Interactions and the minimal conductivity of graphene
Phonon-phonon interactions and the elastic properties of graphene

M. I. Katsnelson
V. Parente
C. Gomez-Navarro
J. Gomez
G. Lopez-Polin
F. Perez-Murano

also M. M. Fogler,
M. Polini

Outline

- Ballistic graphene
- Tunneling and dissipation
- Phonon-phonon interactions in graphene
- Defects and elastic constants

Experiments

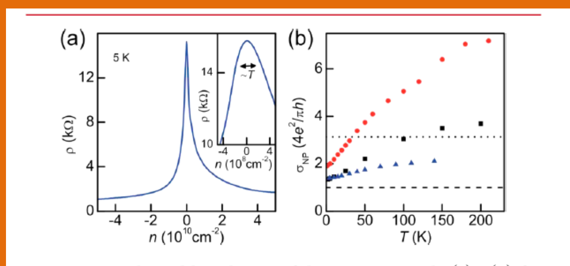
NANO LETTERS

Letter

pubs.acs.org/NanoLett

How Close Can One Approach the Dirac Point in Graphene Experimentally?

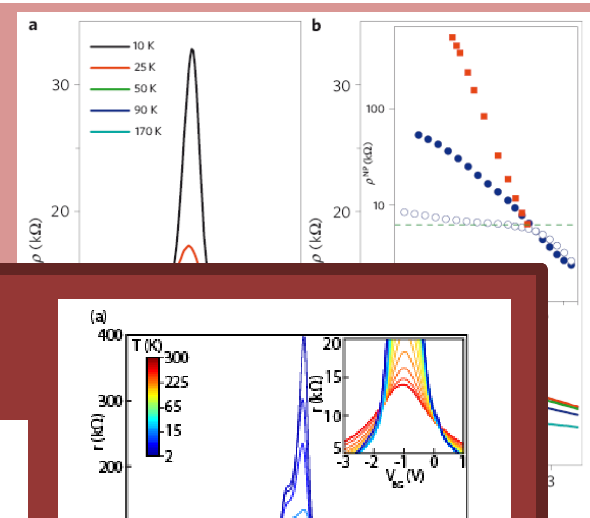
Alexander S. Mayorov,*,† Daniel C. Elias,† Ivan S. Mukhin,‡ Sergey V. Morozov,§ Leonid A. Ponomarenko,† Kostya S. Novoselov,† A. K. Geim,†,‡ and Roman V. Gorbachev†,‡



LETTERS
PUBLISHED ONLINE: 9 OCTOBER 2011 | DOI: 10.1038/NPHYS2114
nature physics

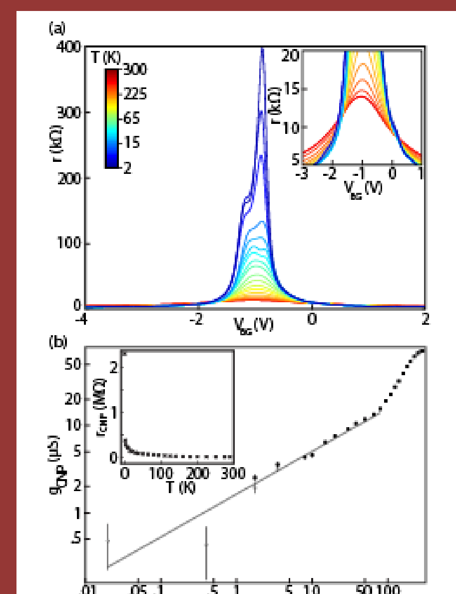
Tunable metal–insulator transition in double-layer graphene heterostructures

L. A. Ponomarenko[1], A. K. Geim[1,2], A. A. Zhukov[2], R. Jalil[2], S. V. Morozov[1,3], K. S. Novoselov[1], I. V. Grigorieva[1], E. H. Hill[2], V. V. Cheianov[4], V. I. Fal'ko[4], K. Watanabe[5], T. Taniguchi[5] and R. V. Gorbachev[2]*



Insulating behavior at the neutrality point in single-layer graphene

F. Amet,[1] J. R. Williams,[2] K. Watanabe,[3] T. Taniguchi,[3] and D. Goldhaber-Gordon[2]

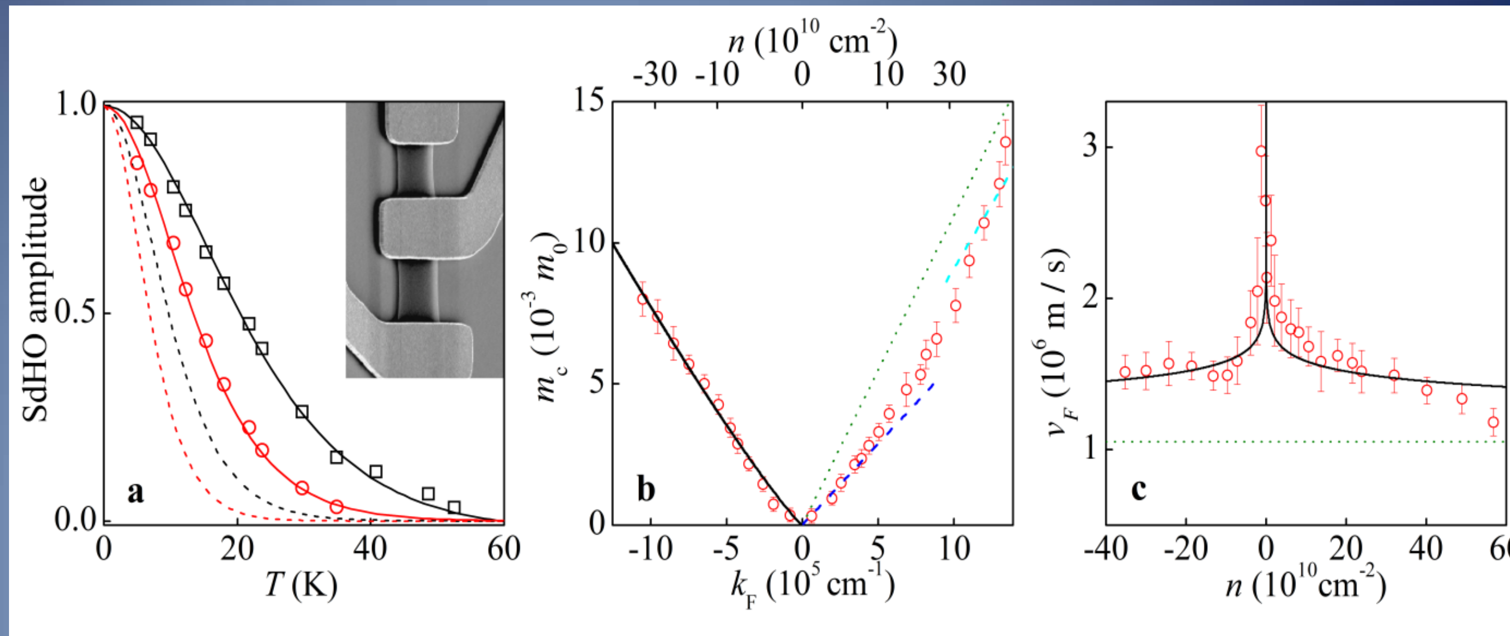


arXiv:1209.6364

Measurements of the effective mass

Suspended samples.
Very high mobility

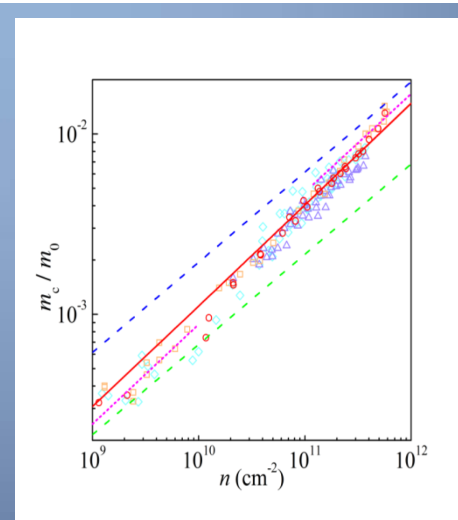
$\mu \approx 10^6 cm^2V^{-1}s^{-1}$



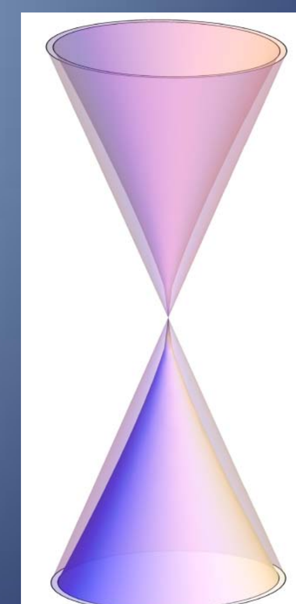
nature physics
LETTERS
PUBLISHED ONLINE: 24 JULY 2011 | DOI: 10.1038/NPHYS2049

