^2

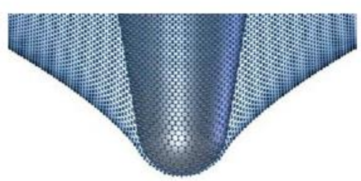




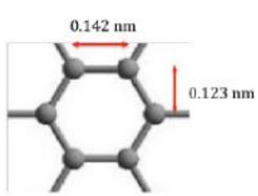
germanene
buckled, sp^2-sp^3



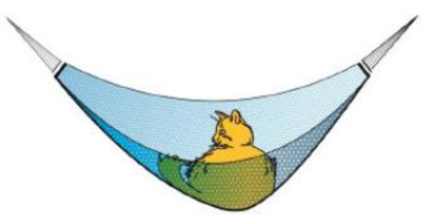
James Hone, Jeffrey Kysar, Changgu Lee and Xiaoding Wei *Science* **321** 385(2008)



breaking strength of 42N/m



density ; 0.77 mg/m².



Graphene is extremely stiff

from Nobel prize site;
an invisible 1 m² hammock
could sustain a 4 Kg cat

Our quantitative theory (Los, Fasolino, MIK) gives a limit 2.7 Kg for a point cat and 8 Kg for a cat uniformly distributed over the hammock

Why a 2D crystal should not exist

3D crystals:

atomic displacements << interatomic distances up to melting (Lindemann)

$$< \vec{u}^2_{n,j} > << d^2$$

harmonic approximation valid up to high temperature

2D crystals

large fluctuations, harmonic approximations fails

Peierls and Landau concluded (~1930) that **2D crystals should not exist**

Graphene invites to review their arguments later revisited by Mermin and Wagner

For a review: *Graphene as a prototype crystalline membrane*
M. I. Katsnelson, A. Fasolino, *Acc. Chem. Res.*, ***46***, 97 (2013)

Lattice dynamics of graphene

Expand V(R) to 2nd order around equilibrium

$$V\left(\vec{R}_{n,j}\right) = V\left(\vec{R}^{(0)}_{n,j}\right) + \frac{1}{2}\sum_{n,n'}\sum_{i,j}\sum_{\alpha\beta} A^{\alpha\beta}_{ni,n'j} u^{\alpha\beta}_{ni} u^{\alpha\beta}_{n'j}$$

Phonons $\omega^2_{\xi}(\vec{q})$ eigenvalues of

$$D^{\alpha\beta}_{ij}(\vec{q}) = \sum_{n} \frac{A^{\alpha\beta}_{0i,nj}}{\sqrt{M_i M_j}} exp(i\vec{q}\cdot\vec{r}_n)$$

2D, 3D translational invariance

no forces for rigid shift:

$$\sum_{nj} A^{\alpha\beta}_{0i,nj} = 0 \quad \xrightarrow[\vec{q}\to 0]{} \quad \omega^2 \propto q^2$$

linear acoustic modes

2D rotational invariance

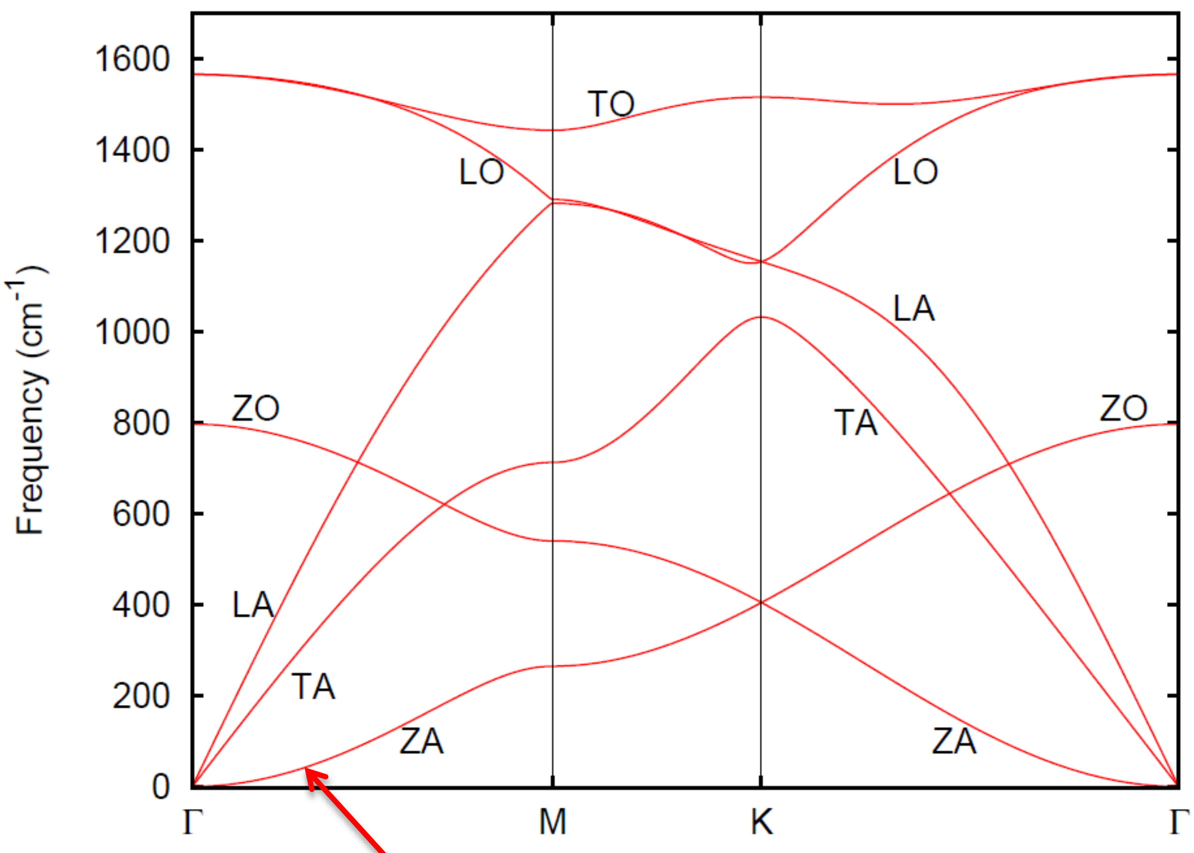
no torques for rigid rotation

$$\sum_{nj} A^{zz}_{0i,nj} r^{\alpha}_{n} r^{\beta}_{n} = 0 \quad \xrightarrow[\vec{q}\to 0]{} \quad \omega^2_{ZA}(q) \propto q^4$$

$$(\alpha, \beta = x, y)$$

quadratic ZA mode

Phonons of graphene (atomistic simulations)



quadratic dispersion
'soft' out of plane mode

$$\omega_{\mathrm{ZA}}(\boldsymbol{q}) = \sqrt{\frac{\kappa}{\rho_{2D}}}|\boldsymbol{q}|^2$$

Finite temperatures

In the harmonic approximations, the mean square displacement is

$$< u_{nj}^{\alpha} u_{nj}^{\beta} > = \sum_{\lambda} \frac{\hbar}{2N_0 M_j \omega_\lambda} \left(e_{\lambda j}^{\alpha} \right)^{*} \left(e_{\lambda j}^{\beta} \right) coth \left(\frac{\hbar \omega_\lambda}{2T} \right)$$

2D : in plane deformations diverge logarithmically due to acoustic branches.

Cut at $q_{min} \sim L^{-1}$

$$< x_{nj}^2 > = < y_{nj}^2 > \approx \frac{T}{2\pi M c_s^2} \ln \left(\frac{L}{d} \right)$$

➡ Landau, Peierls**: 2D crystals cannot exist**

2D in 3D out of plane deformations, $\omega_{ZA}^2(q) \propto q^4$ ➡ stronger divergence

$$< h_{nj}^2 > \propto \frac{T}{E_{at}} \sum_{q} \frac{1}{q^4} \propto \frac{T}{E_{at}} L^2$$

out of plane fluctuations grow as L, flat phase unstable!

