

Graphene@KITP, January 2012

Graphene

an Electronic Crystalline Membrane

Doron Gazit

Racah Institute of Physics

Center for Nanoscience and Nanotechnology

האוניברסיטה העברית בירושלים
The Hebrew University of Jerusalem



Introduction

- Crystalline membranes – solid-like structures with $2D$ character – are very common in our world, in biophysics and condensed matter.
- Graphene is the ultimate crystalline membrane:
 - Can be used as a toy model, as it is simple enough for simulations.
- In addition, structure is a prominent part of quality control and design of graphene applications, as well as in transport properties.
- However,
 - **Experiments** show that **graphene possesses intrinsic ripples**, of sizes 100-300 Å.
 - The **theory** of crystalline membranes predicts a **scale invariant cascade of corrugations**, for a suspended, tension-less membrane.



Introduction

- ***What is the origin of the difference?***
 - I argue that the origin is an **interplay** between the **free electrons** on the surface, and the **elastic energy** of the lattice.
 - Indeed, **Graphane** shows reduced curvature (Elias et al., Science (2009)).
- The same microscopic intrinsic source leads to two disorder phenomena:
 - **Ripples** – topographic disorder
 - **Charge inhomogeneity** - electron hole puddles.



Outline

- Crystalline membranes.

DG, Phys. Rev. E **80**, 041117 (2009)

- Graphene as an electronic crystalline membrane.

- Connecting structure and the creation of electron hole puddles.

DG, Phys. Rev. B **80**, 161406 (2009)

- Stress induced by doping.

- Spontaneous buckling?
- An asymmetry in the transport properties of hole and electron doped graphene.

DG, Phys. Rev. B **79**, 113411 (2009)

- Summary



Outline

- **Crystalline membranes.**

DG, Phys. Rev. E **80**, 041117 (2009)

- Graphene as an electronic crystalline membrane.

- Connecting structure and the creation of electron hole puddles.

DG, Phys. Rev. B **80**, 161406 (2009)

- Stress induced by doping.

- Spontaneous buckling?
- An asymmetry in the transport properties of hole and electron doped graphene.

DG, Phys. Rev. B **79**, 113411 (2009)

- Summary



Fluctuations of crystalline membranes

Out of plane mode

$$F[\vec{u}, \mathbf{h}] = \frac{1}{2} \int d^2\vec{x} \left[k (\nabla^2 \mathbf{h})^2 + \left[(u_{ii})^2 + 2m u_{ij} u_{ij} \right] \right]$$

In-plane modes

Bending (curvature) energy

Strain energy

Deformation tensor:

$$u_{ij} = \frac{1}{2} (\nabla_i u_j + \nabla_j u_i) + \frac{1}{2} \nabla_i \mathbf{h} \times \nabla_j \mathbf{h} + \frac{1}{2} \partial_i u_k \partial_j u_k$$



The “size” of the 3rd dimension in graphene

- A 3D material is fully characterized by:

- 2 elastic constants:

$$\mu \text{ and } \lambda,$$

or alternatively

Young's modulus K_0 and Poisson ratio ν .

- The three constants in 2D elasticity are not independent!

- can be expressed in terms of the

3D young modulus, 3D Poisson ratio, and lateral size h :

$$h = \sqrt{12(1 - \nu^2) \frac{\kappa}{K_0}}$$

- Thus, the “elastic thickness” of graphene is less 1Å
- *Smaller than the lattice size!*
- Graphene, in the continuum limit, is the ultimate membrane!



Flat phase of crystalline membranes

$$F[\vec{u}, \mathbf{h}] = \frac{1}{2} \int d^2\vec{x} \left[K (\nabla^2 \mathbf{h})^2 + \lambda (u_{ii})^2 + 2\mu u_{ij} u_{ij} \right]$$

→ $F_{eff}[\mathbf{h}] = \frac{1}{2} \int d^2\vec{x} \left[K (\nabla^2 \mathbf{h})^2 + K_0 \left(\frac{1}{2} P_{ij}^T \partial_i \mathbf{h} \partial_j \mathbf{h} \right)^2 \right]$

$$K_0 = \frac{4\lambda(\mu + \lambda)}{2\lambda + \mu}$$

Harmonic part

Anharmonic term

Tensor:
 $u_{ij} \circ \frac{1}{2} (\partial_i u_j + \partial_j u_i) - \frac{1}{2} \nabla_i \mathbf{h} \times \nabla_j \mathbf{h}$



Remarks

- The harmonic approximation leads to unstable flat phase.

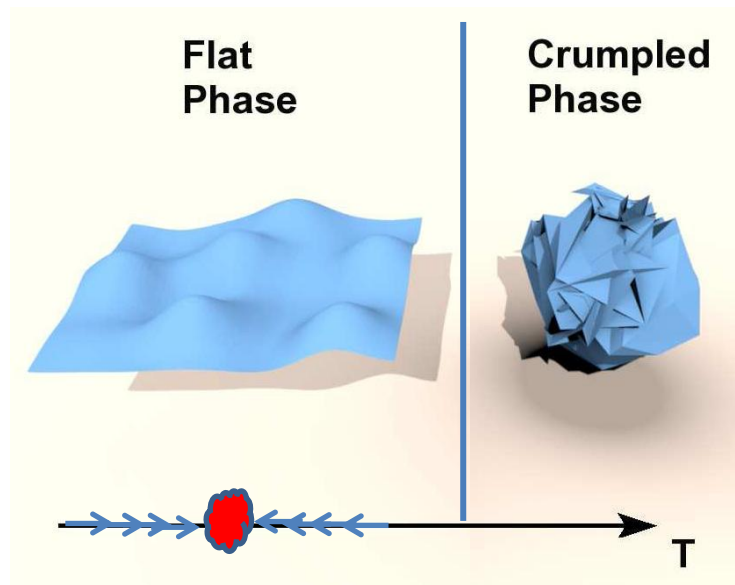
$$\vec{n} = \frac{\hat{z} - \vec{\nabla}h}{\sqrt{1 + |\vec{\nabla}h|^2}}$$

$$G(q) = 1 - \langle |n|^2 \rangle \sim \frac{\hbar}{2\rho} \langle |\vec{q}\mathbf{h}|^2 \rangle \sim \frac{\hbar}{L^{-1}} \frac{d^2\vec{q}}{(2\rho)^2} \frac{q^2}{kq^4} \sim \ln L$$



Remarks

- The harmonic approximation leads to unstable flat phase.
- Stable flat phase is due to anharmonic coupling between bending and stretching mode.
- An indication of the non-trivial, attractive, fixed point in the RG analysis of the problem.
- Confirmed using ε -expansion.