Dirac cones reshaped by interaction effects in suspended graphene

D. C. Elias[1], R. V. Gorbachev[1], A. S. Mayorov[1], S. V. Morozov[2], A. A. Zhukov[3], P. Blake[3], L. A. Ponomarenko[1], I. V. Grigorieva[1], K. S. Novoselov[1], F. Guinea[4]* and A. K. Geim[1,3]



Fits to Renormalization Group calculations

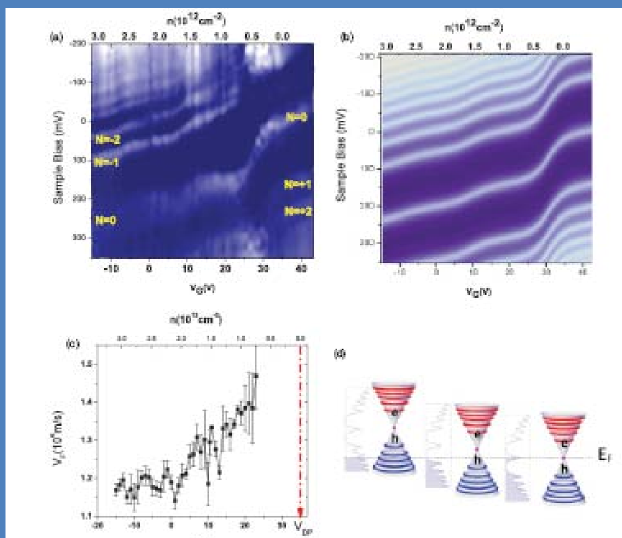


Other recent measurements

PHYSICAL REVIEW B 83, 041405(R) (2011)

Quantized Landau level spectrum and its density dependence in graphene

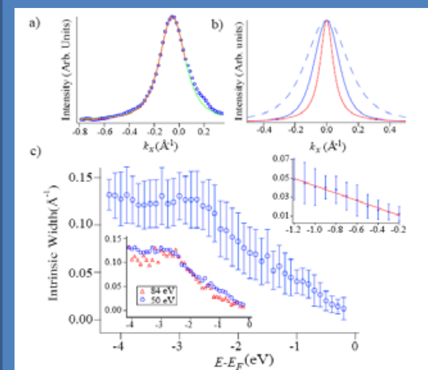
Adina Luican, Guohong Li, and Eva Y. Andrei

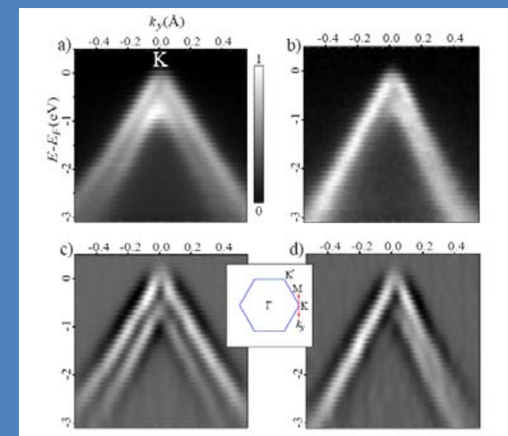


PHYSICAL REVIEW B 84, 115401 (2011)

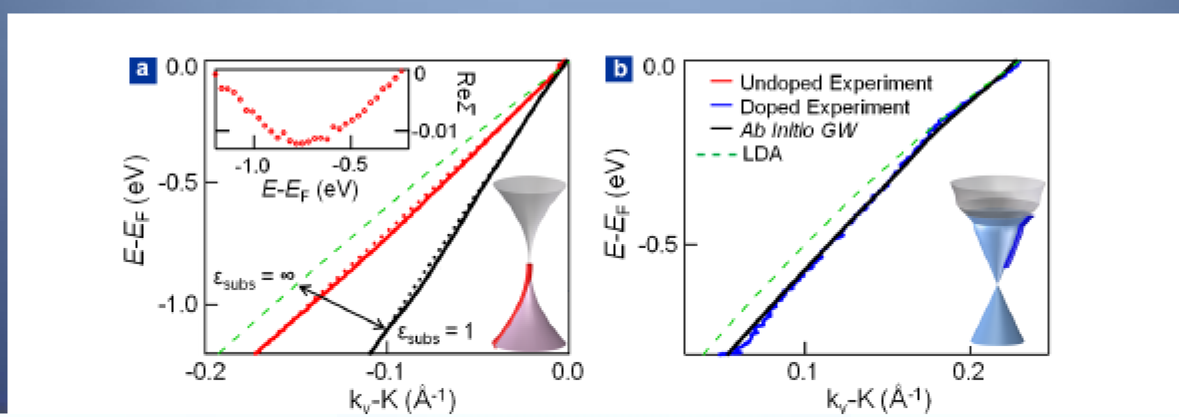
Making angle-resolved photoemission measurements on corrugated monolayer crystals: Suspended exfoliated single-crystal graphene

Kevin R. Knox,[1,2] Andrea Locatelli,[3] Mehmet B. Yilmaz,[4] Dean Cvetko,[5,6] Tevfik Onur Menteş,[3] Miguel Ángel Niño,[3,7] Philip Kim,[1] Alberto Morgante,[5,8] and Richard M. Osgood Jr.[2]





David A. Siegel, Cheol-Hwan Park, Choongyu Hwang, Jack Deslippe, Alexei V. Fedorov, Steven G. Louie, and Alessandra Lanzara, PNAS **108**, 11365 (2011)



Theory I

PHYSICAL REVIEW B **86**, 165413 (2012)

Conductivity of suspended graphene at the Dirac point

I. V. Gornyi,[1,2] V. Yu. Kachorovskii,[1,2,3] and A. D. Mirlin[1,3,4]

$$\sigma_{\mathrm{ee+ph}} = \frac{e^2}{\hbar}\frac{N\ln 2}{2\pi\left[C_2 Z^2 g^2 (T/\Delta_c)^\eta + C_3 g_e^2 N\right]}.$$

$$g_e = \frac{g_e^0}{1 + (g_e^0/4)\ln(\Delta/T)}$$

Flexural modes

Electron-electron interaction

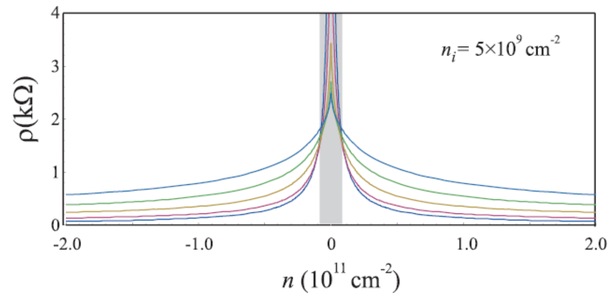


FIG. 8. (Color online) Resistivity as a function of electron concentration at $n_i = 5\times10^9\mathrm{cm}^{-2}$ and different temperatures ($T/1\mathrm{K} = 5,40,90,150,230$) increasing from the bottom to the top at large n. Within the grey area temperature dependence is "insulating," while outside this region it is "metallic."

At the neutrality point the conductivity increases as the temperature decreases

See also: L. Fritz, J. Schmalian, M. Müller, and S. Sachdev, Phys. Rev. B **78**, 085416 (2008).
V. Juricic, O. Vafek, and I. F. Herbut, Phys. Rev. B, **82**, 235402 (2010).