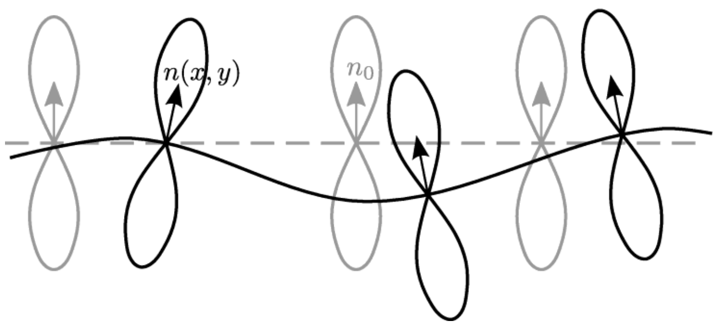
Anharmonicities are crucial

2D $\cancel{< \vec{u}^2_{n,j} > \ll d^2}$

Harmonic approximation (uncoupled modes) never works
due to divergent contribution of acoustic modes

Trick to remain stable: become rippled (like crumpled paper)

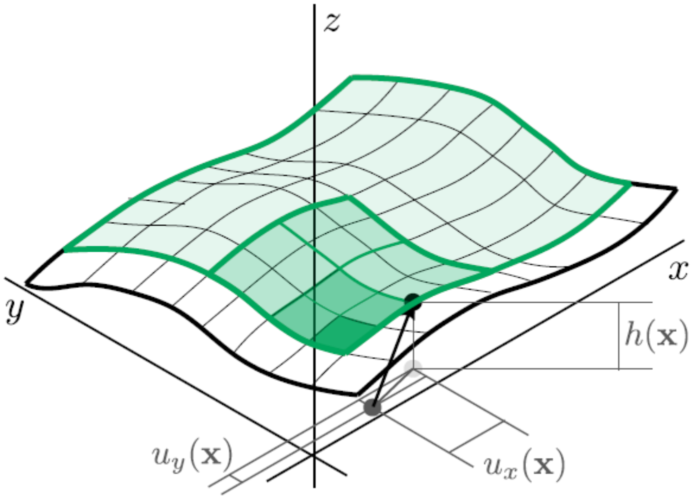
Consider **coupling of acoustic in-plane and out of plane (ZA) modes**
(Nelson,Peliti 1987)



This stabilizes the 2D layer

- Height fluctuations $h \sim L \;\; \to h \sim L^{\zeta} \qquad \zeta < 1$
- Deviations from complete flatness at any $T \neq 0$, thermal ripples
- Critical, power-law behaviour of correlation functions

Crystalline membrane - phenomenology



Elastic energy

$$E = \int d^2x \left[\frac{\kappa}{2} \left(\nabla^2 h \right)^2 + \mu \overline{u}^2_{\alpha\beta} + \frac{\lambda}{2} \overline{u}^2_{\alpha\alpha} \right]$$

Strain tensor

$$\overline{u}_{\alpha\beta} = \frac{1}{2} \left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} + \frac{\partial h}{\partial x_\alpha} \frac{\partial h}{\partial x_\beta} \right)$$

Minimization of elastic energy: Föppl – von Karman equations

$$\kappa \Delta^2 h - \left(\frac{\partial^2 \phi}{\partial y^2} \frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 \phi}{\partial x^2} \frac{\partial^2 h}{\partial y^2} - \frac{\partial^2 \phi}{\partial x \partial y} \frac{\partial^2 h}{\partial x \partial y} \right) = P$$

$$\Delta^2 \phi - Y \left(\frac{\partial^2 h}{\partial x^2} \frac{\partial^2 h}{\partial y^2} - \left(\frac{\partial^2 h}{\partial x \partial y} \right)^2 \right) = 0$$

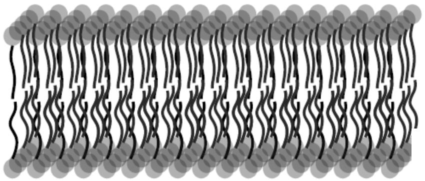
ϕ Airy stress function (potential for in-plane stress tensor)

Crystalline membrane - fluctuations

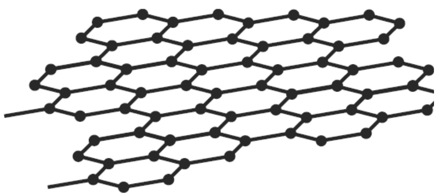
D. R. Nelson, T. Piran & S. Weinberg (Editors),
Statistical Mechanics of membranes and Surfaces
World Sci., 2004

$$P[h(\mathbf{x}), u_i(\mathbf{x})] = Z^{-1} \mathrm{e}^{-\frac{E}{k_B T}}$$

thermal distribution



lipid bilayers



graphene

In harmonic approximation (free fields)

$$G_0(\vec{q}) = \left\langle \left| h_{\vec{q}} \right|^2 \right\rangle_0 = \frac{T}{\kappa q^4},$$

$$P_{\alpha\beta}(\vec{q}) = \frac{q_\alpha q_\beta}{q^2}$$

$$D_0{}^{\alpha\beta}(\vec{q}) = \langle u_{\alpha\vec{q}}{}^* u_{\beta\vec{q}} \rangle_0 = P_{\alpha\beta}(\vec{q}) \frac{T}{(\lambda + 2\mu) q^2} + \left[\delta_{\alpha\beta} - P_{\alpha\beta}(\vec{q}) \right] \frac{T}{\mu q^2}$$

$\langle h^2 \rangle \sim \dfrac{T}{\kappa} L^2$ and the correlation function $\langle \vec{n}_0 \vec{n}_{\vec{R}} \rangle$

does not tend to constant at $R \to \infty$

Membrane cannot be flat in harmonic approximation, nonlinearities are crucial

Crystalline membrane – fluctuations II

Effective interacting field theory

Integrating out u-field: $$\frac{\int D\vec{u}\exp\left(-\frac{1}{2}\vec{u}\hat{L}\vec{u}-\vec{f}\vec{u}\right)}{\int D\vec{u}\exp\left(-\frac{1}{2}\vec{u}\hat{L}\vec{u}\right)}=\exp\left(\frac{1}{2}\vec{f}\hat{L}^{-1}\vec{f}\right)$$

$$Z=\int Dh(\vec{r})\exp\left\{-\beta\Phi\left[h(\vec{r})\right]\right\}$$

$$\Phi=\frac{1}{2}\sum_{\vec{q}}\kappa q^4\left|h_{\vec{q}}\right|^2+\frac{Y}{8}\sum_{\vec{q}\vec{k}\vec{k}'}R\left(\vec{k},\vec{k}',\vec{q}\right)\left(h_{\vec{k}}h_{\vec{q}-\vec{k}}\right)\left(h_{\vec{k}'}h_{-\vec{q}-\vec{k}'}\right)$$

$$R\left(\vec{k},\vec{k}',\vec{q}\right)=\frac{\left(\vec{q}\times\vec{k}\right)^2\left(\vec{q}\times\vec{k}'\right)^2}{q^4}$$

Y is 2D Young modulus

Crystalline membrane – fluctuations III

Nonlinearities lead to scaling (like at critical point, but for *any* finite temperature

$$G(q) = \frac{T}{\kappa_R(q) q^4}$$ Effective bending rigidity $$\kappa_R(q) \sim q^{-\eta}$$

$$q \leq q^* = \sqrt{\frac{3TY}{16\pi\kappa^2}}$$ strong coupling regime

$$\lambda_R(q), \mu_R(q) \sim q^{\eta_u}$$

$$D^{\alpha\beta}(\vec{q}) = \langle u_{\alpha\vec{q}}{}^* u_{\beta\vec{q}} \rangle \sim \frac{1}{q^{2+\eta_u}}$$

$$\eta_u = 2 - 2\eta$$

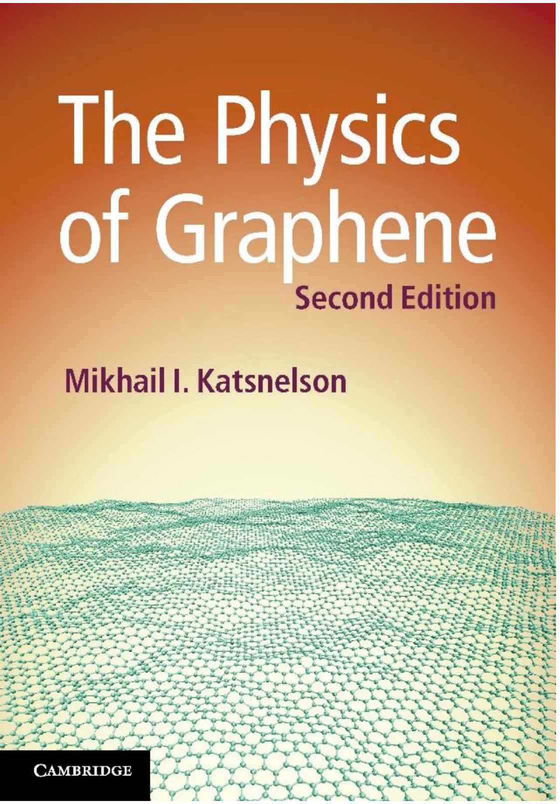
$$\langle h^2 \rangle \sim L^{2\zeta}$$

$$\zeta = 1 - \frac{\eta}{2}$$

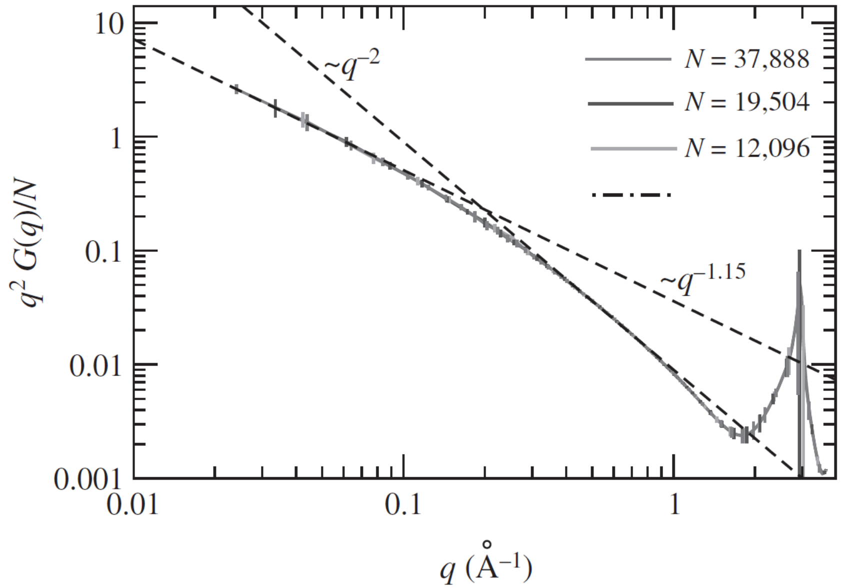
Effective elastic moduli tend to zero, effective bending rigidity to infinity