Remarks

- The harmonic approximation leads to unstable flat phase.
- Stable flat phase is an indication of a non-trivial fixed point.

$$\langle |\mathbf{h}|^2 \rangle = \int_{L^{-1}} \frac{d^D \vec{q}}{(2\rho)^D} \frac{k_B T}{k_R(q) q^4} \sim L^{2z} \quad 0 < z < 1$$

- Normal-normal correlation function:

$$G(q) = \langle |n|^2 \rangle = \sum \langle |\vec{q}\mathbf{h}|^2 \rangle \sim \int_{L^{-1}} \frac{d^2 \vec{q}}{(2\rho)^2} \frac{q^2}{k_R(q) q^4} \sim L^{2z-2} \xrightarrow{L \rightarrow \infty} 0$$

- An asymptotically flat surface, with scale invariant structure of softly diverging corrugations.
- Computing the anomalous exponents has been a huge challenge.



Crystalline Membranes – Partial History

- **80's – understanding the problem:**

1. D. R. Nelson and L. Peliti, J. Phys. France **48**, 1085 (1987).
2. J. A. Aronovitz and T. C. Lubensky, Phys. Rev. Lett. **60**, 2634 (1988).
3. M. Kardar and D. R. Nelson, Phys. Rev. A **38**, 966 (1988).
4. F. David and E. Guitter, Europhys. Lett. **5**, 709 (1988).
5. E. Gutter, F. David, S. Leibler, and L. Peliti, J. Phys. France **50** 1787 (1989)
6. J. Aronovitz, L. Golubovic, and T. Lubensky, J. Phys. France **50**, 609 (1989)

- **90's – understanding the solution – theory, simulations and experiment:**

1. P. Le Doussal and L. Radzihovsky, Phys. Rev. Lett. **69**, 1209 (1992)
2. Z. Zhang, H. T. Davis, and D. M. Kroll, Phys. Rev. E **48**, 651(R) (1993).
3. L. Radzihovsky and J. Toner, Phys. Rev. Lett. **75**, 4752 (1995)
4. L. Radzihovsky and J. Toner, Phys. Rev. E **57**, 1832 (1998).
5. C. Schmidt, K. Svoboda, N. Lei, I. Petsche, L. Berman, C., Safinya, and G. Grest, Science **259**, 952 (1993).
6. Z. Zhang, H. T. Davis, and D. M. Kroll, Phys. Rev. E **53**, 1422 (1996).
7. Mark J. Bowick, Simon M. Catterall, Marco Falcioni, Gudmar Thorleifsson, and Konstantinos N. Anagnostopoulos, J. Phys. I **6**, 1321 (1996)
8. M. Falcioni, M. J. Bowick, E. Gutter, and G. Thorleifsson, Europhys. Lett. **38**, 67 (1997).

- **“Graphene induced” revival:**

1. J.-P. Kownacki and D. Mouhanna, Phys. Rev. E **79**, 040101(R) (2009)
2. J. H. Los, M. I. Katsnelson, O. V. Zazyev, K. V. Zakharchenko, and A. Fasolino, Phys. Rev. B **80**, 121405(R) (2009).
3. D. Gazit, Phys. Rev. E **80**, 041117 (2009).
4. Zakharchenko, K. V.; Roldán, R.; Fasolino, A.; Katsnelson, M. I., Phys. Rev. B **82**, 125435.
5. Essafi, K.; Kownacki, J. -P.; Mouhanna, D. arXiv: 1011.6173
6. Hasselmann, N.; Braghin, F. L., arXiv: 1012.0313.



Self Consistent Screening Approximation

$$F[\vec{u}, \mathbf{h}] = \frac{1}{2} \int d^D \vec{x} \left[k (\nabla^2 \mathbf{h})^2 + l (u_{ii})^2 + 2m u_{ij} u_{ij} \right]$$

In general dimensionality (d -world, D -membrane, $d_C = d - D$):

$$F_{eff}[\vec{u}, \mathbf{h}] = \frac{1}{2} \int \frac{d^D \vec{q}}{(2\pi)^D} \left\{ k q^4 |\mathbf{h}_{\vec{q}}|^2 + \right.$$

$= 0$ for $D=2$

$$\frac{d^D \vec{k}'}{(2\pi)^D} \frac{R^{(D)}(\vec{q}, \vec{k}, \vec{k}')}{4(d-D)}$$

$k_i k_j k'_l k'_m \vec{r}_{ij,lm}(\vec{q})$

$$\mathbf{h}_{\vec{k}} \times \mathbf{h}_{\vec{q}-\vec{k}} \mathbf{h}_{\vec{k}'} \times \mathbf{h}_{-\vec{q}-\vec{k}'}$$

$$\vec{r} = 2m \vec{N}(\vec{q}) + 2b \vec{M}(\vec{q})$$

$$N_{ij,lm}(\vec{q}) = \frac{1}{D-1} P_{ij}^T(\vec{q}) P_{lm}^T(\vec{q})$$

$$M_{ij,lm}(\vec{q}) = \frac{1}{2} \left(P_{il}^T(\vec{q}) P_{jm}^T(\vec{q}) + P_{im}^T(\vec{q}) P_{jl}^T(\vec{q}) \right) - N_{ij,lm}(\vec{q})$$

$$b = \frac{m(2m + D/l)}{2m + l}$$



Self Consistent Screening Approximation

A diagrammatic expansion:

1. Every interaction introduces a $1/d_C$ factor.
2. Since the h propagator:

$$\langle \mathbf{h}(\vec{q}) \mathbf{h}(-\vec{q}) \rangle = \mathbf{I}_{d_C, d_C} k_B T G(q)$$

Every loop introduces a d_C factor.