PHYSICAL REVIEW B **85**, 195451 (2012)

Disorder by order in graphene

S. Das Sarma, E. H. Hwang, and Qiuzi Li

Theory II

The pseudodiffusive regime

Eur. Phys. J. B **51**, 157–160 (2006)
DOI: 10.1140/epjb/e2006-00203-1
THE EUROPEAN PHYSICAL JOURNAL B

Zitterbewegung, chirality, and minimal conductivity in graphene

M.I. Katsnelson[a]

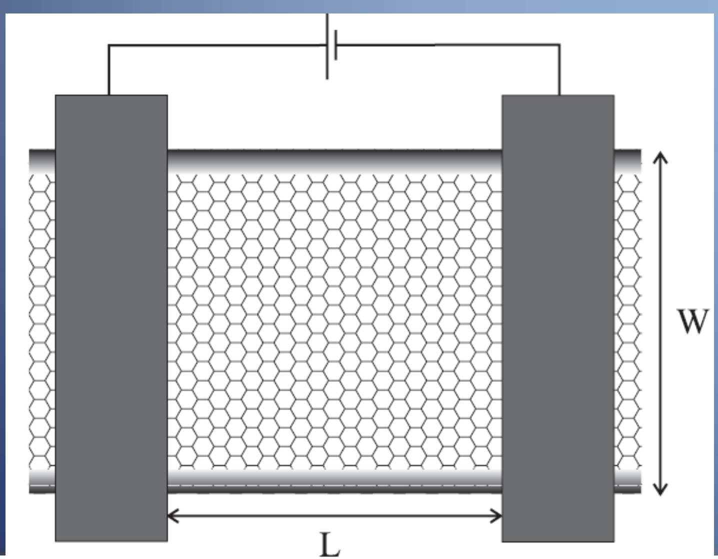
PRL **96,** 246802 (2006) PHYSICAL REVIEW LETTERS week ending 23 JUNE 2006

Sub-Poissonian Shot Noise in Graphene

J. Tworzydło,[1] B. Trauzettel,[2] M. Titov,[3] A. Rycerz,[2,4] and C. W. J. Beenakker[2]

$$T(k_y) \propto e^{-k_y L_x}$$

$$G = \sum_{k_y} T(k_y) \propto \frac{L_y}{L_x}$$



See also

- **Pseudodiffisive transport in graphene**, E. Prada, P. San Jose, B. Wunsch, F. G., Phys. Rev. B **75**, 113407 (2007).
- **Transport through evanescent waves in graphene quantum dots**, M. I. Katsnelson, F. G., Phys. Rev. B **79**, 075417 (2008)

Tunneling and interactions

PHYSICAL REVIEW LETTERS

VOLUME 46 — 26 JANUARY 1981 — NUMBER 4

Influence of Dissipation on Quantum Tunneling in Macroscopic Systems

A. O. Caldeira and A. J. Leggett

School of Mathematical and Physical Sciences, University of Sussex, Brighton BN1 9QH, Sussex, United Kingdom

ELSEVIER

Annals of Physics

Volume 149, Issue 2, September 1983, Pages 374–456

Quantum tunnelling in a dissipative system

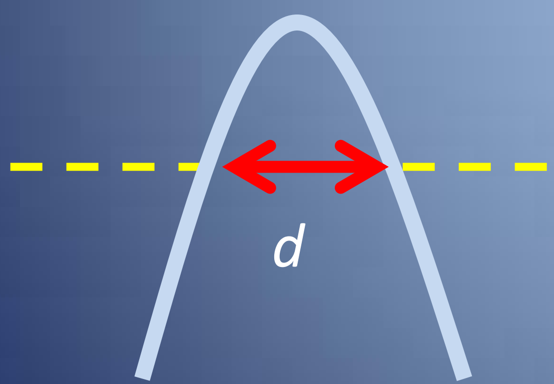
A.O Caldeira

Instituto de Fisica "Gleb Wataghin" Universidade Estadual de Campinas, Cidade Universitaria, Barao Geraldo, 13–100 Campinas, Sao Paulo, Brazil

A.J Leggett*

School of Mathematical and Physical Sciences, University of Sussex, Falmer, Brighton BN1 9QH, England

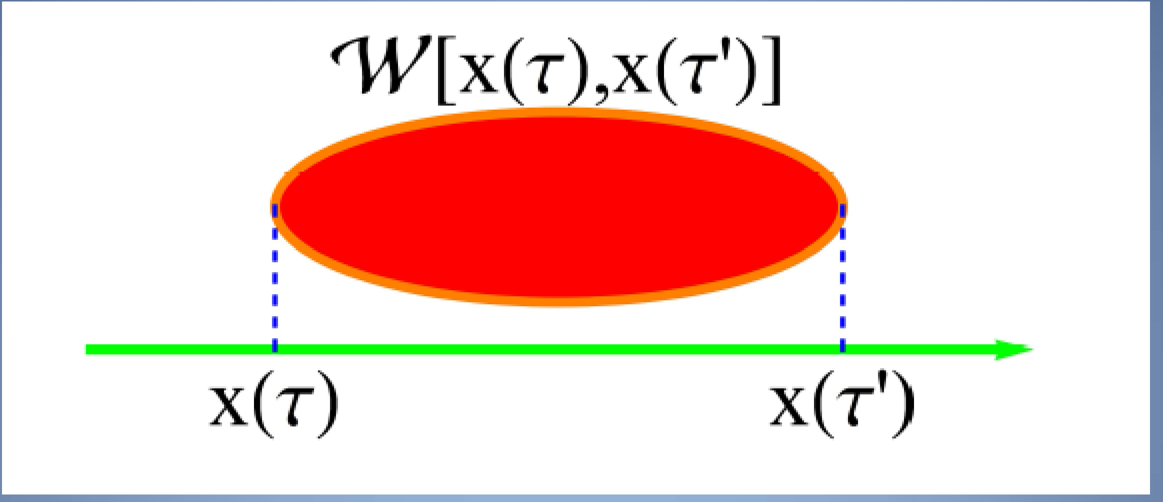
$$Mq'' + \eta q' = -dV/dq + F_{ext}(t)$$



$$T = T_0 e^{-c\frac{\eta d^2}{\hbar}}$$

- Semiclassical analysis
- The excitations of the environment are treated as a set of independent bosons

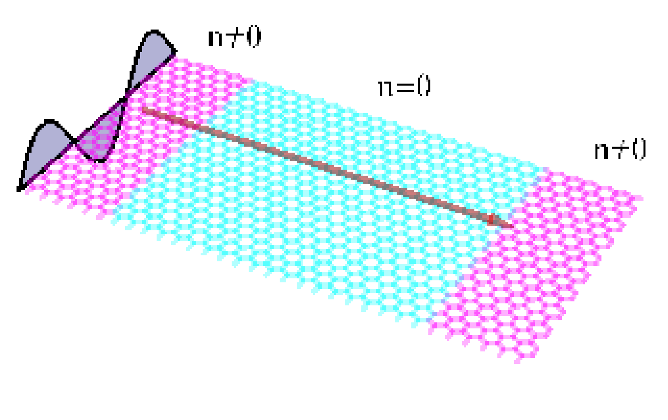
The Caldeira-Leggett model

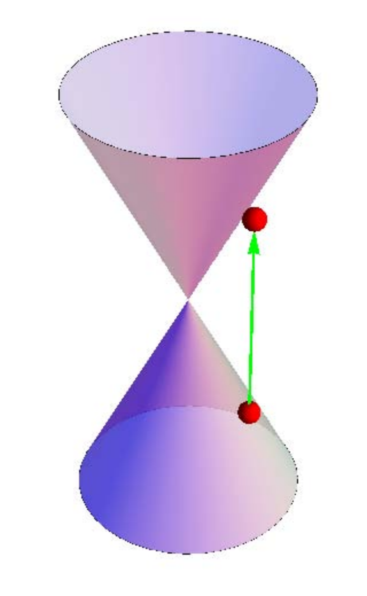


$$\delta S = \int_{-\infty}^{+\infty} d\tau \int_0^{\beta} d\tau' \int_{-\infty}^{+\infty} \frac{dq}{2\pi} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{iq[x(\tau)-x(\tau')]} e^{-\omega|\tau-\tau'|} \,\mathrm{Im}[W(q,\omega)]$$

$$W_{CL}[x(\tau)-x(\tau'),\tau-\tau'] = \frac{\eta}{2\pi} \frac{[x(\tau)-x(\tau')]^2}{[\tau-\tau']^2}$$