Crystalline membrane – fluctuations IV

Computer simulations for graphene (Jan Los, Annalisa Fasolino, MIK)



Snapshot from Monte Carlo simulations @RT



$$\eta \approx 0.85$$

$$q^* \approx 0.2\ \text{Å}^{-1}$$

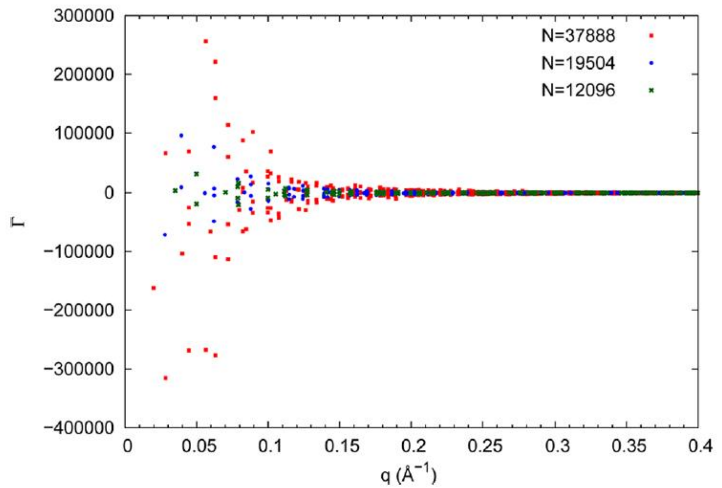
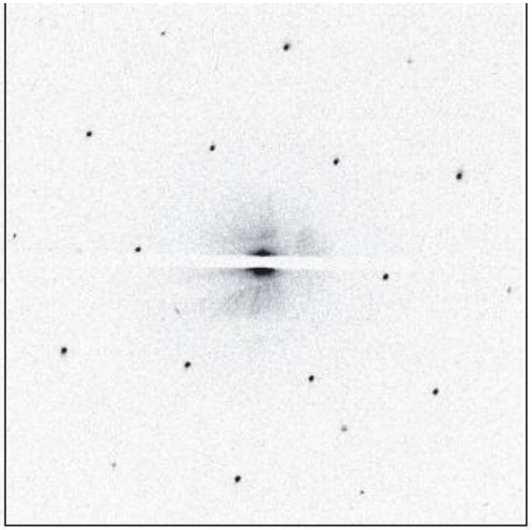


FIGURE 3. Function $\Gamma(q)$ for three values of N.

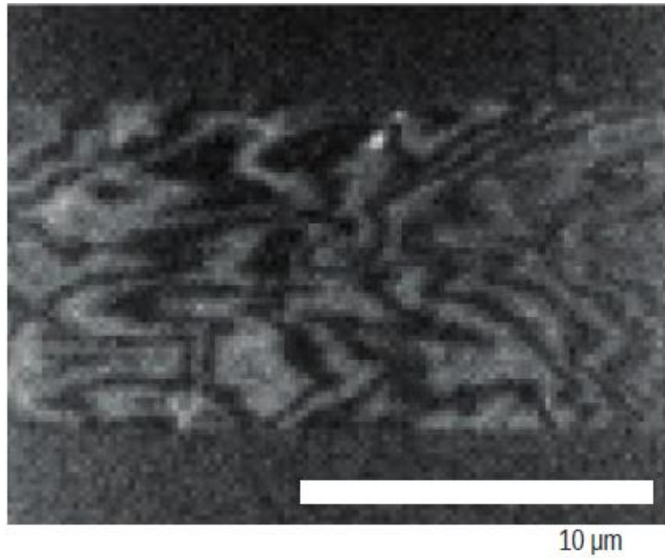
$$\Gamma_{\vec{q}} = \left\langle (u_x)_{\vec{q}} \left(h^2\right)_{-\vec{q}} \right\rangle$$

Strong anharmonic coupling at small q

Ripples and corrugations: Experiment

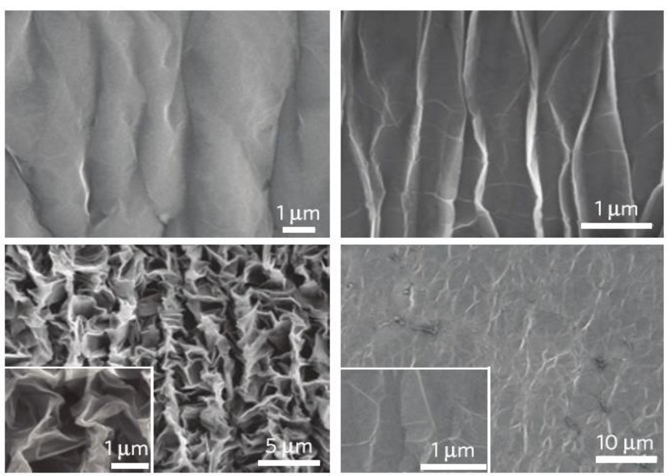


static ripples free-standing graphene ($\lambda \approx 10$ nm, $h \approx 1$nm)
Broadening of Bragg peaks [1]



static ripples in free-standing graphene ($\lambda \approx 1$ µm, $h \approx 100$nm)
interference microscopy image [2]

[1] J.C. Meyer et al., Nature 446, 60 (2007)
[2] M. Blees et al., Nature 524, 204 (2015)



wrinkles and crumples under strain
scanning electron microscopy images [5]

[5] J. Zang et al., Nature Mater. 12, 321 (2013)

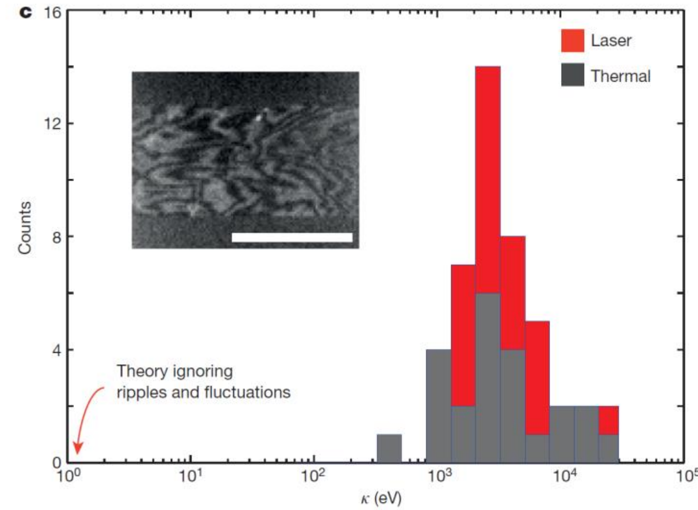
Experiment and simulations confirm scaling