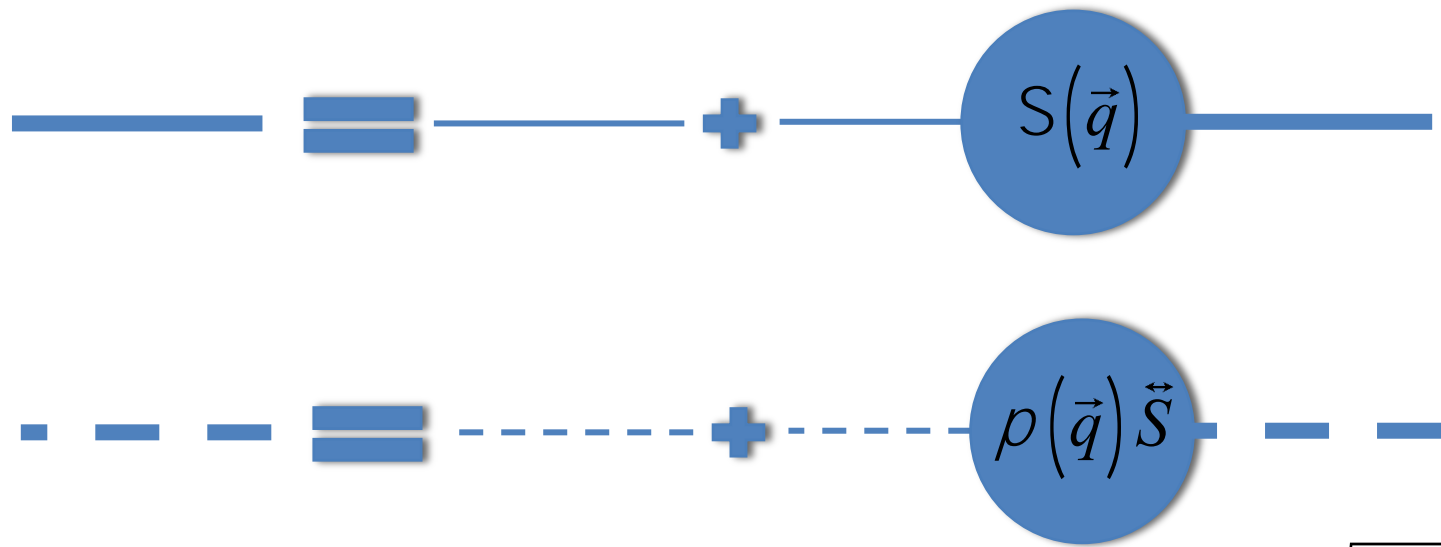
A $1/d_C$ expansion is called for.

Order of expansion: $n = \text{Number of interactions} - \text{Number of loops}$

Radzihovsky, Le-Doussal, PRL **69**, 1209 (1992);
DG, PRE **80**, 041117 (2009)



Self Consistent Screening Approximation



The long-wavelength approximation: $q \ll q_T = \sqrt{\frac{K_0 k_B T}{k^2}}$

$$K_0(\vec{q}) \underset{q \rightarrow 0}{\sim} q^{h_u} \quad k(q) \underset{q \rightarrow 0}{\sim} S(q) \sim q^{-h}$$

A general result:

$$h_u = 4 - D - 2h$$

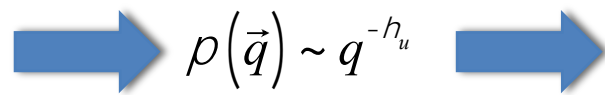


Self Consistent Screening Approximation

A Dyson equation for the interaction: $\vec{r}_R = \vec{r} - \rho(q) \vec{r} \times \vec{S} \times \vec{r}_R$

$$m_R(\vec{q}) = \frac{m}{1 + 2m\rho(\vec{q})}$$

$$b_R(\vec{q}) = \frac{b}{1 + (D+1)b\rho(\vec{q})}$$



$$\rho(\vec{q}) \sim q^{-h_u}$$

$$\lim_{q \rightarrow 0} \frac{l(q)}{m(q)} = -\frac{2}{D+1}$$

$D \neq 1, 2$

A universal negative Poisson's Ratio for $D \neq 1, 2$

D=2: simulations give $\nu = -0.32(1)$,
extrapolation of SCSA $\nu = -1/3$.

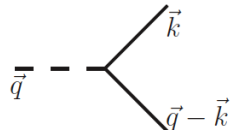
Falcioni *et al*, *Europhys. Lett.* **38**, 67 (1997)

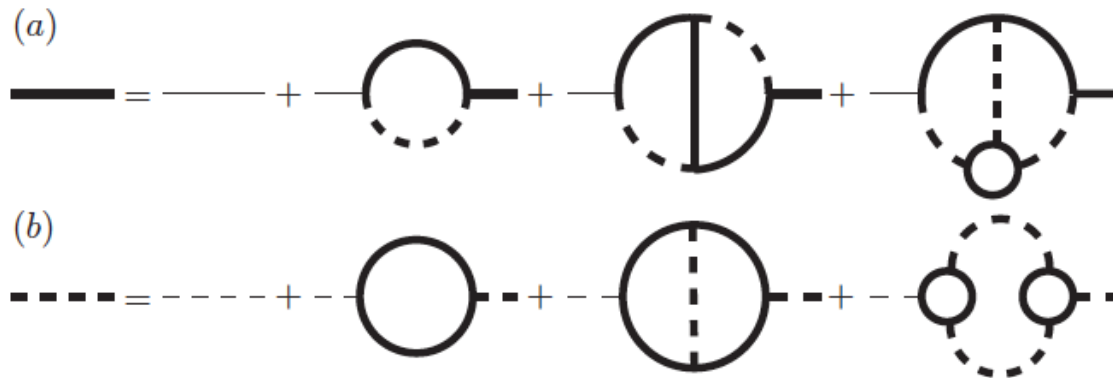


SCSA Results for physical membranes

$(\beta\kappa q^4)^{-1}$  **h** propagator

βK_0  Interaction propagator

$-\frac{1}{2}[\hat{q} \times \vec{k}]^2$  Interaction vertex





SCSA Results for physical membranes

1st order

- A one loop expansion.
- Recovers all other expansions.

$$Z = 0.590\dots$$

$$\lim_{q \rightarrow 0} \frac{\sqrt{k_B T K_R(q)}}{q K_R(q)} = 3.351\dots$$

$$\lim_{q \rightarrow 0} \frac{l(q)}{m(q)} \stackrel{D^{1,2}}{=} -\frac{2}{D+1}$$

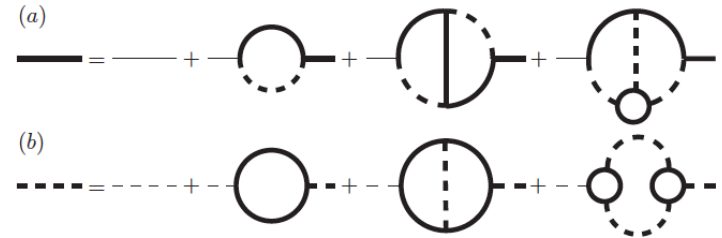
2nd order

- Gives a result **iff** regarded as a $1/d_C$ expansion.

$$Z = 0.605\dots$$

$$\lim_{q \rightarrow 0} \frac{\sqrt{k_B T K_R(q)}}{q K_R(q)} = 3.573\dots$$

$$\lim_{q \rightarrow 0} \frac{l(q)}{m(q)} \stackrel{D^{1,2}}{=} -\frac{2}{D+1}$$