Graphene as a dissipative environment





$$\operatorname{Im} W(q,\omega) = \operatorname{Im} \frac{v_q}{\varepsilon(q,\omega)} = \operatorname{Im} \frac{v_q}{1 + v_q \chi_{1D}(q,\omega)}$$

$$v_q \approx \begin{cases} -\dfrac{2e^2}{\varepsilon_0} \operatorname{Log}(qL_y) & qL_y << 1 \\ \dfrac{2\pi e^2}{\varepsilon_0 q L_y} & qL_y >> 1 \end{cases}$$

$$\chi_{1D}(q,\omega) \approx \begin{cases} \dfrac{L_y q^2}{4\sqrt{\mathrm{v}_F^2 q^2 - \omega^2}} & \text{graphene} \\ \dfrac{\nu_{1D} D q^2}{i\omega + Dq^2} & \text{diffusive metal, } q \le \ell_{el}^{-1} \\ \dfrac{\nu_{1D} \mathrm{v}_F q}{i\omega + \mathrm{v}_F q} & \text{ballistic metal,} \ell_{el}^{-1} \le q \le k_F \end{cases}$$

$$q_c \approx \operatorname{Max}\left(L_x^{-1}, \mathrm{v}_F / T, \ell_B^{-1} \right)$$

Results

$$\delta S_G \approx \frac{L_x}{8\pi L_y}\frac{\alpha^2}{4\sqrt{2}+\alpha}\log\left(\frac{L_x}{a}\right)$$

$$\delta S_M \approx \frac{L_x^2}{4\pi g \ell L_y} + \frac{L_x}{8\pi L_y}\log(g)$$

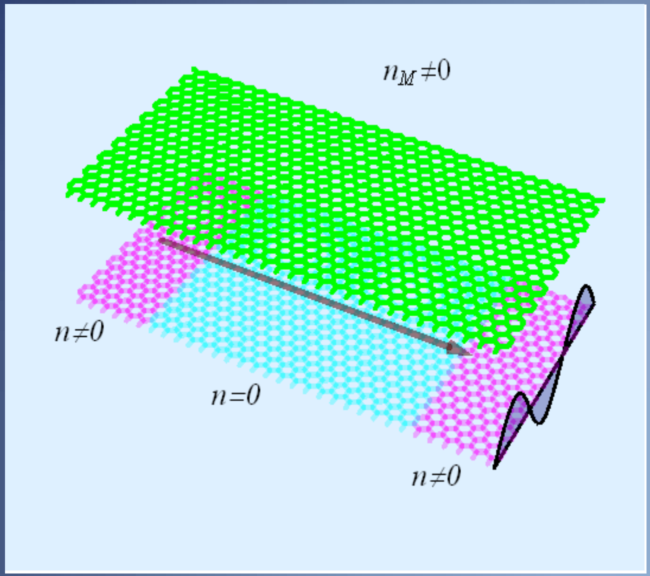
T=B=0

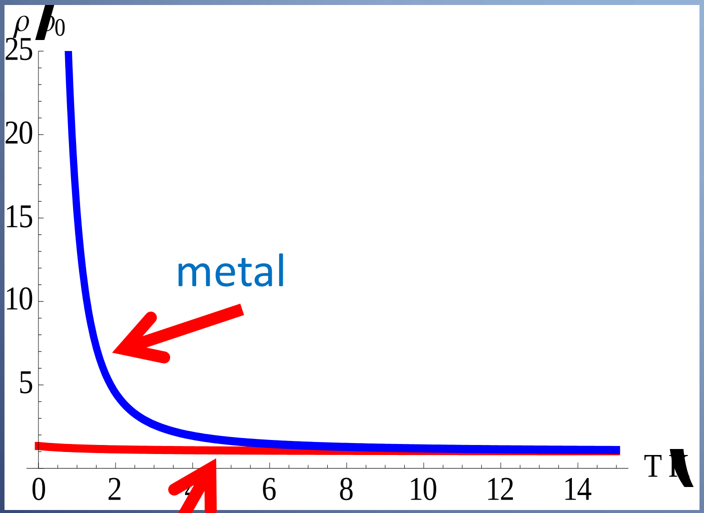
diffusive contribution,

$L_x^{-1} \le q \le \ell^{-1}$

ballistic contribution,

$\ell^{-1} \le q \le k_F$

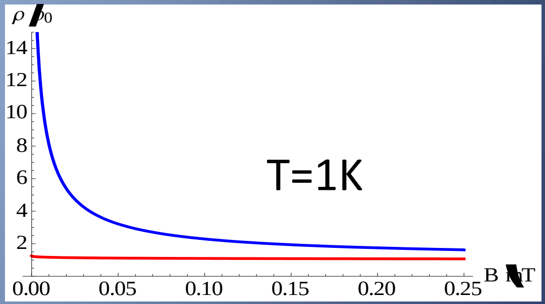




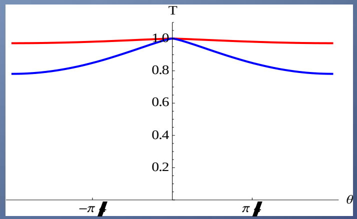
metal

graphene

L_x=4μm
L_y=1μm
$n_M=10^{11}$ cm^{-2}
l=60nm



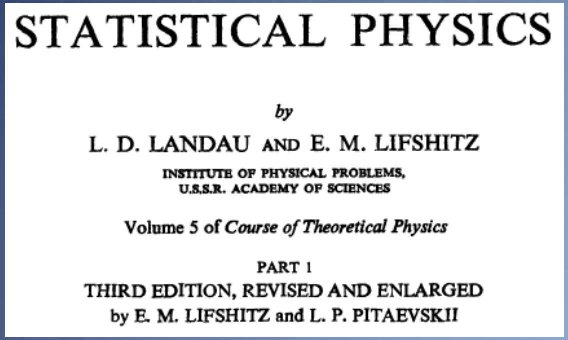
magnetic field



p-n junction

Why are there two dimensional crystals?

Phonon-phonon interactions in graphene



STATISTICAL PHYSICS

by

L. D. LANDAU AND E. M. LIFSHITZ

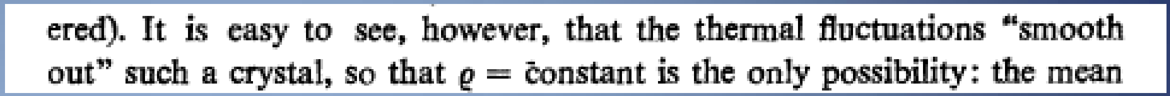
INSTITUTE OF PHYSICAL PROBLEMS, U.S.S.R. ACADEMY OF SCIENCES

Volume 5 of *Course of Theoretical Physics*

PART 1

THIRD EDITION, REVISED AND ENLARGED

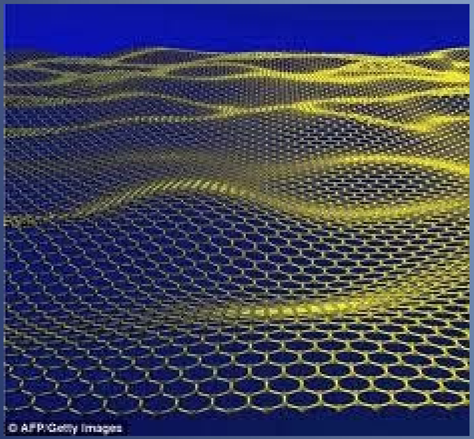
by E. M. LIFSHITZ and L. P. PITAEVSKII



ered). It is easy to see, however, that the thermal fluctuations "smooth out" such a crystal, so that ϱ = constant is the only possibility: the mean

Thermal fluctuations:

$$\langle \vec{u}(L)\vec{u}(0)\rangle \approx \frac{k_B T}{B}\log\left(\frac{L}{d}\right)$$



$B_{graphene}$ =22 eV Å^{-2} = 352 N/m

$B_{diamond}$ x d=52.4 N/m

T=300K

L=1Km

$$\langle \vec{u}(L)\vec{u}(0)\rangle \approx 0.03\text{Å}^2$$

GRAPHENE'S SUPERLATIVES

- Thinnest imaginable material
- largest surface area (~2,700 m^2 per gram)
- strongest material 'ever measured' (theoretical limit)
- stiffest known material (stiffer than diamond)
- most stretchable crystal (up to 20% elastically)
- record thermal conductivity (outperforming diamond)
- highest current density at room T (106 times of copper)
- completely impermeable (even He atoms cannot squeeze through)
- highest intrinsic mobility (100 times more than in Si)
- conducts electricity in the limit of no electrons
- lightest charge carriers (zero rest mass)
- longest mean free path at room T (micron range)