Graphene kirigami

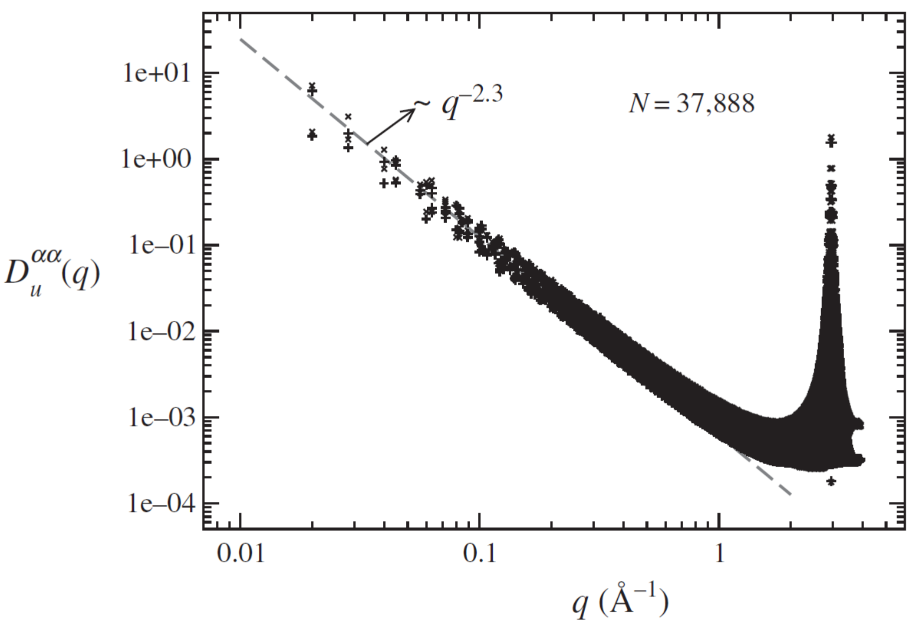
Melina K. Blees[1], Arthur W. Barnard[2], Peter A. Rose[1], Samantha P. Roberts[1], Kathryn L. McGill[1], Pinshane Y. Huang[2], Alexander R. Ruyack[3], Joshua W. Kevek[1], Bryce Kobrin[1], David A. Muller[2,4] & Paul L. McEuen[1,4]

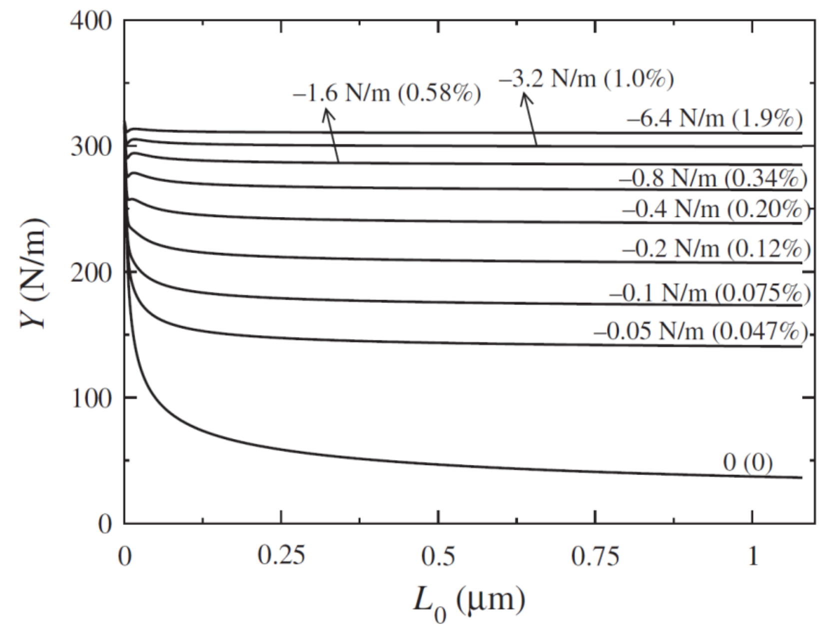
Bending rigidity $\varkappa$ increases with size as L^{η} with $\eta \approx 0.85$

The effect is very strong (many orders of magnitude)



Renormalization of in-plane phonons and elastic moduli





J.H. Los, A. Fasolino, M.I. Katsnelson, PRL 116, 015901 (2016)

How to calculate η analytically?

Generalization: $$H = \frac{1}{2}\int \mathrm{d}^D x \left[\kappa(\partial^2 \mathbf{r})^2 + \lambda U_{\alpha\alpha}^2 + 2\mu U_{\alpha\beta}U_{\alpha\beta}\right]$$

$$U_{\alpha\beta} = \frac{1}{2}(\partial_\alpha \mathbf{r}\cdot\partial_\beta \mathbf{r} - \delta_{\alpha\beta})$$ strain tensor

$\mathbf{r} = (\mathbf{x}+\mathbf{u}, \mathbf{h})$, where $\mathbf{u} \in \mathbb{R}^D$ and $\mathbf{h} \in \mathbb{R}^{d-D}$

Physical situation: $D = 2$, $d = 3$ but
as usual better keep as parameters

Importantly: nonlinearity in out-of-plane displacements is crucial
but nonlinearity in in-plabe displacements can be skipped

$$u_{\alpha\beta} = \frac{1}{2}(\partial_\alpha u_\beta + \partial_\beta u_\alpha + \partial_\alpha \mathbf{h}\cdot\partial_\beta \mathbf{h})$$

strain tensor

nonlinear coupling between curvature and stretching

Self-consistent screening approximation

Le Doussal and Radzihovsky, 1992

Diagrammatic expansion neglecting vertex

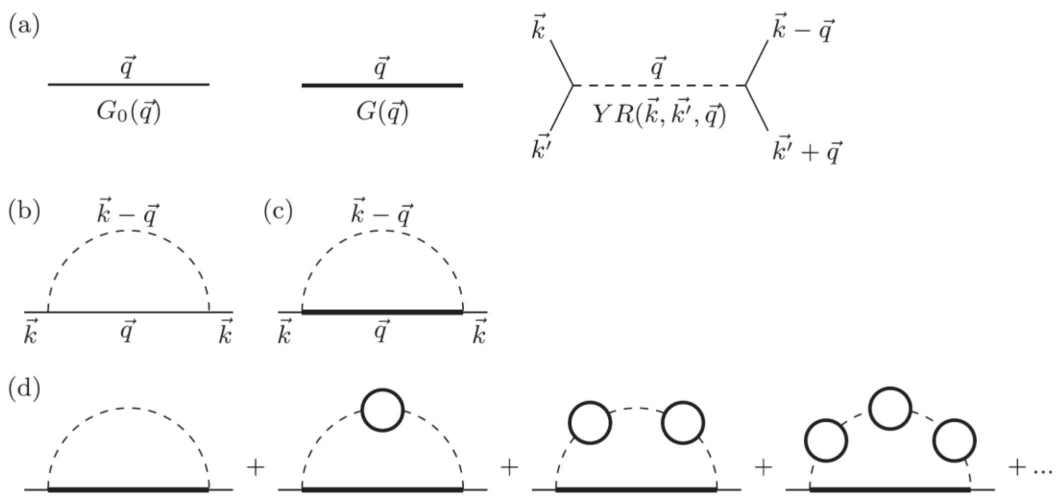


Fig. 9.7 (a) Basic elements of the diagram technique (see the text). (b) The lowest-order perturbation expression for the self-energy corresponding to Eq. (9.96). (c) The self-consistent version of the previous diagram corresponding to Eq. (9.131). (d) The diagram summation equivalent to the SCSA.

$$G^{-1}(\vec{q}) = G_0{}^{-1}(\vec{q}) + \Sigma(\vec{q})$$

$$Y_{ef}\left(\vec{k}\right) = \frac{Y}{1+\frac{Y}{2T}I\left(\vec{k}\right)}$$

$$\Sigma(\vec{q}) = \int \frac{d^2\vec{k}}{(2\pi)^2}\frac{Y_{ef}\left(\vec{k}\right)}{T}\left[\frac{\left(\vec{q}\times\vec{k}\right)^2}{k^2}\right]^2 G\left(\vec{k}-\vec{q}\right)$$

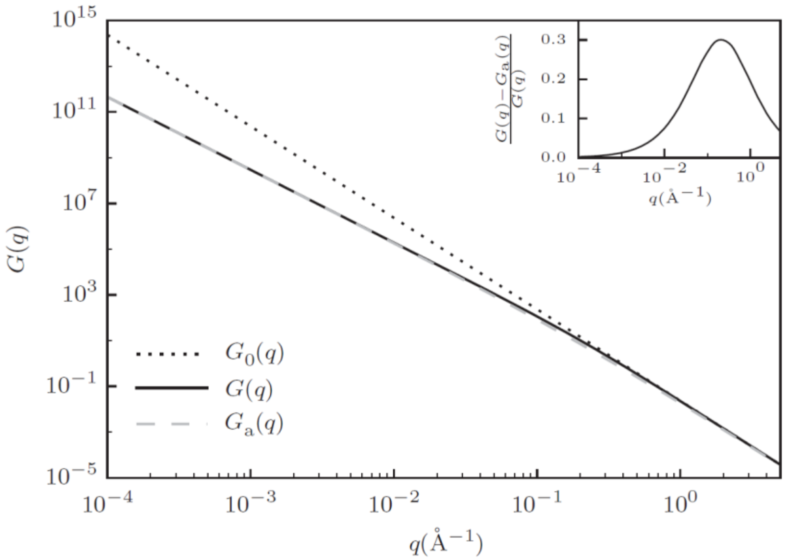
$$I\left(\vec{k}\right) = \int \frac{d^2\vec{p}}{(2\pi)^2}\left(\frac{\left(\vec{k}\times\vec{p}\right)^2}{k^2}\right)^2 G(\vec{p})G\left(\vec{k}-\vec{p}\right)$$