Crystalline membranes and graphene

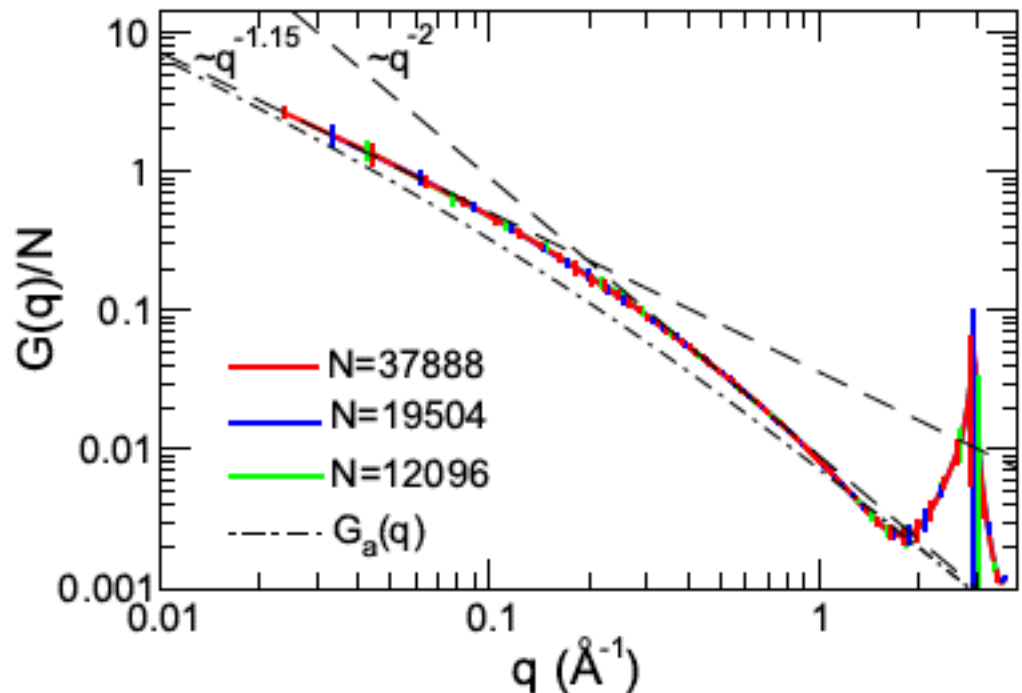
- Going to second order has not changed the general results:
 - Scale free structure at wavelengths much longer than the thermal wavelength ≈ 1.2 nm in graphene.
- Numerical solution of the SCSA equation to first order leads to the same conclusion.

Zakharchenko, Roldán, Fasolino, Katsnelson, Phys. Rev. B **82**, 125435.



Atomistic simulations of graphene

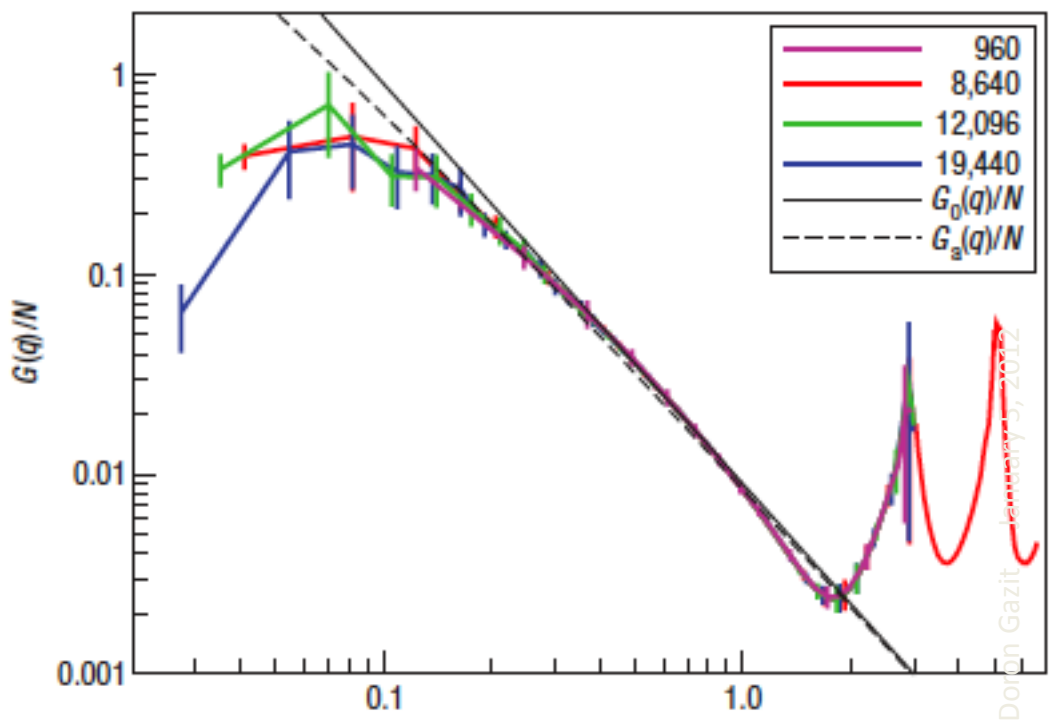
- Los et al. [PRB(R) (2009)] have used carbon-carbon potential to calculate *normal-normal correlation*.
- They found a behavior consistent with the theory of crystalline membranes.
- **No sign of ripples.**



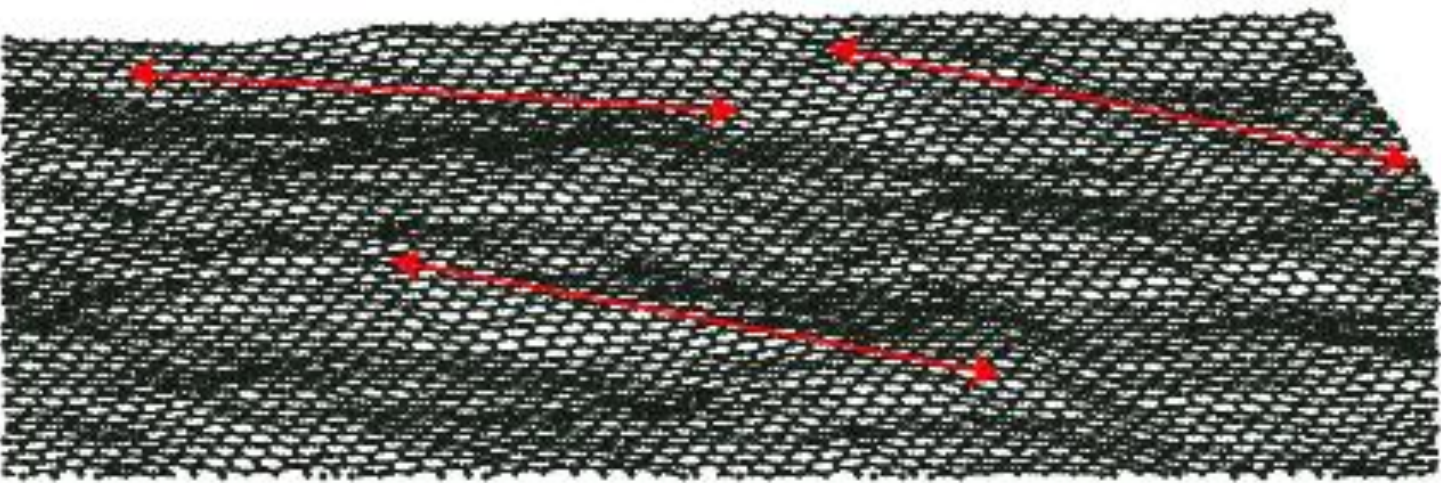


- How should ripples look?