Elastic properties of graphene

Measurement of the Elastic Properties and Intrinsic Strength of Monolayer Graphene

Changgu Lee,[1,2] Xiaoding Wei,[1] Jeffrey W. Kysar,[1,3] James Hone[1,2,4]*

We measured the elastic properties and intrinsic breaking strength of free-standing monolayer graphene membranes by nanoindentation in an atomic force microscope. The force-displacement behavior is interpreted within a framework of nonlinear elastic stress-strain response, and yields second- and third-order elastic stiffnesses of 340 newtons per meter ($N\ m^{-1}$) and –690 $N\ m^{-1}$, respectively. The breaking strength is 42 $N\ m^{-1}$ and represents the intrinsic strength of a defect-free sheet. These quantities correspond to a Young's modulus of E = 1.0 terapascals, third-order elastic stiffness of D = –2.0 terapascals, and intrinsic strength of σ_{int} = 130 gigapascals for bulk graphite. These experiments establish graphene as the strongest material ever measured, and show that atomically perfect nanoscale materials can be mechanically tested to deformations well beyond the linear regime.

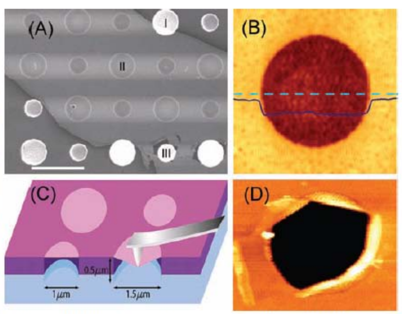


Fig. 1. Images of suspended graphene membranes. (**A**) Scanning electron micrograph of a large graphene flake spanning an array of circular holes 1 μm and 1.5 μm in diameter. Area I shows a hole partially covered by graphene, area II is fully covered, and area III is fractured from indentation. Scale bar, 3 μm. (**B**) Noncontact mode AFM image of one membrane, 1.5 μm in diameter. The solid blue line is a height profile along the dashed line. The step height at the edge of the membrane is about 2.5 nm. (**C**) Schematic of nanoindentation on suspended graphene membrane. (**D**) AFM image of a fractured membrane.

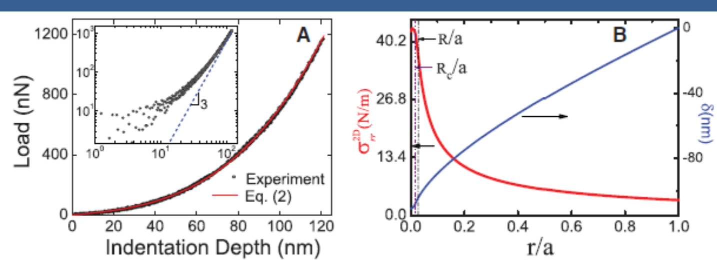


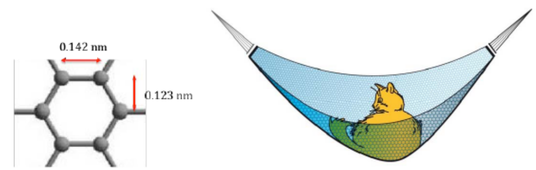
Fig. 2. (**A**) Loading/unloading curve and curve fitting to Eq. 2. The curve approaches cubic behavior at high loads (inset). (**B**) Maximum stress and deflection of graphene membrane versus normalized radial distance at maximum loading (simulation based on nonlinear elastic behavior in Eq. 1). The dashed lines indicate the tip radius R and contact radius R_c.

KUNGL. VETENSKAPS-AKADEMIEN

THE ROYAL SWEDISH ACADEMY OF SCIENCES

OCTOBER 5, 2010

Appendix, some properties of graphene



CLAIM #1: GRAPHENE CAN HOLD AN ELEPHANT

"…graphene as the strongest material ever measured, some 200 times stronger than structural steel. … If a sheet of cling film (which typically has a thickness of around 100 μm) were to have the same strength as pristine graphene, it would require a force of over 20,000 N to puncture it with a pencil,"."

Jim Hone, Columbia U

physicsworld.com

Graphic: Sci. Am., 11/2011

courtesy from M. M. Fogler

VOLUME 69, NUMBER 8 PHYSICAL REVIEW LETTERS 24 AUGUST 1992

Self-Consistent Theory of Polymerized Membranes

Pierre Le Doussal[a]
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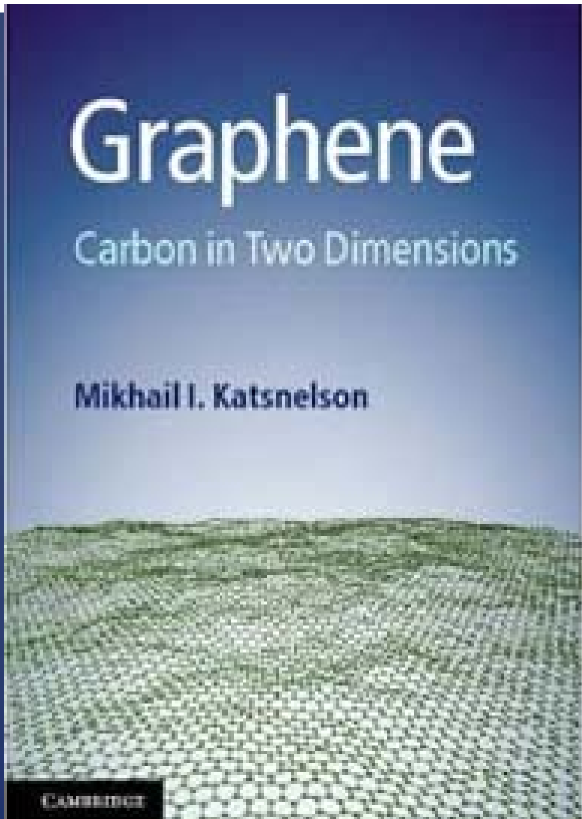
Leo Radzihovsky
Lyman Laboratory, Harvard University, Cambridge, Massachusetts 02138
(Received 18 May 1992)



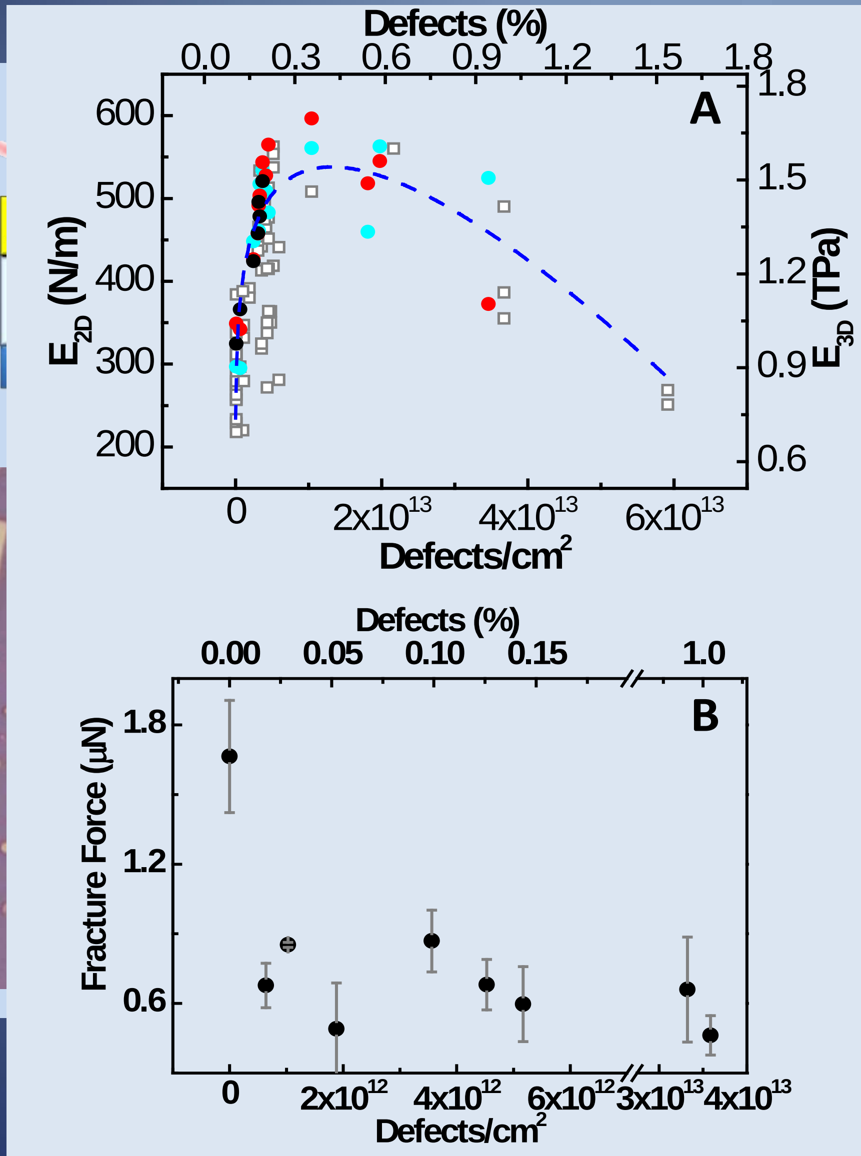
y a nontrivial fixed point, but with *anomalous*
stants $\lambda(q) \sim \mu(q) \sim q^{\eta_u}$, $\eta_u > 0$, with η_u

