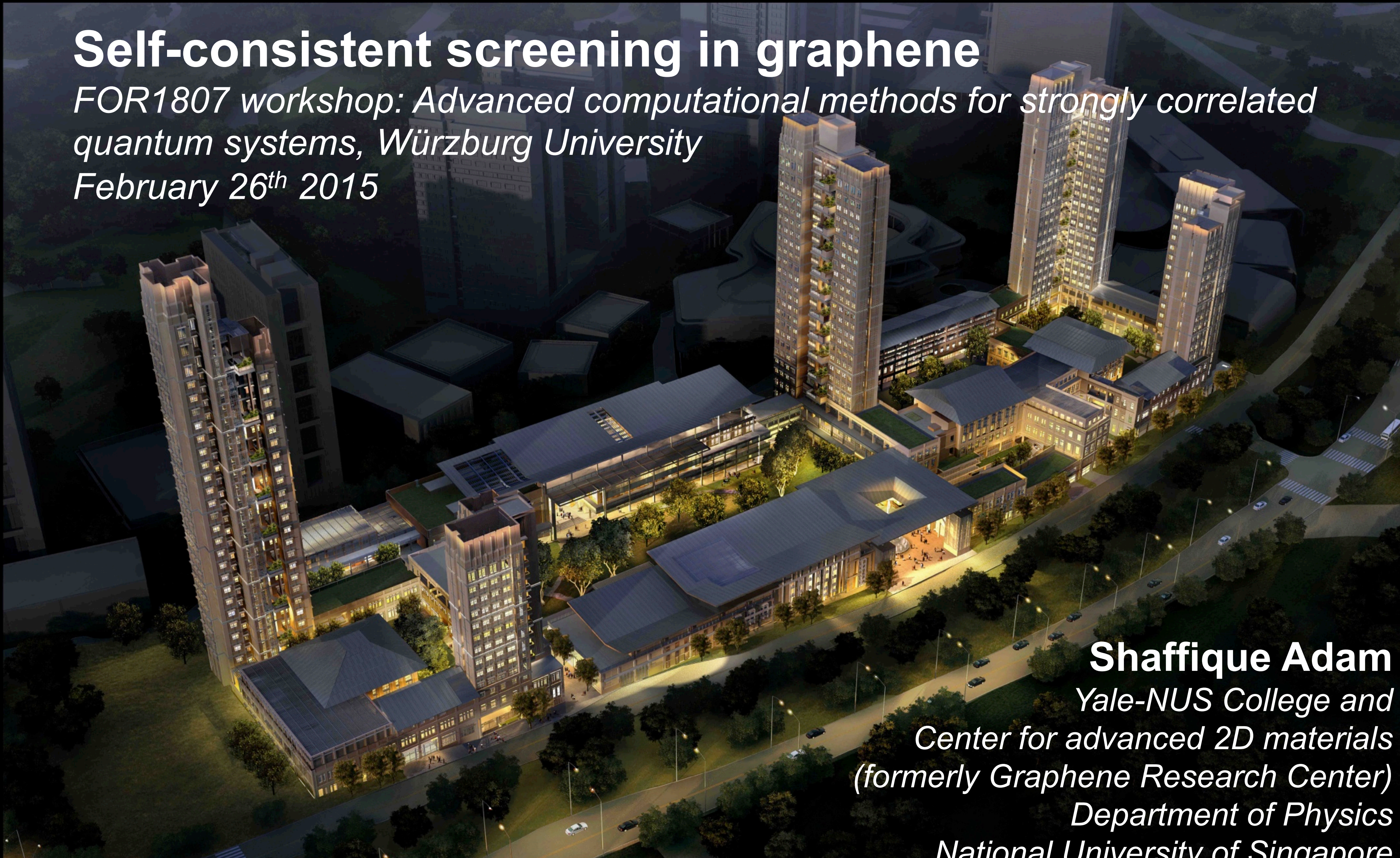
Self-consistent screening in graphene

FOR1807 workshop: Advanced computational methods for strongly correlated quantum systems, Würzburg University

February 26th 2015



Shaffique Adam

Yale-NUS College and

Center for advanced 2D materials

(formerly Graphene Research Center)

Department of Physics

National University of Singapore

Yale NUS College

NUS National University of Singapore

NATIONAL RESEARCH FOUNDATION
PRIME MINISTER'S OFFICE
SINGAPORE

Center for Advanced 2D materials (formerly Graphene Research Center)

Showing NUS physicists and collaborators… (not shown: chemists, engineers, people at NTU etc.)