Los, Fasolino, Katsnelson, Nature Materials 6, 858 [2007].



Graphene@KITP - Dordon Gazit - January 5, 2012





Physical membranes:

Method	ζ	References
1 st order SCSA	0.590...	Radzihovsky, Le-Doussal, PRL, 69 , 1209 (1992)



Crystalline membranes and graphene

- Going to second order has not changed the general results:
 - Scale free structure at wavelengths much longer than the thermal wavelength ≈ 1.2 nm in graphene.
- Numerical solution of the SCSA equation to first order leads to the same conclusion.
- No signature of ripples using state of the art atomic carbon-carbon interaction in QMC or MD simulations.
- Existence of intrinsic ripples in graphene implies that:

Graphene is not a regular crystalline membrane.



Outline

- Crystalline membranes.

DG, Phys. Rev. E **80**, 041117 (2009)

- **Graphene as an electronic crystalline membrane.**

- Connecting structure and the creation of electron hole puddles.

DG, Phys. Rev. B **80**, 161406 (2009)

- Stress induced by doping.
 - Spontaneous buckling?
 - An asymmetry in the transport properties of hole and electron doped graphene.

DG, Phys. Rev. B **79**, 113411 (2009)

- Summary



What about the π electrons?





An interplay between charge inhomogeneities and corrugations

- In the presence of corrugations, the surface area changes:

$$\delta S \sim a^2 u_{ii}$$

- This changes the ion density, and thus the electron density.
- As a result, the electron's chemical potential is locally changed
→ an effective induced electric field:

$$V(r) = D u_{ii} ; D = 10 - 30 eV$$

Suzuura, Ando PRB, 65, 235412 (2002)
Katsnelson, Perreira, Castro-Neto, Guinea,
Geim, Kim, Fogler, Horovitz, ...



The total Classical free energy

Charge inhomogeneity

Electron-electron interaction

$$F[u, h, \delta n] = E_{ee}[\delta n] + \frac{1}{2} \int d^2 \vec{x} \kappa (\Delta h)^2 + \frac{1}{2} \int d^2 \vec{x} [2\mu u_{ij}^2 + \lambda u_{ii}^2 + 2D u_{ii} \delta n]$$

Elastic energy

Coupling between structure and charge inhomogeneity

$$E_{ee} = \frac{e^2}{2\epsilon} \int \int d^2 x d^2 y \frac{\delta n(\vec{x}) \delta n(\vec{y})}{|\vec{x} - \vec{y}|} = \frac{1}{2\epsilon} \int \frac{d^2 q}{(2\pi)^2} \frac{|\delta n(\vec{q})|^2}{q}$$



Intrinsic ripples in graphene

$$F_{eff}(\mathbf{h}) = \frac{1}{2} \frac{d^2 \vec{q}}{(2\rho)^2} \left[k(q^2 \mathbf{h})^2 + \underbrace{K(q)}_{F(h(\vec{x})) = \frac{1}{2} P_{ij}^T \parallel_i h \parallel_j h} F^2(q) \right]$$

$$K(q) = K_0 \frac{1 - \frac{2\mu + \lambda}{\mu + \lambda} \frac{q}{q_0}}{1 - \frac{q}{q_0}} \quad \xi_0 = \frac{2\pi}{q_0} \equiv \frac{D^2 \frac{E}{e^2}}{2\mu + \lambda}$$

- The screening factor was estimated using RPA calculations

V. N. Kotov, B. Uchoa, and A. H. Castro Neto, Phys. Rev. B **78**, 035119 (2008)

- For 2D materials, this means inherent competition between bending and stretching.
- Ripples compensate this competition.



Intrinsic ripples in graphene

The long wavelength limit is not changed, however a new scale comes into play due to the free electrons on the membrane.

 (q)

Need to solve:

$$\begin{cases} y(q) = 1 + \left(\frac{q_T}{q}\right)^2 \Sigma(q) \\ z(q) = 1 + \frac{1}{2} \left(\frac{q_T}{q}\right)^2 \Psi(q) \end{cases} \quad \text{around } q \approx q_0$$