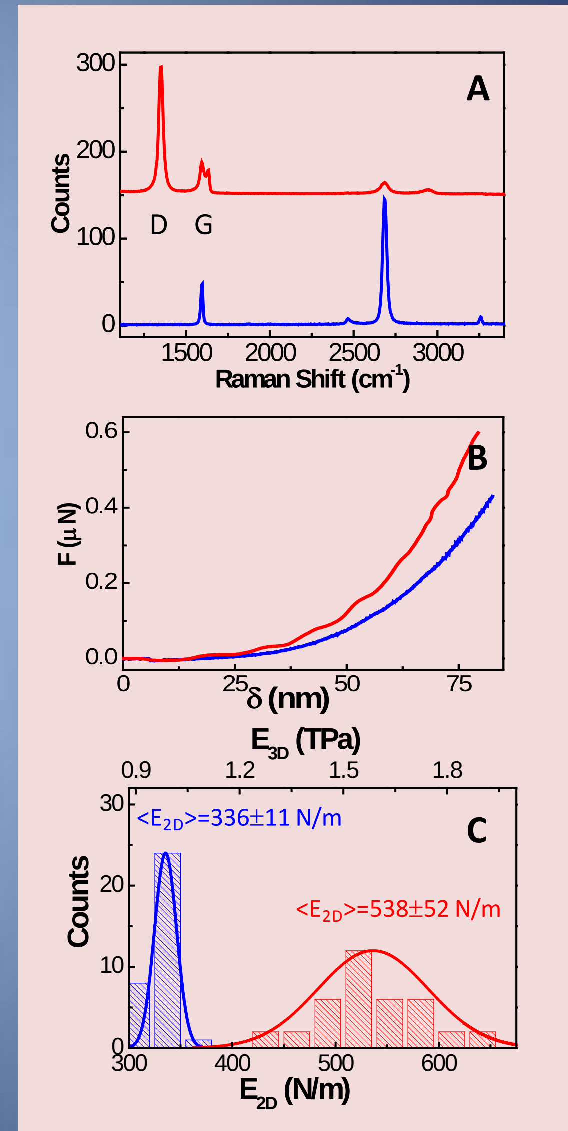
of the order of a^{-1} to make A dimensionless. One can assume also a renormalization of effective Lamé constants:

$$\lambda_R(q),\ \mu_R(q) \sim q^{\eta_u}, \tag{9.103}$$

Experiments

C. Gomez-Navarro, J. Gomez, G. Lopez-Polin, F. Perez-Murano



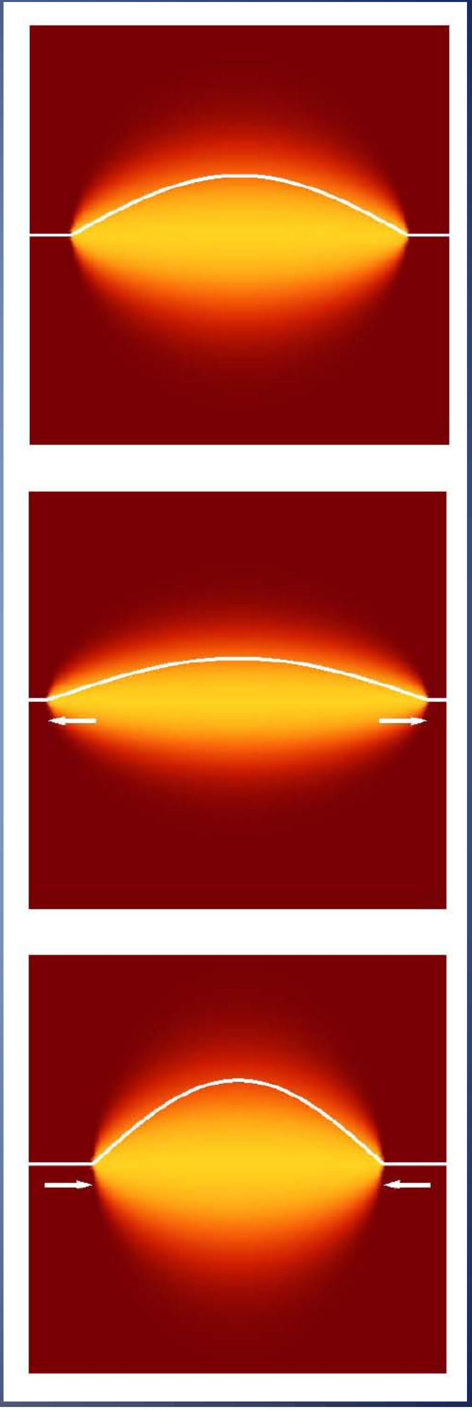


Out of plane fluctuations renormalize the in plane elastic constants

$$E \approx \left(c_1 Y \overline{u} + c_2 \frac{\kappa}{\ell^2} \right) h^2$$

$$F \approx T \log \left(\frac{T}{c_1 Y \overline{u} + c_2 \frac{\kappa}{\ell^2}} \right)$$

$$\delta Y = \frac{1}{\ell^2} \frac{\partial^2 F}{\partial \overline{u}^2} \propto -\frac{Y^2 T \ell^2}{\kappa^2}$$



Anharmonic effects: thermal expansion coefficient in graphene and graphite

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]

$$\alpha \approx -\frac{k_B}{8\pi\kappa}\log\left(\frac{\kappa^3\rho}{\hbar^2 Y^2}\right)$$

graphite: crossover wavelength

$$q_c^* \approx \sqrt{\frac{g/d^2}{\lambda+2\mu}}$$

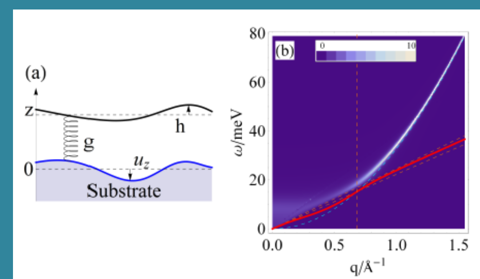
g≈30meV/Å²
d≈ 3.3Å
λ+2μ≈22eV/Å²

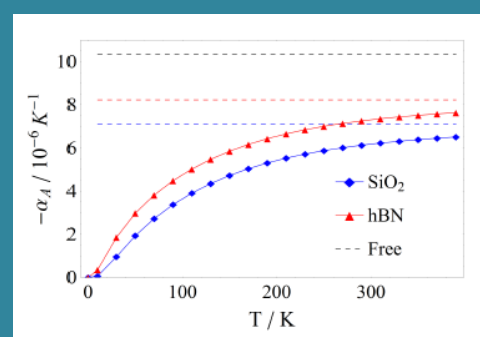
$1/q_c^* \approx 5.5$Å^{-1}

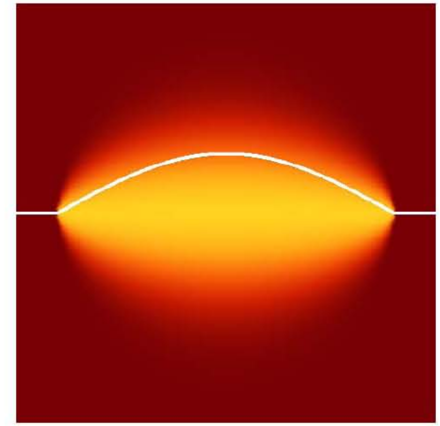
The flexural modes of graphene on a substrate