Theory colleagues

Antonio Castro Neto

Giovanni Vignale

Baowen Li

Feng Yuan Ping

Zhang Chun

Hsin Lin

Su Ying Quek

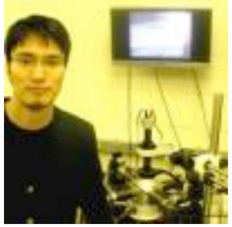
Vitor Pereira

Experimental colleagues

Barbaros Özyilmaz

Kian Ping Loh

Andrew Wee



Goki Eda

Jens Martin

Slaven Garaj

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Peter Ho

Sow Chorng Haur

Ji Wei

Jose Gomes

Lay-Lay Chua

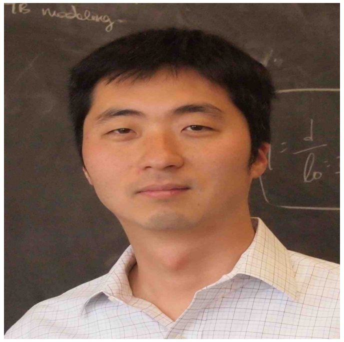
Wei Chen

Christian Nijhuis

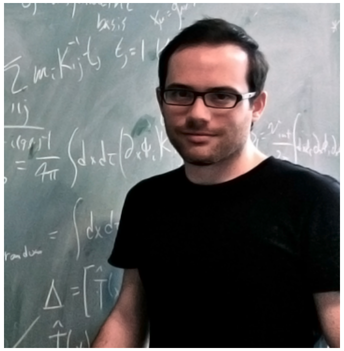
Research Group

Yale NUS College | NUS National University of Singapore | National Research Foundation

Postdoctoral Research Fellows



Jeil Jung



Mirco Milletari

Joao Rodrigues

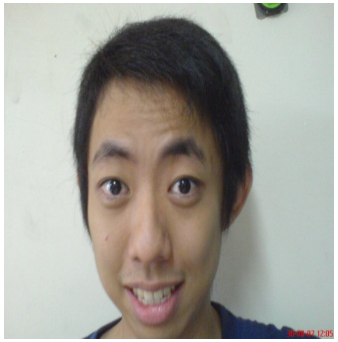
Derek Ho

Graduate Student Researchers

Indra Yudhistira

Navneeth Ramakrishnan

Tang Ho Kin



Jia Ning Leaw

The perfect 2DEG

Graphene is all surface and no bulk

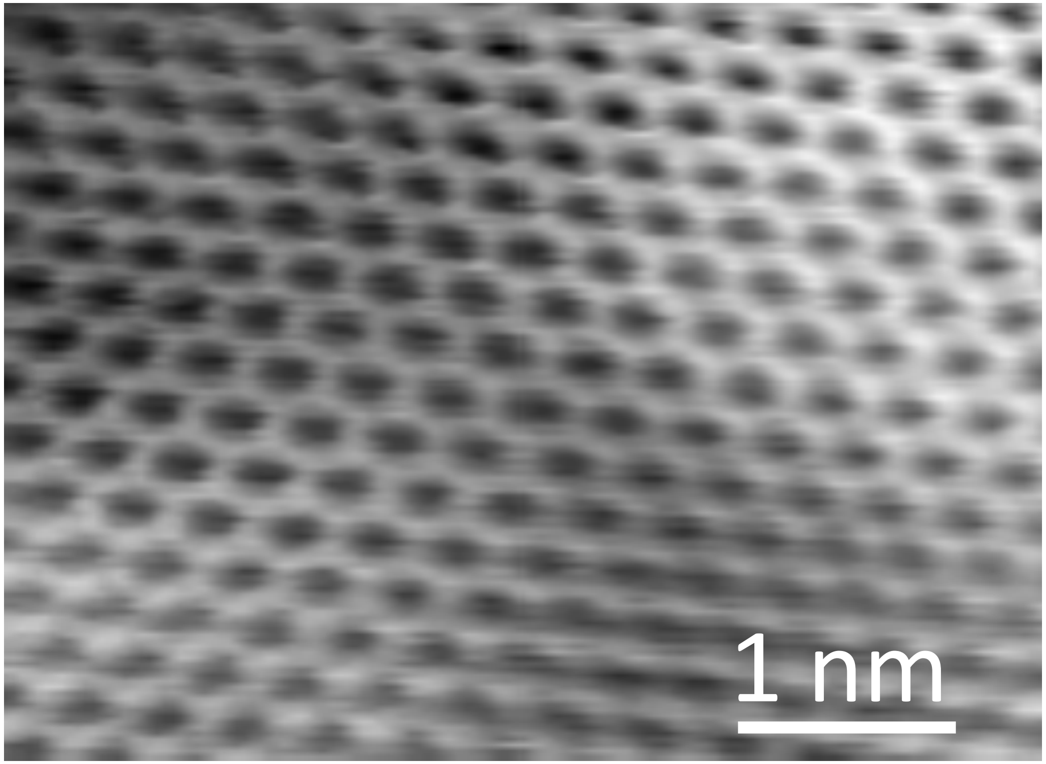
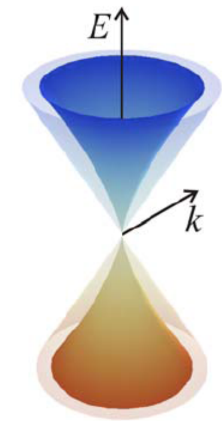