$D=2$, $d=3$ for simplicity, otherwise additional tensor structure

Self-consistent screening approximation II

For $D = 2, d = 3$ $\qquad \eta = \dfrac{4}{1+\sqrt{15}} \approx 0.821$ $\qquad$ close to our $\eta \approx 0.85$

Parameters for graphene



Simple interpolation

$$G_{\mathrm{a}}{}^{-1}(q) = \frac{\kappa q^4}{T} + \left(\frac{\kappa}{T}\right)^{1-\frac{\eta}{2}} \frac{q_0{}^{\eta} q^{4-\eta}}{\alpha}$$

works pretty well

For any d and D

$$G_{ij}(\mathbf{q}) = z\delta_{ij}|\mathbf{q}|^{-4+\eta'}$$

$$\frac{d_c}{2} = \frac{\Gamma(\frac{\eta'}{2})\Gamma(2-\eta')\Gamma(D+\eta')\Gamma(2-\frac{\eta'}{2})}{\Gamma(\frac{D}{2}+\frac{\eta'}{2})\Gamma(2-\eta'-\frac{D}{2})\Gamma(\frac{D}{2}+\eta')\Gamma(\frac{D}{2}+2-\frac{\eta'}{2})}$$

Formally exact in the limit $d_{\mathrm{c}} = d - D \to \infty$ but not too bad for physical case (for unknown reasons)

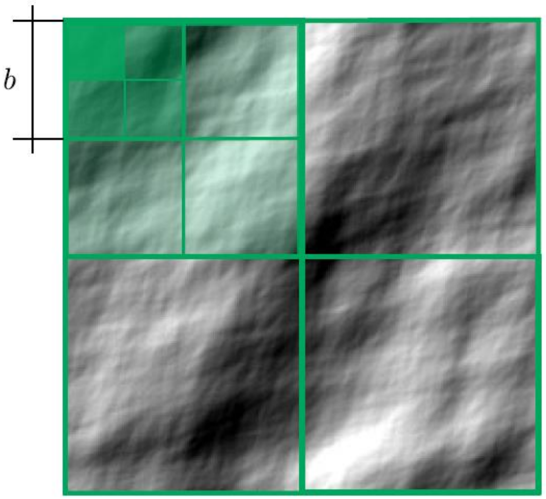
Modification of the model and ε-expansion

Scaling behavior of crystalline membranes: An ε-expansion approach

Achille Mauri *, Mikhail I. Katsnelson

Nuclear Physics B 956 (2020) 115040

Quantum field-theory RG based on the idea of scaling invariance



$$\kappa \to \kappa_{\mathrm{R}}(b) \propto b^{\eta}$$

renormalized bending rigidity

$$\lambda \to \lambda_{\mathrm{R}}(b) \propto b^{-\eta_u}$$

$$\mu \to \mu_{\mathrm{R}}(b) \propto b^{-\eta_u}$$

renormalized elastic moduli

Instead of working with initial model we introduce a new model (Gaussian curvature interaction, GCI model) coinciding with the correct one for $D = 2$ only)

Analogy:

Heisenberg model is either $O(n)$ model for $n = 3$ or $SU(N)$ for $N = 2$

GCI model

Hubbard-Stratonovich transformation

$$P[\mathbf{h}(\mathbf{x})] = \int [\mathrm{d}\lambda] \mathrm{e}^{-\mathcal{H}[(\mathbf{x}),\lambda(\mathbf{x})]}$$

$$\mathcal{H} = \int \mathrm{d}^D x \left[\frac{1}{2}(\partial^2 \mathbf{h})^2 + \frac{1}{2Y_0}(\partial^2 \lambda)^2 + i\lambda K \right]$$

local representation
consistent with locality in renormalization amplitudes

highly non-local interaction

$$E_{\text{eff}} = \frac{\kappa}{2} \int \mathrm{d}^2 x (\partial^2 h)^2 + \frac{Y}{16\pi} \int \mathrm{d}^2 x \int \mathrm{d}^2 x' |\mathbf{x} - \mathbf{x}'|^2 \ln \frac{|\mathbf{x} - \mathbf{x}'|}{a} K(\mathbf{x}) K(\mathbf{x}')$$

effective field theory for out-of-plane fluctuations in D=2-dimensional membranes

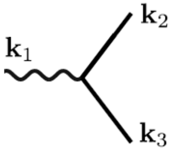
$$K(\mathbf{x}) = -\frac{1}{2}(\delta_{ij}\partial^2 - \partial_i \partial_j)(\partial_i h \partial_j h)$$

approximate Gaussian curvature

diagrammatic rules

$\mathbf{k}$ $\qquad$ $\mathbf{k}$

$\frac{1}{k^4}$ $\qquad$ $\frac{Y_0}{k^4}$

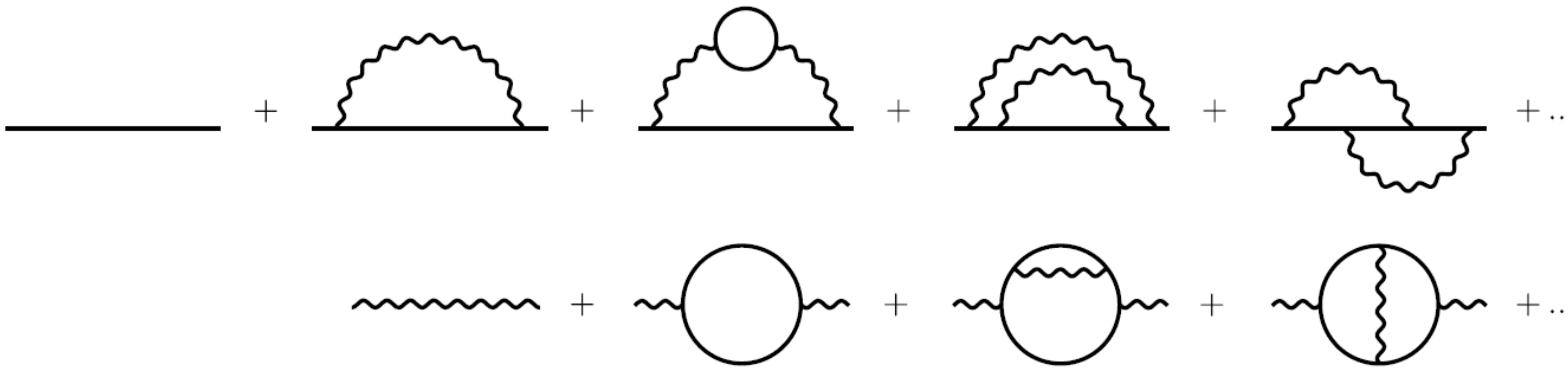


$$-i\left(k_1^2 k_2^2 - (\mathbf{k}_1 \cdot \mathbf{k}_2)^2\right)$$
$$= -i\left(k_2^2 k_3^2 - (\mathbf{k}_2 \cdot \mathbf{k}_3)^2\right)$$
$$= -i\left(k_3^2 k_1^2 - (\mathbf{k}_3 \cdot \mathbf{k}_1)^2\right)$$

and now we will consider this model for a generic D

As usual, $D = 4$ is a special case where interactions are marginal

GCI model II



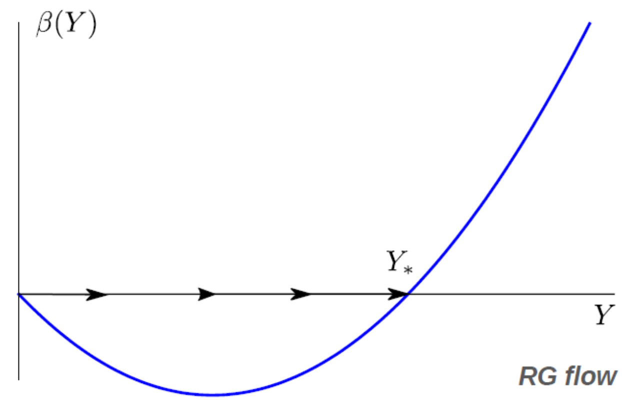
amplitude renormalization counterterm

$$\tilde{H} = \int \mathrm{d}^D x \left[\frac{Z}{2} (\partial^2 \mathbf{h})^2 + \frac{1}{2 Z_Y Y} (\partial^2 \lambda)^2 + i \lambda K \right]$$