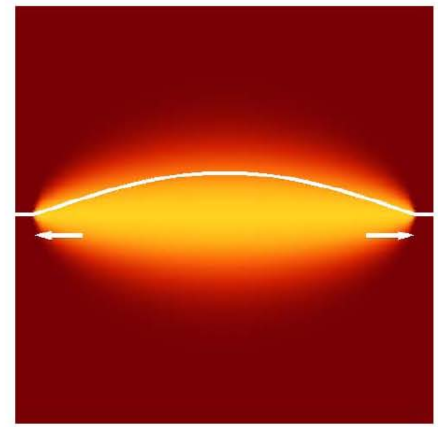
Bruno Amorim[1] and Francisco Guinea[1]

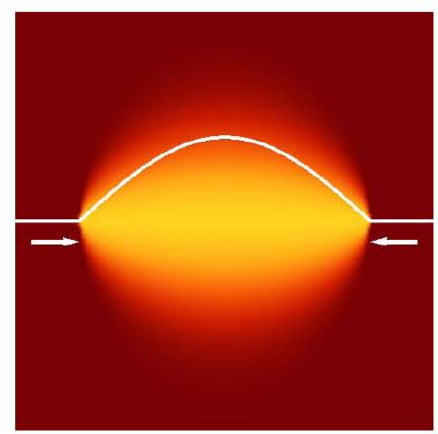
Arxiv:1304.6567











Vacancies and flexural modes

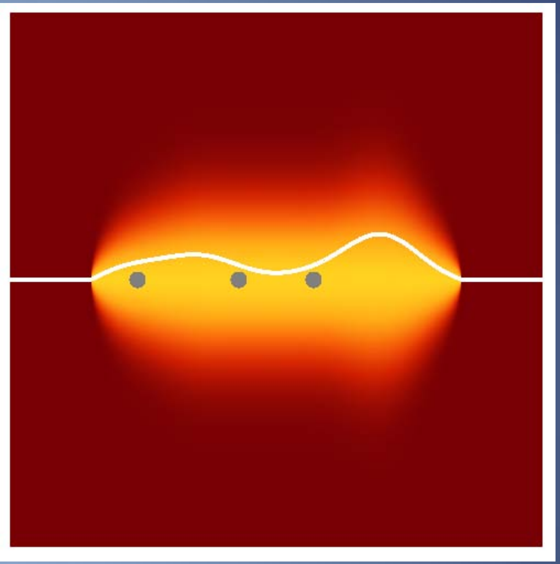
$$G(q,\omega)=\frac{1}{\rho\omega^2-\kappa q^4-\Sigma(q,\omega)}$$

T-matrix approximation

$$\Sigma(\omega)\approx\begin{cases} n_V\sqrt{\kappa\rho\omega^2} & h^2=0 \\ n_V\dfrac{\sqrt{\kappa\rho\omega^2}}{\log\left(\dfrac{\kappa}{a^4\rho\omega^2}\right)} & |\nabla h|^2=0 \end{cases}$$

infinite mass

vacancies



localization length

$$\frac{\kappa}{\ell^4}\approx\Sigma\left(\sqrt{\frac{\kappa}{\rho\ell^4}}\right)$$

$$\ell\approx n_V^{-1/2}$$

- Vacancies localize flexural modes
- Long wavelength flexural modes do not contribute to the screening of the elastic constants

geometric factor

percolation

$$Y \approx K\left(\frac{1}{R^2}+\frac{1}{\ell_0^2}+n_V\right)^{\frac{\eta_u}{2}}\left[1-c\left(\frac{1}{\ell_0^2}+n_V\right)\right]$$

intrinsic localization length

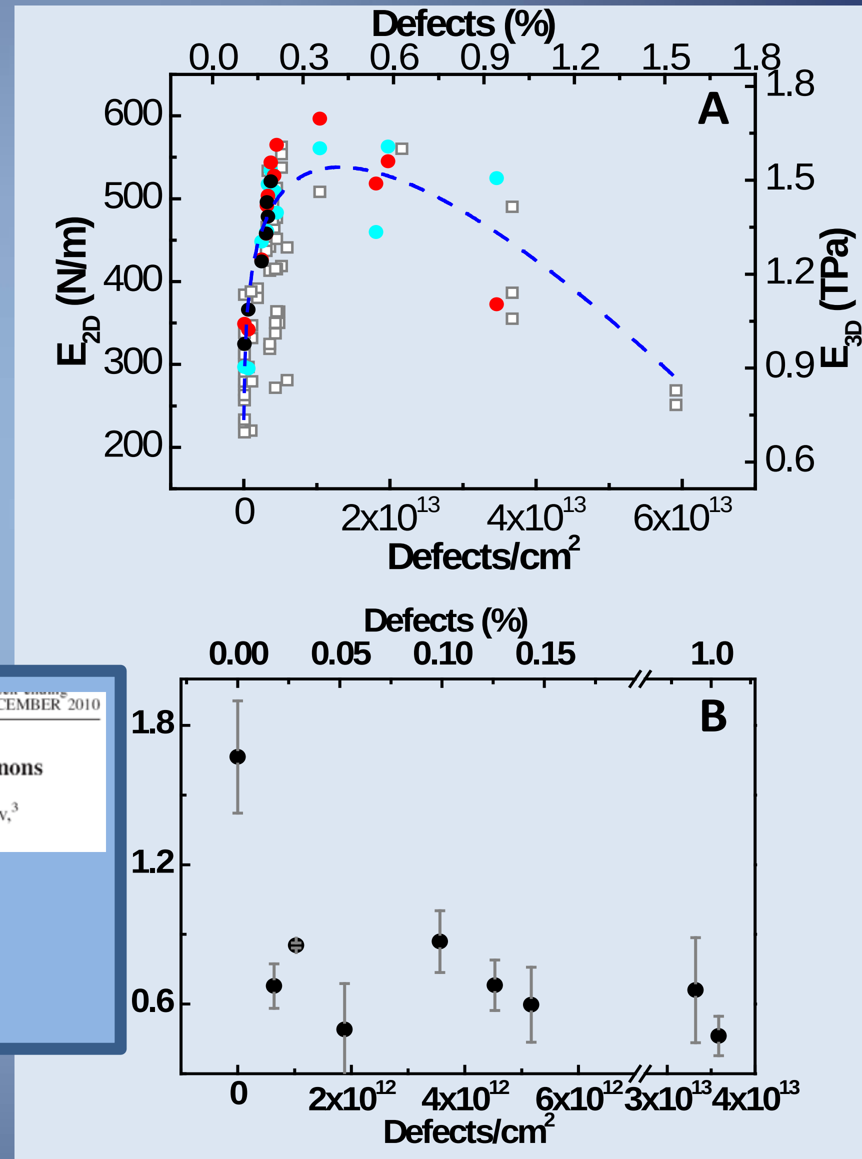
PRL **105**, 266601 (2010) PHYSICAL REVIEW LETTERS 31 DECEMBER 2010

Limits on Charge Carrier Mobility in Suspended Graphene due to Flexural Phonons

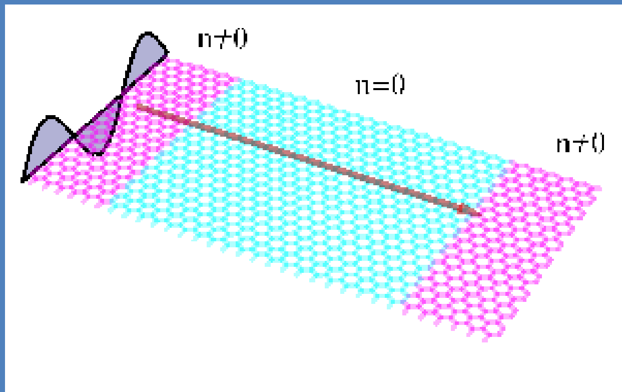
Eduardo V. Castro,[1] H. Ochoa,[1] M. I. Katsnelson,[2] R. V. Gorbachev,[3] D. C. Elias,[3] K. S. Novoselov,[3] A. K. Geim,[3] and F. Guinea[1]