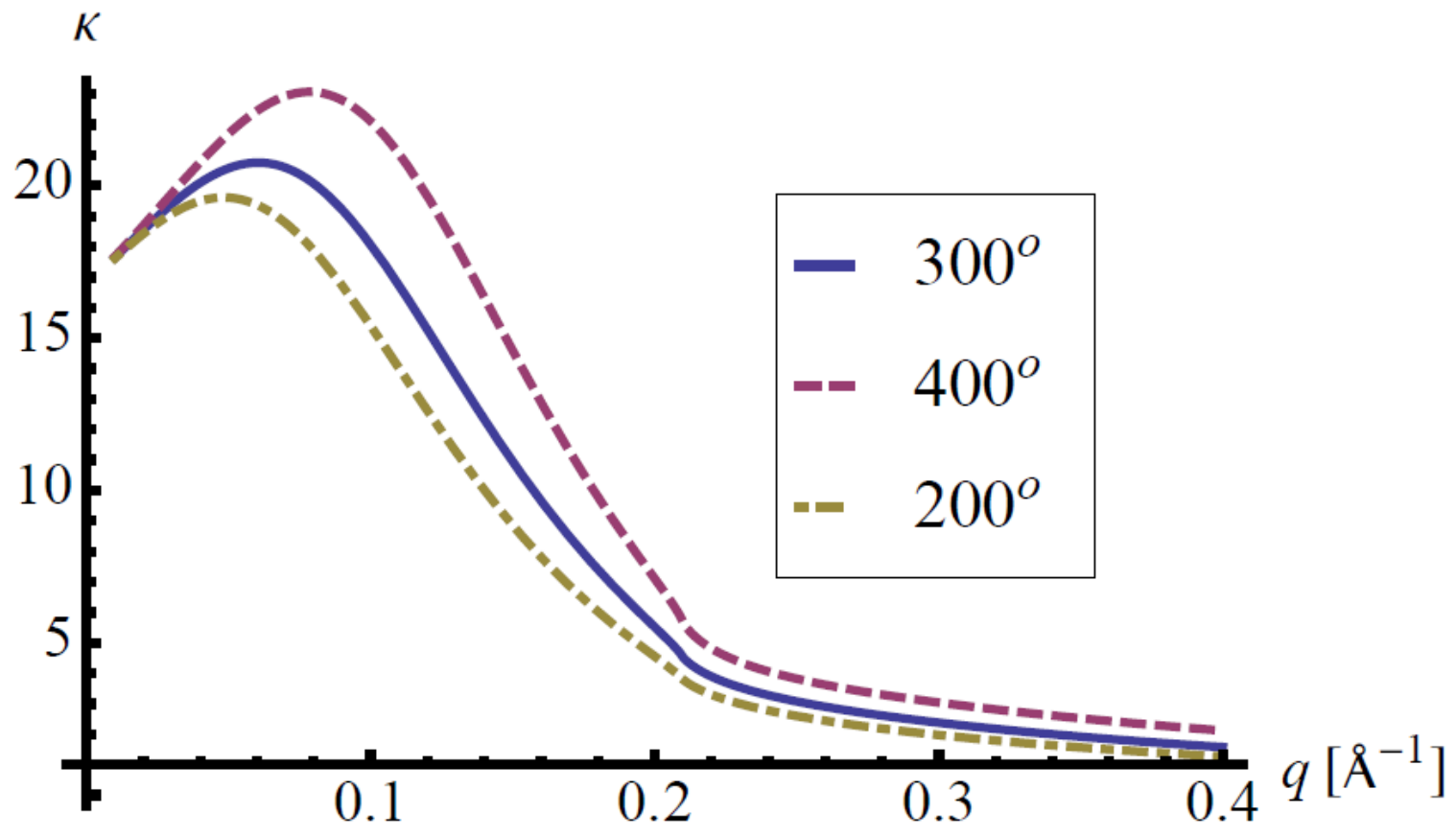
$$\Sigma(q) = \mathcal{P} \int \frac{d^2 \vec{k}}{(2\pi)^2} \frac{K(qk)}{K_0} \frac{|\hat{q} \times \hat{k}|^4}{|\hat{q} - \hat{k}|^4}$$



Normal-Normal Correlation

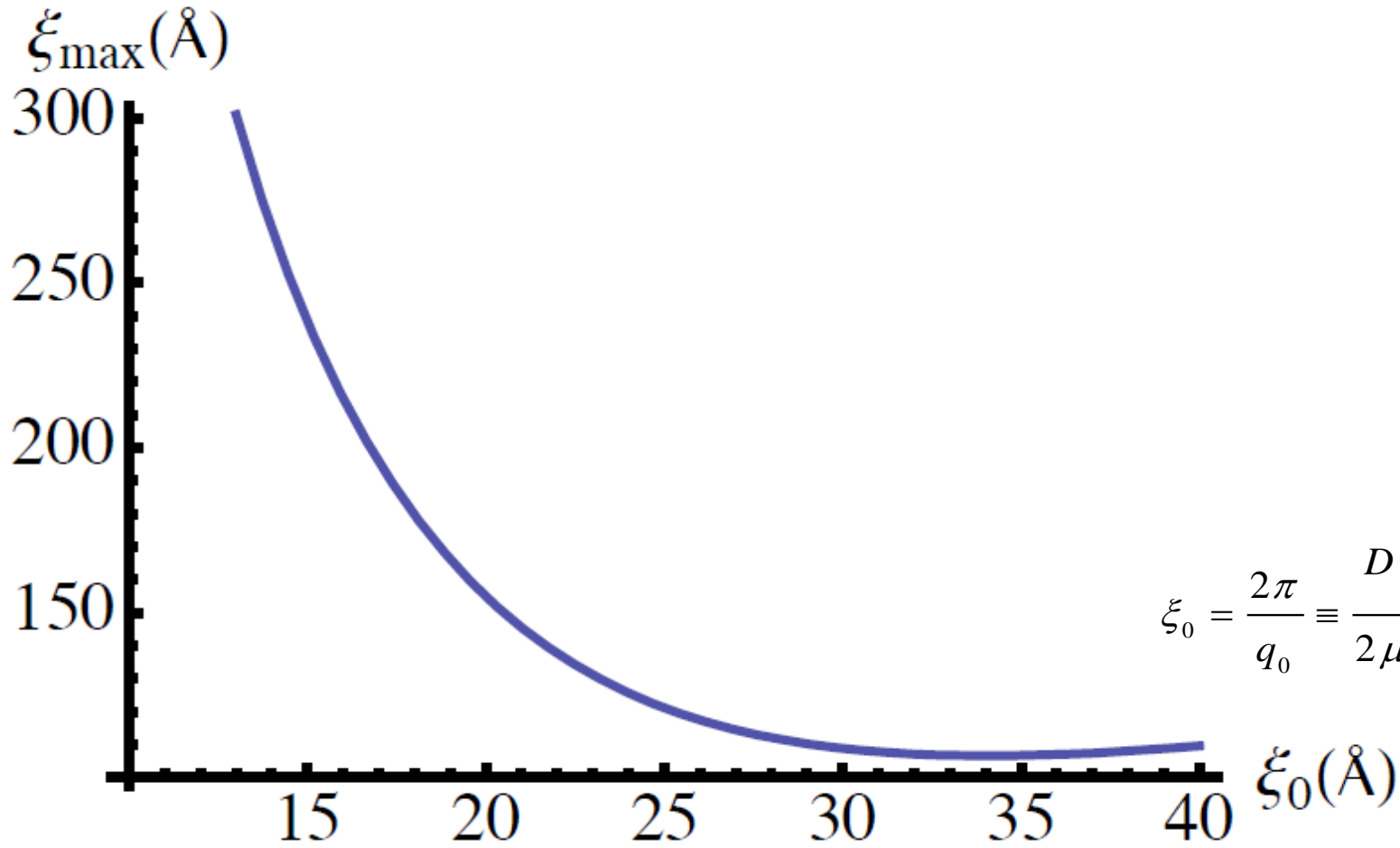
Function

$$\frac{G(q,T) K_0}{K}$$





Characteristic Size of Ripples



$$\xi_0 = \frac{2\pi}{q_0} \equiv \frac{D^2 \frac{E}{e^2}}{2\mu + \lambda}$$



Characteristics of Ripples

- Wavelength: 100-300Å.
 - Recovers measurements of Meyer et al. (2007).
- Amplitude: 5-20 Å.
- Correlation between charge inhomogeneities and ripples:
 - Circumstantial evidence: **Graphane's** structure is consistent with no ripples!
 - This model indicates that the charge inhomogeneities will be correlated to the Gaussian curvature.

$$dn \propto S_e^h(x) \propto -\frac{1}{2} \left(d_{ij}^2 - \frac{1}{h_i h_j} \right) \frac{1}{h_i h_j}$$

Marco Gibertini et al., arXiv:1111.6280.