coupling renormalization counterterm

dimensional regularization
D= 4- ε

$$Y_0 = M^{\varepsilon} \frac{Z_Y Y}{Z^2}$$

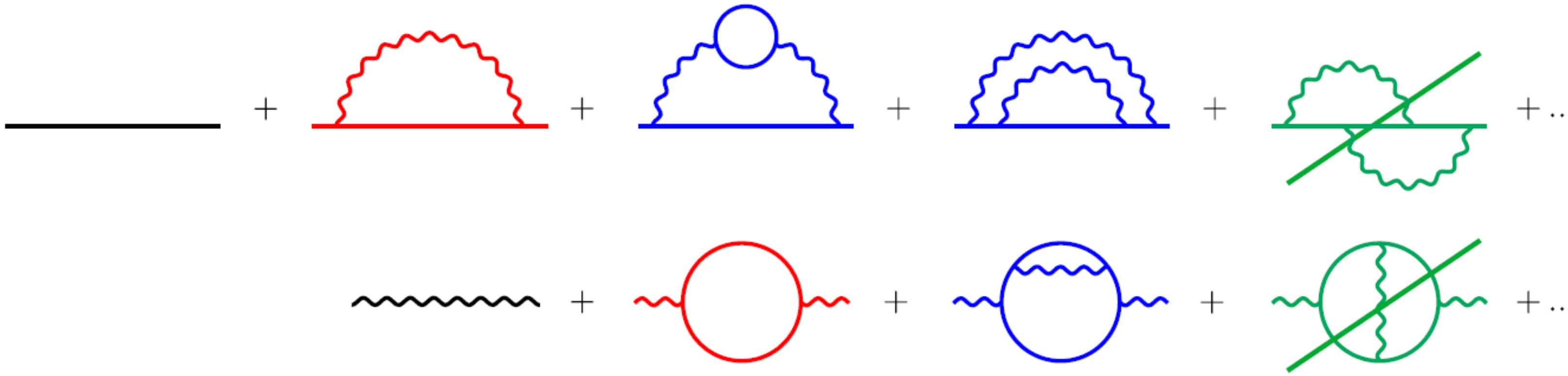


Parameters of the model:

$d_c = N$, the number of components of field ***h***

$D = 4 - \varepsilon$

GCI model III



cancellation of leading
vertex corrections
to $O(\varepsilon^2)$ value of the exponent

self-consistent screening approximation
exact at $O(\varepsilon^2)$

$$\eta = \frac{2\varepsilon}{N+4} - \frac{N(2-N)}{6(N+4)^3}\varepsilon^2 + \ldots$$

$$\to 0.8 - 0.005\bar{3} + \ldots$$

at $N = 1$ and $\varepsilon = 2$

$$\eta = \frac{2\varepsilon}{5} - \frac{\varepsilon^2}{750} + O(\varepsilon^3) \qquad \text{for } N = 1$$

Despite $\varepsilon = 2$ ε-expansion works amazingly well due to small numerical factors; 2 << 1

Scaling invariance without conformal invariance

Scale without conformal invariance in membrane theory

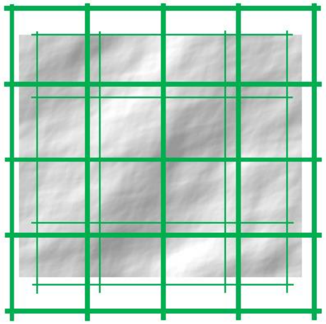
Achille Mauri *, Mikhail I. Katsnelson

Nuclear Physics B 969 (2021) 115482

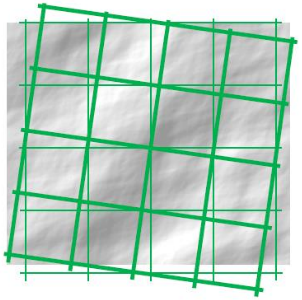
Motivation: Conformal invariance (if it holds) is the most powerful tool to calculate e.g. critical exponents with enormous accuracy – see recent results by Rychkov et al on 3D Ising model

The conformal bootstrap: Theory, numerical techniques, and applications
David Poland, Slava Rychkov, and Alessandro Vichi
Rev. Mod. Phys. **91**, 015002 (2019) - Published 11 January 2019

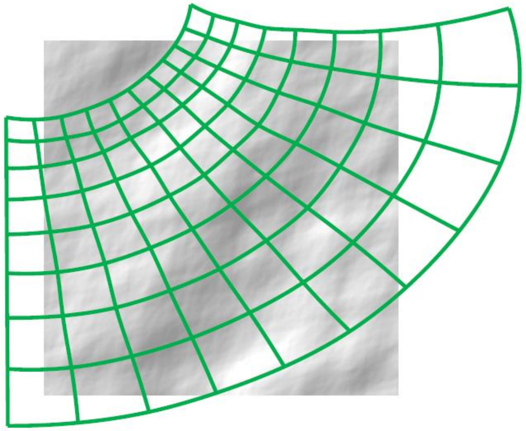
In 2D this is especially poweful but this is not our case, since embedding space is not 2D, so, we do not have infinite set of generators etc.



scale symmetry



rotation symmetry



conformal invariance

$$x'_\alpha = \frac{x_\alpha - b_\alpha x^2}{1 - 2(\mathbf{b}\cdot\mathbf{x}) + b^2 x^2}$$

Scaling invariance without conformal invariance II

$$[D, P_\alpha] = iP_\alpha$$

Poincaré group + dilatations

$$[P_\alpha, L_{\beta\gamma}] = i(\delta_{\alpha\beta}P_\gamma - \delta_{\alpha\gamma}P_\beta)$$

$$[L_{\alpha\beta}, L_{\gamma\delta}] = i(\delta_{\beta\gamma}L_{\alpha\delta} + \delta_{\alpha\delta}L_{\beta\gamma} - \delta_{\alpha\gamma}L_{\beta\delta} - \delta_{\beta\delta}L_{\alpha\gamma})$$

$$[D, K_\alpha] = -iK_\alpha$$

special conformal transformations

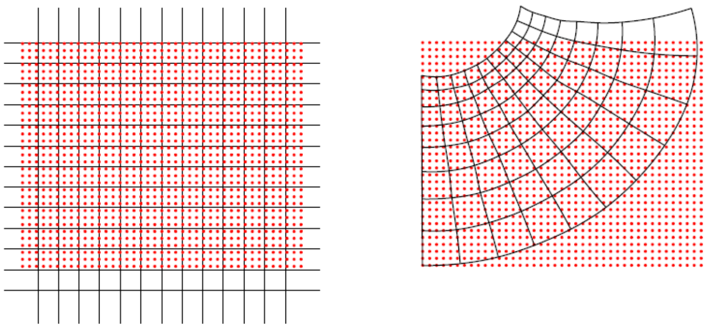
$$[K_\alpha, L_{\beta\gamma}] = i(\delta_{\alpha\beta}K_\gamma - \delta_{\alpha\gamma}K_\beta)$$

$$[K_\alpha, P_\beta] = 2i(\delta_{\alpha\beta}D - L_{\alpha\beta})$$

conformal generator

$$(d+1)(d+2)/2 \quad \text{generators}$$

Scaling invariance without conformal invariance III



$$\delta\mathcal{H} = -\int \mathrm{d}^D x T_{\alpha\beta}\partial_\alpha\epsilon_\beta$$

response to non-uniform Wilson's RG

energy-momentum tensor

$x'_\alpha = x_\alpha + \epsilon_\alpha(\mathbf{x})$

rotational invariance

$T_{\alpha\beta} = T_{\beta\alpha}$ $\qquad \epsilon_\alpha = \omega_{\alpha\beta}x_\beta \qquad \omega_{\alpha\beta} = -\omega_{\beta\alpha}$

scale invariance

$T_{\alpha\alpha} = \partial_\alpha V_\alpha$ $\qquad \epsilon_\alpha = \epsilon x_\alpha$

conformal invariance $\quad V^\alpha = j^\alpha + \partial_\beta L^{\alpha\beta}$ where j^α is conserved $(\partial_\alpha j^\alpha = 0)$

V^α is a local field, the 'virial current'

V^α must have a scaling dimension exactly equal to $\{V^\alpha\} = D - 1$ since $\{T_{\alpha\beta}\} = D$

Usually non-conserving currents for interacting fields acquires anomalous dimension and thus should vanish – therefore generally speaking scaling leads to conformal symmetry (if there are no special reasons to protect dimension of nonconserving vector current)

Scaling invariance without conformal invariance IV

Unitary theories in two dimensions

Wilson-Fisher fixed point

Unitary theories in four dimensions

Critical 3D Ising model

scale implies conformal invariance

Linear elasticity theory: an example of scale-invariant but non-conformal field theory

What about our case of anharmonic (nonlinear) elasticity?

$$\mathcal{H} = \frac{1}{2}\int \mathrm{d}^D x[(\partial^2 \mathbf{h})^2 + \lambda_0 (u_{\alpha\alpha})^2 + 2\mu_0 u_{\alpha\beta} u_{\alpha\beta}$$

$$u_{\alpha\beta} = (\partial_\alpha u_\beta + \partial_\beta u_\alpha + \partial_\alpha \mathbf{h}\cdot\partial_\beta \mathbf{h})/2$$