Figure from G. Rutter

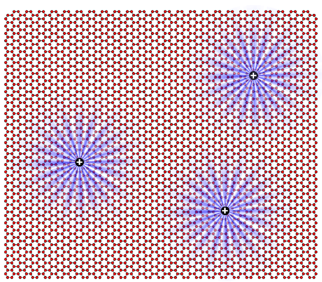
"*God made the bulk; surfaces were invented by the devil*"
– Wolfgang Pauli

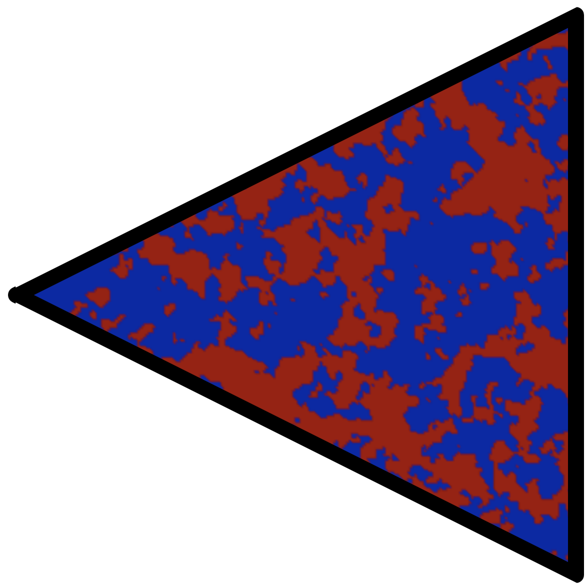
Delicate interplay between disorder, interactions and quantum effects

Most experiments are in the regime, where all these effects are relevant, but not dominant!

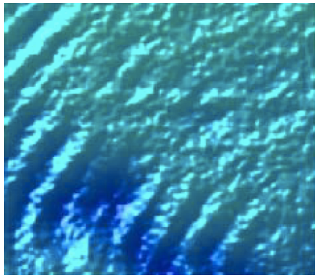


Electron Interactions





Disorder



Quantum Interference

See e.g.

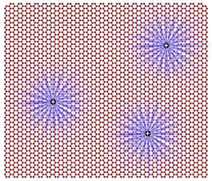
M. S. Fuhrer and S. Adam, *Nature*, news and views, **458** 38 (2009); and