- previous theories and measurements searched for correlations in the mean curvature.

Castro-Neto, Kim, EPL (2008); Deshpande et al. PRB (2009)



Outline

- Crystalline membranes.

DG, Phys. Rev. E **80**, 041117 (2009)

- Graphene as an electronic crystalline membrane.

- Connecting structure and the creation of electron hole puddles.

DG, Phys. Rev. B **80**, 161406 (2009)

- **Stress induced by doping.**

- Spontaneous buckling?
- An asymmetry in the transport properties of hole and electron doped graphene.

DG, Phys. Rev. B **79**, 113411 (2009)

- Summary



Doped Graphene

- Until now, we neglected the dynamics of the electrons.
- In other words, the Dirac action should be taken into account:

$$S = - \int_{n=1}^2 \int_0^b dt d^2\vec{x} \bar{Y}_n(t, \vec{x})$$

$$\left\{ g_0 \frac{\partial}{\partial t} + i \left(D_{\vec{u}} + \mu \right) + v_f \vec{g} \cdot \left(\vec{\nabla} + g_5 \vec{A} \right) \right\} Y_n(t, \vec{x})$$

Deformation Energy

Chemical potential

Pseudo-Magnetic gauge fields

$$\vec{A}(\vec{r}) = \frac{g_2}{v_f} \begin{pmatrix} 2u_{xy} & 0 \\ u_{xx} - u_{yy} & 0 \end{pmatrix} \quad g_2 \sim 1 - 3 \text{ eV}$$



π electrons effect on the surface structure

- The surface structure is determined by the elastic free energy:
 - A low q expansion of the free energy.
 - The contribution of the σ electrons – elasticity.
- At low q , the π electrons are well described by the Dirac picture.
- All we have to do is to evaluate the π electrons contribution to the free-energy.
- The acoustic velocity is much smaller than the Fermi velocity:


$$v_{ph} \approx 2 \cdot 10^6 \frac{\text{cm}}{\text{sec}} \ll v_f \approx 10^8 \frac{\text{cm}}{\text{sec}}$$

- Thus – one can integrate out the degrees of freedom of the electrons (Average the effect of the free electrons).

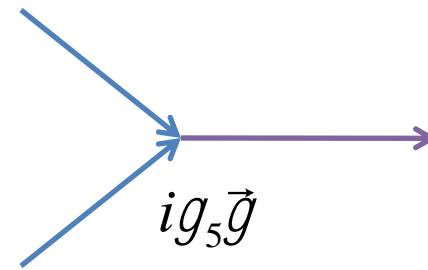


Feynman Diagrams for π -Electrons

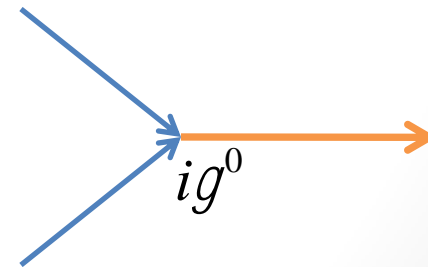
- Fermion propagator
- No Vector/Electro-chemical potential propagator.


$$\frac{i}{g_m k^m}$$

- Vector pot./Fermion vertex



- Electro-chem. Pot/Fermion vertex

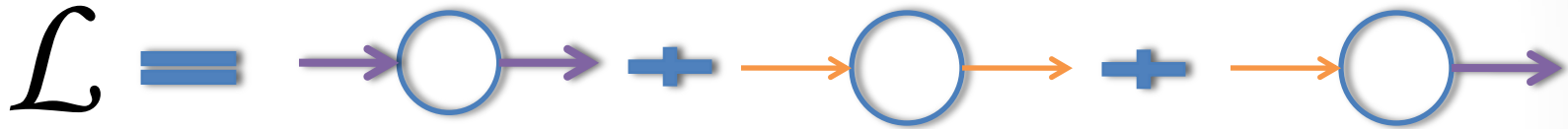




Integrating out the π -electrons

- The resulting (perturbative) Lagrangian is pure gauge.

$$\mathcal{L} = \frac{1}{2} A_i P_{ij}^A A_j + \frac{1}{2} P^V V^2$$





“Structure” Polarization operators

$$P^V(q_0 = 0; \vec{q}) = \frac{1}{b} \int_{S=1}^{w_f} \int_{w_f} \frac{d^2 \vec{k}}{(2\rho)^2} \text{Tr} \left[\frac{g^a k_a}{k^2} g^0 \frac{g^b (k+q)_b}{(k+q)^2} g^0 \right]$$

$$P_A^{ij}(q_0 = 0; \vec{q}) = \frac{1}{b} \int_{S=1}^{w_f} \int_{w_f} \frac{d^2 \vec{k}}{(2\rho)^2} \text{Tr} \left[\frac{g^a k_a}{k^2} g_5 g^i \frac{g^b (k+q)_b}{(k+q)^2} g_5 g^j \right]$$

$$w_f = \frac{2\rho}{b} \left(n + \frac{1}{2} \right) \quad k^m = (w_f, \vec{k})$$