Important symmetries (incl. rotations of membrane in embedding space)

$$\mathbf{h} \to \mathbf{h} + \mathbf{A}_\alpha x_\alpha \ ,$$

$$u_\alpha \to u_\alpha - (\mathbf{A}_\alpha \cdot \mathbf{h}) - \frac{1}{2}(\mathbf{A}_\alpha \cdot \mathbf{A}_\beta) x_\beta$$

for any set of D vectors $\mathbf{A}_\alpha$ in $(d-D)$-dimensional space

Scaling invariance without conformal invariance V

$$T_{\alpha\alpha} = \overbrace{\frac{\varepsilon}{2}\left[(\partial^2 \mathbf{h})^2 + \lambda_0 (u_{\alpha\alpha})^2 + 2\mu_0 u_{\alpha\beta} u_{\alpha\beta}\right]}^{\text{scale-breaking term}} - E_\alpha u_\alpha + \partial_\alpha V_\alpha$$

trace of improved symmetric energy-momentum tensor

u_α field equation of motion

$$E_\alpha = \partial_\beta \sigma_{\alpha\beta}$$

$$\sigma_{\alpha\beta} = \lambda_0 \delta_{\alpha\beta} u_{\gamma\gamma} + 2\mu_0 u_{\alpha\beta}$$

virial current

$$V_\alpha = \left[(D-2)\lambda_0 + 2\mu_0\right] u_\alpha u_{\gamma\gamma} - 4\mu_0 u_\beta u_{\alpha\beta}$$

≠0 also at the fixed point
and $\neq \partial_\beta L_{\alpha\beta}$

Virial current does not vanish at the fixed point and does not obtain anomalous dimension (direct RG calculation)

Related to additional symmetries of the problem (incl. rotations in embedding space); the same conclusion for GCI model

A. Mauri and M.I. Katsnelson, NPB 969, 115482 (2021)

Quantum membranes: Graphene at low T

Phonons are Bose-particles with Planck distribution function

This provides third-low of thermodynamics: entropy $S \to 0$ at temperature $T \to 0$

Heat capacity also $\to 0$ at $T \to 0$. Harmonic approximation:

$$C_V(T) = \sum_{\lambda} C_{\lambda} \qquad C_{\lambda} = \left(\frac{\hbar\omega_{\lambda}}{T}\right)^2 \frac{\exp\left(\frac{\hbar\omega_{\lambda}}{T}\right)}{\left[\exp\left(\frac{\hbar\omega_{\lambda}}{T}\right) - 1\right]^2}$$

Thermal expansion coefficient

$$\alpha_p = \frac{1}{\Omega}\left(\frac{\partial \Omega}{\partial T}\right)_p$$

Ω is the volume for three-dimensional crystals and area for two-dimensional ones; p is the pressure

also should $\to 0$ since $\left(\frac{\partial \Omega}{\partial T}\right)_p = -\left(\frac{\partial S}{\partial p}\right)_T$ (Maxwell relation)

Quantum membranes II

Quasiharmonic approximation (Grüneisen law)

$$\alpha_p = \frac{\gamma C_V(T)}{\Omega B_T} \qquad \gamma = \frac{\sum_\gamma \gamma_\lambda C_\lambda}{\sum_\gamma C_\lambda} \qquad \gamma_\lambda = -\frac{\partial \ln \omega_\lambda}{\partial \ln \Omega}$$

microscopic Grüneisen parameters

PHYSICAL REVIEW B **86**, 144103 (2012)

Bending modes, anharmonic effects, and thermal expansion coefficient in single-layer and multilayer graphene

P. L. de Andres,[1] F. Guinea,[1] and M. I. Katsnelson[2]

$$\gamma_{\vec{q}} = -\frac{B}{2\kappa q^2}$$

$$\alpha_p \approx -\frac{1}{4\pi\kappa}\int_{q^*}^{q_T}\frac{dq}{q} = -\frac{1}{8\pi\kappa}\ln\frac{T}{\hbar\omega^*} \approx -\frac{1}{16\pi\kappa}\ln\frac{\kappa^3\rho}{\hbar^2 Y^2}$$

Negative and *T*-independent!!!

For flexural phonons, Grüneisen parameters diverge at $q \to 0$

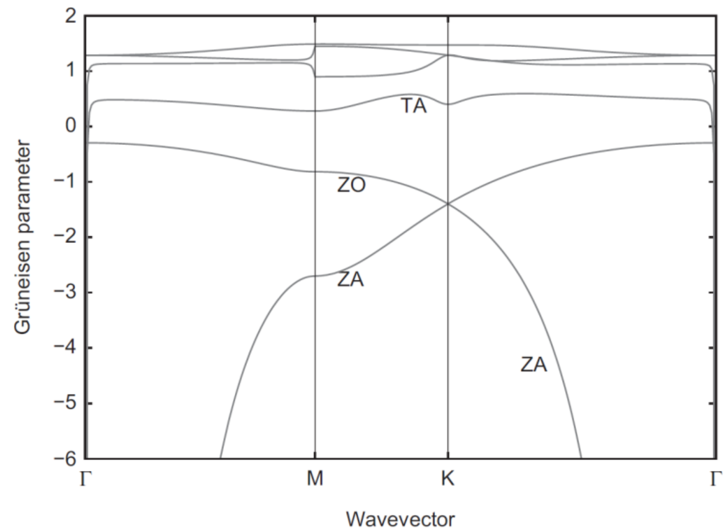


Fig. 9.9 Grüneisen parameters calculated in graphene with the potential LCBOBII.
(Reproduced with permission from Katsnelson & Fasolino, 2013.)

Quantum membranes III

One needs *quantum* theory of *anharmonic* flexural phonons!

PHYSICAL REVIEW B **94**, 195430 (2016)

Quantum elasticity of graphene: Thermal expansion coefficient and specific heat

I. S. Burmistrov,[1,2] I. V. Gornyi,[1,3,4,5] V. Yu. Kachorovskii,[1,3,4,5] M. I. Katsnelson,[6] and A. D. Mirlin[1,3,4,7]

Correct results with some heuristic arguments

PHYSICAL REVIEW B **105**, 195434 (2022)

Editors' Suggestion

Perturbative renormalization and thermodynamics of quantum crystalline membranes

Achille Mauri* and Mikhail I. Katsnelson

Full quantum field theory RG consideration

Partition function:

$$\mathcal{Z} = \int [d\mathbf{h}(\mathbf{x},\tau) du_\alpha(\mathbf{x},\tau)] e^{-S/\hbar}$$

$$\lambda = \hbar\tilde{\lambda}/(\tilde{\rho}\tilde{\kappa}^3)^{1/2}$$

$$\mu = \hbar\tilde{\mu}/(\tilde{\rho}\tilde{\kappa}^3)^{1/2},\ T = (\tilde{\rho}/\tilde{\kappa})^{1/2} k_B \tilde{T}/\hbar$$

areal mass density $\tilde{\rho}$

Quantum action (kinetic energy added):

$$S[\mathbf{r}(\mathbf{x},\tau)] = \int_0^{\hbar/(k_B\tilde{T})} d\tau \int d^2x \left\{ \frac{\tilde{\rho}}{2}\dot{\mathbf{r}}^2 + \frac{\tilde{\kappa}}{2}(\partial^2\mathbf{r})^2 + \frac{\tilde{\lambda}}{2}(U_{\alpha\alpha})^2 + \tilde{\mu} U_{\alpha\beta} U_{\alpha\beta} \right\}$$

Quantum membranes IV

Bare Green functions for in-plane (D) and out-of-plane (G) phonons

$$\bar{D}^{(0)}_{\alpha\beta}(\omega,\mathbf{k}) = \frac{\hbar k_\alpha k_\beta}{(\tilde{\rho}\omega^2 + (\tilde{\lambda} + 2\tilde{\mu})|\mathbf{k}|^2 + \tilde{\kappa}|\mathbf{k}|^4)k^2} + \frac{\hbar(k^2\delta_{\alpha\beta} - k_\alpha k_\beta)}{(\tilde{\rho}\omega^2 + \tilde{\mu}|\mathbf{k}|^2 + \tilde{\kappa}|\mathbf{k}|^4)k^2},$$

$$\bar{G}^{(0)}_{ij}(\omega,\mathbf{k}) = \frac{\hbar\delta_{ij}}{\tilde{\rho}\omega^2 + \tilde{\kappa}|\mathbf{k}|^4}.$$

Dimensional analysis at $\omega \sim k^2$ $\quad [\mathbf{x}] = -1 \quad [\tau] = -z = -2$

$$[\mathbf{h}] = (2 + z - 4)/2 = 0 \qquad [u_\alpha] = (2 + z - 2)/2 = 1$$

Terms $\tilde{\rho}\dot{u}_\alpha^2/2$ and $\tilde{\kappa}(\partial^2 u_\alpha)^2/2$ in S and $\partial_\alpha u_\gamma \partial_\beta u_\gamma$ in $U_{\alpha\beta}$ should be neglected. Important: all *together*, otherwise we break exact symmetries which lead to wrong results!!!