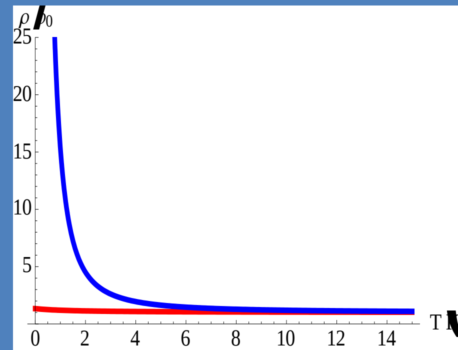
$$\ell_0 \approx 20-100\,\mathrm{nm}$$

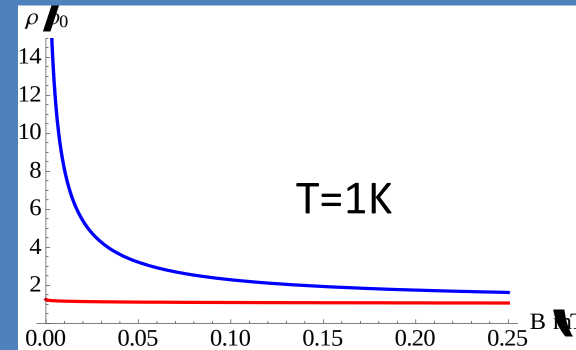
$$\ell_0 \geq k_F^{-1}$$



Ballistic graphene+interactions

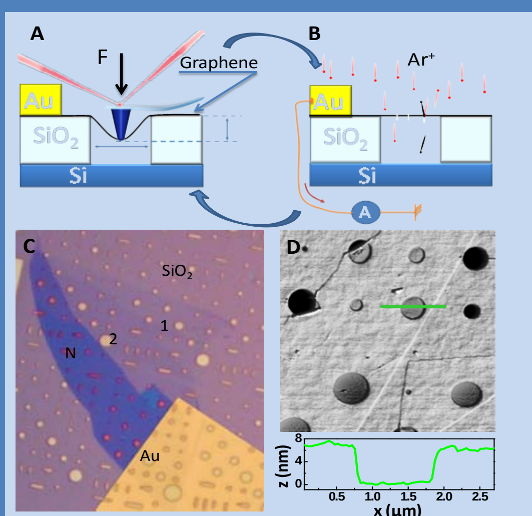


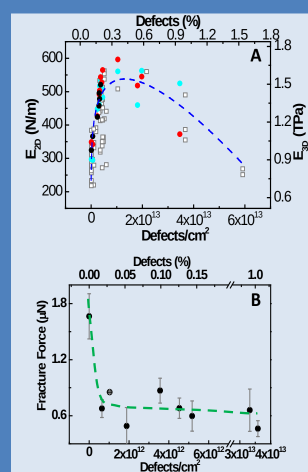


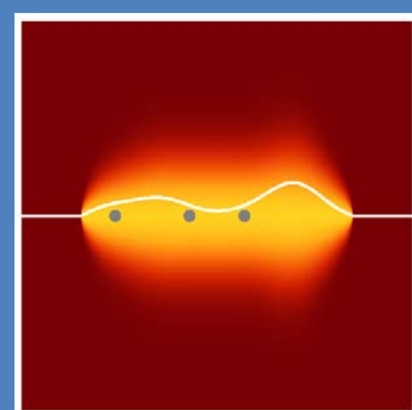


The pseudodiffusive regime is highly sensitive to interactions

Elastic properties of graphene with defects







- Flexural phonons modify the elastic properties
- The value of the Young modulus depends on the experimental setup

PHYSICAL REVIEW B **71**, 205214 (2005)

First-principles determination of the structural, vibrational and thermodynamic properties of diamond, graphite, and derivatives

Nicolas Mounet* and Nicola Marzari†

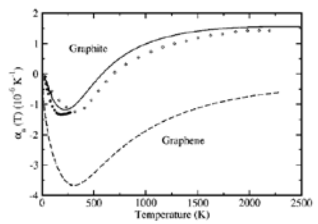


FIG. 15. In-plane coefficient of linear thermal expansion as a function of temperature for graphite (solid line) and graphene (dashed line) from our QHA-GGA *ab initio* study. The experimental results for graphite are from Ref. 14 (filled circles) and Ref. 7 (open diamonds).

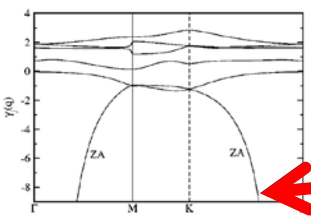


FIG. 17. *Ab initio* mode Grüneisen parameters for graphene.

$=-[a/2\omega_j(\mathbf{q})][d\omega_j(\mathbf{q})/da]$). While not visible in the figure, the Grüneisen parameters for the lowest acoustic branch of graphite become as low as −40, and as low as −80 in

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

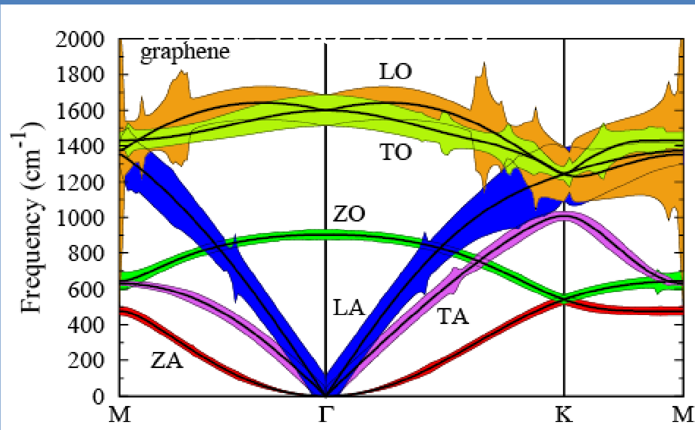
Bending modes, anharmonic effects, and thermal expansion coefficient in single-layer and multilayer graphene

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

$$\gamma_{\vec{q}} = -\frac{\mathcal{A}}{\omega_{\vec{q}}}\frac{\partial\omega_{\vec{q}}}{\partial\mathcal{A}} = -\frac{1}{2\omega_{\vec{q}}}\frac{\partial\omega_{\vec{q}}}{\partial\bar{u}}\bigg|_{\bar{u}=0} = -\frac{\lambda+\mu}{2\kappa|\vec{q}|^2},$$

Anharmonic properties from a generalized third order ab initio approach: theory and applications to graphite and graphene

Lorenzo Paulatto,* Francesco Mauri, and Michele Lazzeri



PHYSICAL REVIEW B **82**, 195436 (2010)

First-principles investigation of graphene fluoride and graphane

O. Leenaerts,[1,*] H. Peelaers,[1,†] A. D. Hernández-Nieves,[1,2,‡] B. Partoens,[1,§] and F. M. Peeters[1,||]

TABLE III. Elastic constants of the different hydrogenated and fluorinated graphene derivatives. The 2D Young's modulus, E', and Poisson's ratio, ν, are given along the cartesian axes. E' is expressed in N m^{-1}.

	Chair	Boat	Zigzag	Armchair
		Graphane		
E'_x	243	230	117	247
E'_y	243	262	271	142
ν_x	0.07	−0.01	0.05	−0.05
ν_y	0.07	−0.01	0.11	−0.03
		Fluorographene		
E'_x	226	238	240	215
E'_y	226	240	222	253
ν_x	0.10	0.00	0.09	0.02
ν_y	0.10	0.00	0.11	0.02

for the chair configurations agree well with recent calculations (245 N m^{-1} and 228 N m^{-1} for graphane and fluorographene, respectively, in Ref. 20). Nair *et al.*[11] performed a nanoindentation experiment on fluorographene and measured a value of 100 ± 30 N m^{-1} for E'_{FG}. This value is approximately half the theoretical value. Because the theoretical values are trustworthy, i.e., they agree with earlier theoretical calculations, and this kind of calculations are believed to be accurate (as in the case of graphene), this suggests that the experimental samples contain an appreciable