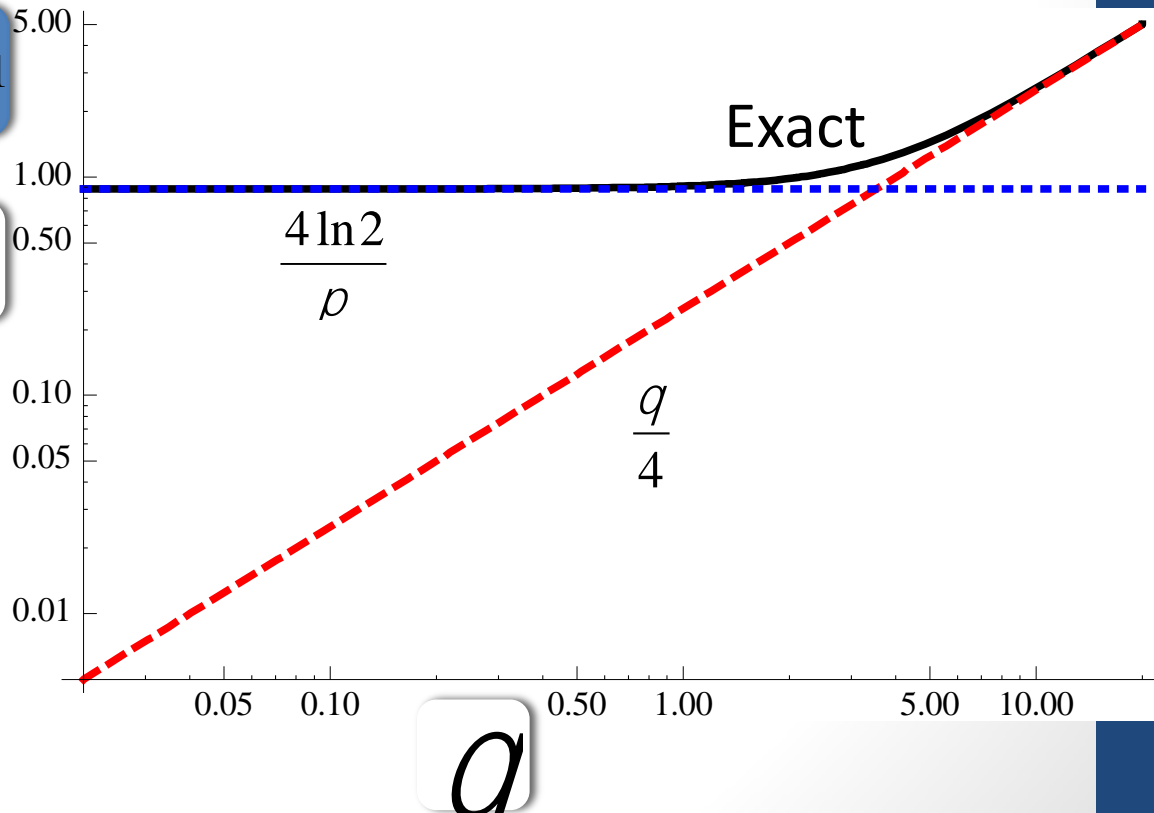
Electro-chemical "Structure" Polarization Operator

$$P^0 (\hbar v_f)^2 b P^V (q^0 \hbar v_f b q) = \frac{4}{\rho} \int_0^1 dx \ln \left[2 \cosh \left(\frac{q}{2} \sqrt{x(1-x)} \right) \right] = \begin{cases} \frac{4 \ln 2}{\rho} & q \ll 1 \\ \frac{q}{4} & q \gg 1 \end{cases}$$

$$\hbar v_f b q \gg 15 \frac{T}{300^\circ \text{K}} \approx \frac{1}{100 \text{A}} \gg 1$$

$$P_{ij}^A(\vec{q}) = \frac{\hbar v_f q}{4} d_{ij} - \frac{q_i q_j}{q^2}$$

$$P^V(\vec{q}) = \frac{q}{4 \hbar v_f}$$





Elastic Free-Energy

$$F[\vec{u}, h] = \frac{1}{2} \int \frac{d^2 \vec{q}}{(2\pi)^2} \hat{e}^i \hat{e}^j k q^4 |h|^2 + l(q) (u_{ii})^2 + 2m(q) (u_{ij})^2 - \frac{\hbar v_f q}{4} |\vec{A} \times \hat{q}|^2$$

$$l(q) = l + \frac{D^2 q}{4\hbar v_f} \quad m(q) = m + \frac{g_2^2 q}{8\hbar v_f}$$

- q dependence of elastic constants.
- Preferred directions.



Effect of an External Electro-chemical potential

$$F(\vec{u}, \hbar) = \frac{1}{2} \int \frac{d^2 \vec{q}}{(2\pi)^2} \left[k q^4 |\hbar|^2 + l(q) (u_{ii})^2 + 2m(u_{ij})^2 + 2D(u_{ii})_{-q} P^V(q; b) \right] dV_q$$

- For constant external potential:

$$dF(\vec{u}, \hbar) = t \int d^2 \vec{x} u_{ii}(\vec{x}) \quad t = \frac{4D \ln 2 \times k_B T}{\rho (\hbar v_f)^2} dV$$

Chemical potential induces additional stress!



Spontaneous Buckling of hole doped graphene

- Take the harmonic approximation:

$$F[h] = \frac{1}{2} \int d^2\vec{x} \left[\kappa (\nabla^2 h)^2 + t (\vec{\nabla} h)^2 \right]$$

$$0 = \frac{\delta F}{\delta h} = \kappa q^4 h + \tau q^2 h \Rightarrow \begin{cases} \tau < 0 & q^* = \sqrt{\frac{|\tau|}{\kappa}} \\ \tau \geq 0 & q^* = 0 \end{cases}$$

negative stress (hole-doping) leads to buckling!

$$\xi = 2\pi \sqrt{\frac{\pi (\hbar v_f)^2 \beta \kappa}{4D \ln 2 \cdot \delta V}} = 144 \text{ \AA} \cdot \left(\frac{T}{300^\circ\text{K}} \right)^{-1/2} \cdot \left(\frac{D}{20\text{eV}} \right)^{-1/2} \cdot \left(\frac{\delta V}{100\text{meV}} \right)^{-1/2}$$

- When using the electric field effect: $e_f \sim \hbar v_f \sqrt{\rho n}$

$$\chi \sim 270 \text{ \AA} \frac{|V_g|}{10\text{V}}^{-1/4}$$



Rippling side-effect: Additional Resistivity

- The disorder phenomena: ripples and charge inhomogeneities are a source for deviation from ballistic conductance.

$$r \approx \frac{\hbar}{e^2} \left(\frac{T}{k} \cdot \frac{\chi}{a} \right)^2 \approx 200 - 600 \Omega \left(\frac{T}{300^\circ K} \right) \cdot \left(\frac{|n|}{10^{12}} \right)^{-1/2}$$

- The different structural response of hole- and electron-doped graphene creates an inherent asymmetry!

Katsnelson and Geim, Phil. Trans. R. Soc. A 366, 195 (2008).



Bolotin et al. 2008

Nevertheless, this large asymmetry is unusual and presently unresolved and, together with the observed n dependence, may point to a scattering behavior in suspended graphene that is more complex than simple electron-phonon interaction.



Summary

- Graphene is an example of a new class of materials:
electronic crystalline membranes,
in which a strong interplay exists between the structure and the free electrons in the membrane.
- The π -electrons induce:
 - **Ripples** due to competition between electron-electron interaction and electron-phonon interaction.
 - Additional stress in the presence of a chemical potential.
 - Can lead to **buckling in the case of hole doping**.
- Outlook:
 - Phase diagram in the presence of impurities and other defects.
 - Effect on transport.