$$\mathcal{S} = \int_0^{1/T} d\tau \int d^2x \left\{ \frac{\dot{\mathbf{h}}^2}{2} + \frac{1}{2}(\partial^2\mathbf{h})^2 + \frac{\lambda}{2}(u_{\alpha\alpha})^2 + \mu u_{\alpha\beta}u_{\alpha\beta} - \sigma\partial_\alpha u_\alpha \right\},$$

Effective action

where $u_{\alpha\beta} = (\partial_\alpha u_\beta + \partial_\beta u_\alpha + \partial_\alpha \mathbf{h}\cdot\partial_\beta\mathbf{h})/2$, $\lambda = \hbar\tilde{\lambda}/(\tilde{\rho}\tilde{\kappa}^3)^{1/2}$, $\mu = \hbar\tilde{\mu}/(\tilde{\rho}\tilde{\kappa}^3)^{1/2}$, $T = (\tilde{\rho}/\tilde{\kappa})^{1/2}k_B\tilde{T}/\hbar$, and $\sigma = \tilde{\sigma}/\tilde{\kappa}$. After

Quantum membranes V

Importantly: at $D = 2$, $D + z = 4$, we are at the critical dimensionality, all divergences are logarithmic, and the theory is renormalizable

Renormalization of bending rigidity and Young modulus

$$\tilde{\kappa} \to \tilde{\kappa}_{\mathrm{r}}(k) = \left[1 + g_0 \ln \frac{\Lambda}{k}\right]^{\theta} \tilde{\kappa} \qquad \tilde{Y} \to \tilde{Y}_{\mathrm{r}}(k) = \left[1 + g_0 \ln \frac{\Lambda}{k}\right]^{3\theta/2-1} \tilde{Y}$$

$$g_0 = \frac{3(d_c + 6)Y}{128\pi} = \frac{3(d_c + 6)\hbar\tilde{Y}}{128\pi(\tilde{\rho}\tilde{\kappa}^3)^{1/2}}$$

$$\theta = 4/(d_c + 6)$$

($d_{\mathrm{c}} = 1$ for real membranes)

$g_0 \simeq 0.02$ for graphene

Bending rigidity increases as $(\log\Lambda)^{4/7}$

Young modulus decreases as $1/(\log \Lambda)^{1/7}$

Violation of Hooke's law: effective bulk modulus

$$\frac{1}{B_{\mathrm{eff}}(\sigma)} \approx \frac{1}{B} + \frac{8}{3Y}\left[\left(1 + \frac{3(d_c + 6)Y}{256\pi} \ln \frac{\Lambda^2}{\sigma}\right)^{\frac{d_c}{d_c+6}} - 1\right]$$

Quantum membranes VI

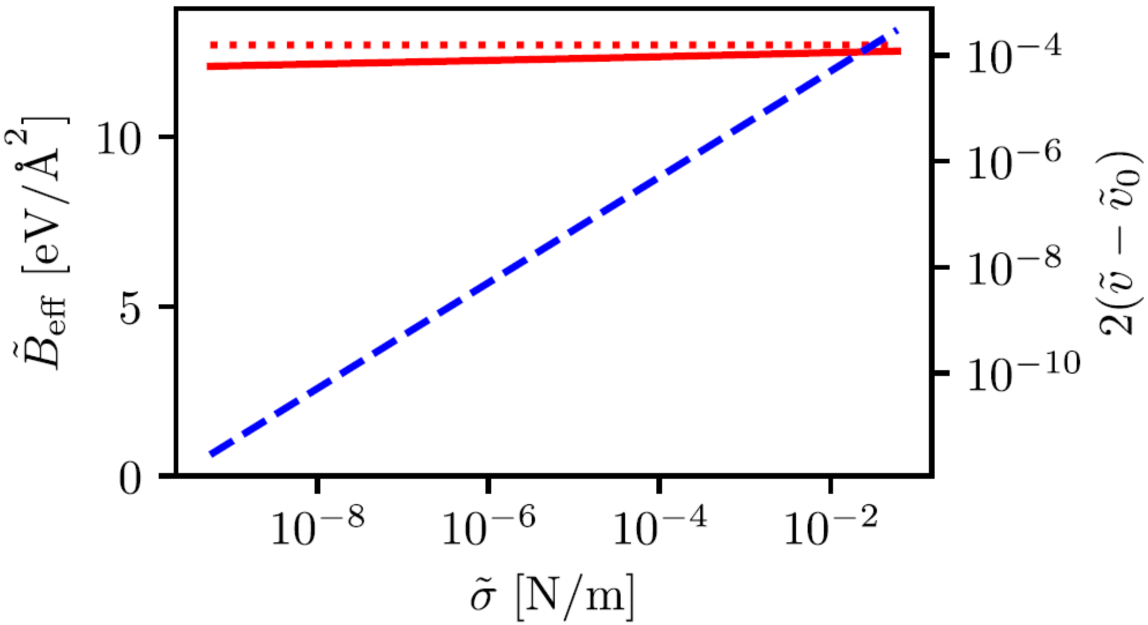


FIG. 2. Anomalous Hooke's law for a graphene membrane at $T = 0$. The red solid line represents the macroscopic bulk modulus $\tilde{B}_{\rm eff} = \frac{1}{2}\partial\tilde{\sigma}/\partial\tilde{v}$ as a function of the applied tension $\tilde{\sigma}$, as described by Eq. (41). The red dotted line is constant as a function of the applied stress and identifies the microscopic bulk modulus $\tilde{B} \simeq 12.7$ eV Å^{-2} controlling the normal Hooke's law for a membrane constrained in two dimension (without quantum-mechanical out-of-plane fluctuations). The strain induced by tension is represented by blue dashed lines. The effective bulk modulus vanishes in the limit $\sigma \to 0$ as $\tilde{B}_{\rm eff}(\sigma) \approx (\ln(1/\sigma))^{-1/7}$. The singularity, however, is very slow. The prediction for the stress-strain relation breaks down when the tension is so large that the stress dominates over bending rigidity at all momentum scales up to the cutoff Λ. Equation (41) is thus valid for $\tilde{\sigma} \ll \tilde{\kappa}\Lambda^2 \simeq 40$ N/m.

Quantum membranes VII

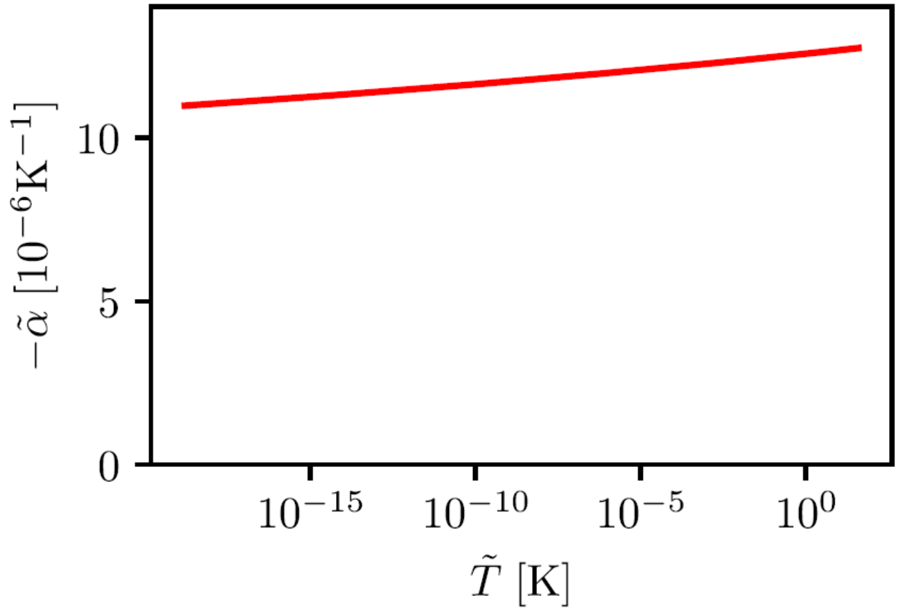


FIG. 3. Negative thermal expansion coefficient for an unstressed graphene membrane as a function of temperature (red solid line). In the limit $T \to 0$, $\tilde{\alpha} \to 0$ as expected from the third law of thermodynamics, but the approach to zero is only logarithmic with $\tilde{T}$.

A very strong prediction: almost constant thermal expansion coefficient for any realistic temperatures (for freely suspended 2D materials). Vanishes at $T \to 0$ but very slowly, as

$$\alpha_T \approx -\frac{d_c}{8\pi} \frac{\ln(\ln(\Lambda^2/T))}{[(g_0/2)\ln(\Lambda^2/T)]^{\theta}}$$

To conclude

1. We have quite good description of scaling properties for classical case
2. Rare example of nontrivial field theory with scaling but without conformal invariance
3. Quantum theory is renormalizable and can be considered quite rigorously.
4. Very unusual thermal expansion, on the border of violation of third law of thermodynamics
5. Beyond this talk: statistical physics of compressed membranes (still unsolved)

MANY THANKS FOR YOUR ATTENTION