S. Das Sarma, S. Adam, E. Hwang and E. Rossi, *Reviews of Modern Physics* **83** 407 (2011)

Image credits: Fuhrer, Geim, Westervelt,

Semi-classical picture

Disorder



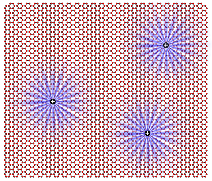
Disorder
Potential

Electron gas

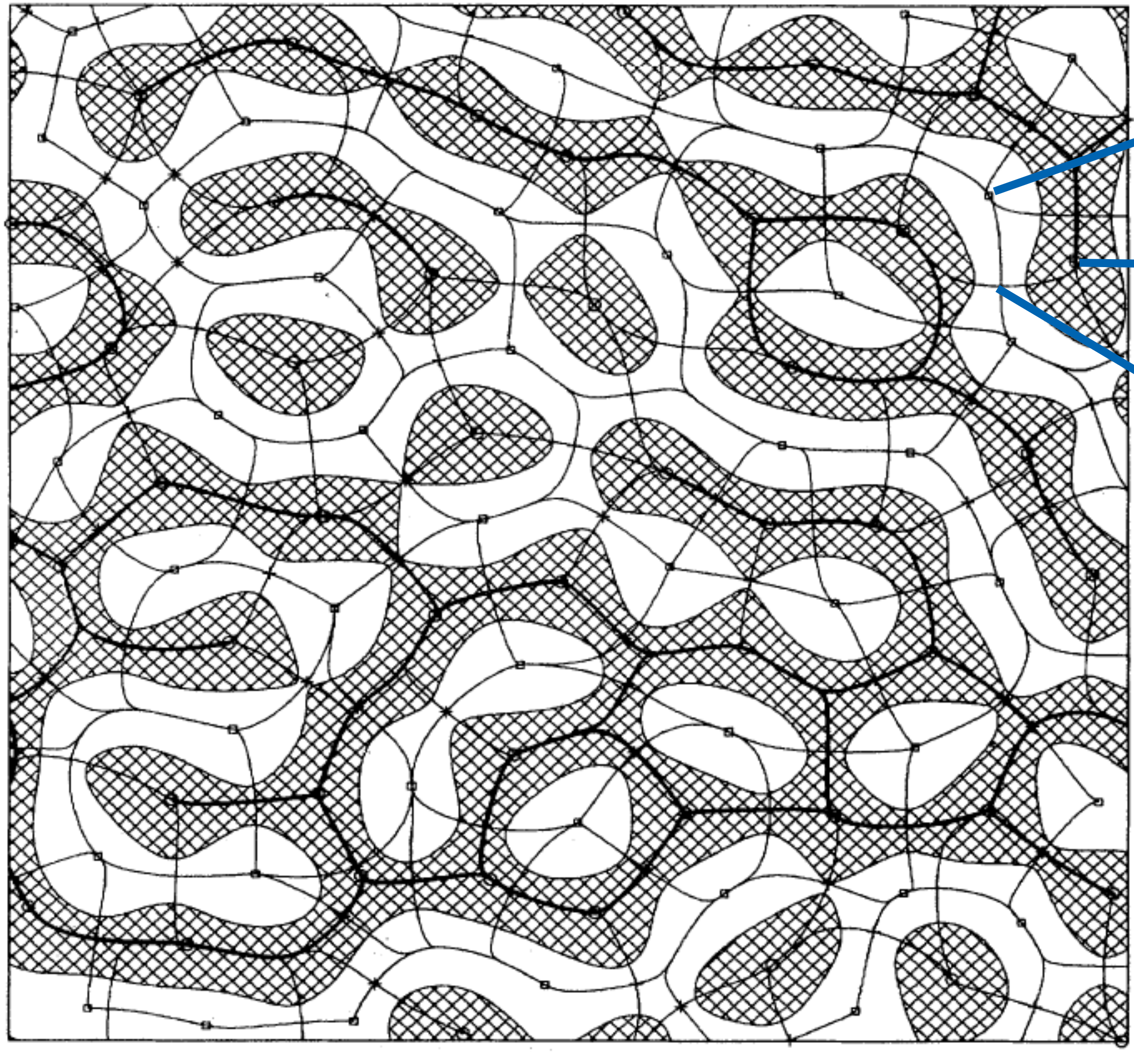
Figure from M. Wayne

Map to classical percolation

Disorder



Unlike conventional 2DEGs, graphene remains metallic even for strong disorder



Potential Maxima

Potential Minima

Saddle Point = bond

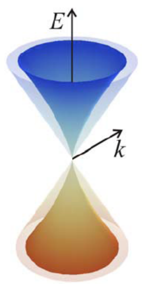
M. Isichenko, Rev. Mod. Phys. (1992)

Metal above percolation threshold,

Insulator below percolation threshold

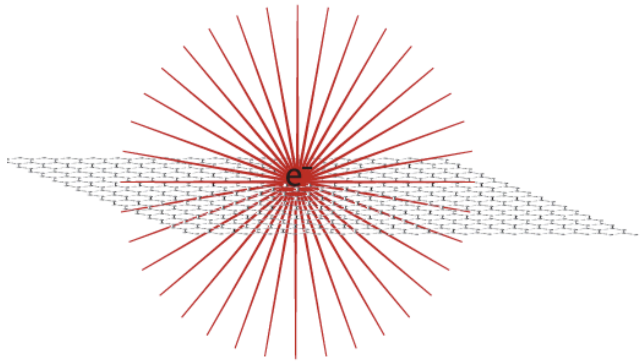
Dirac materials: interaction strength and density tuned independently

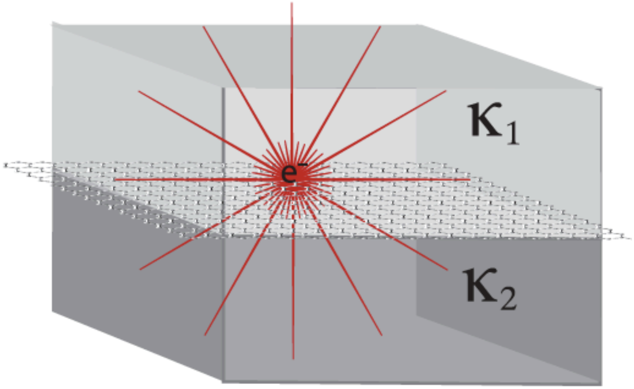
Interactions



$$r_s = \frac{e^2}{\hbar v_F}$$

$$r_s = \frac{e^2}{\hbar v_F(\kappa_1 + \kappa_2)}$$

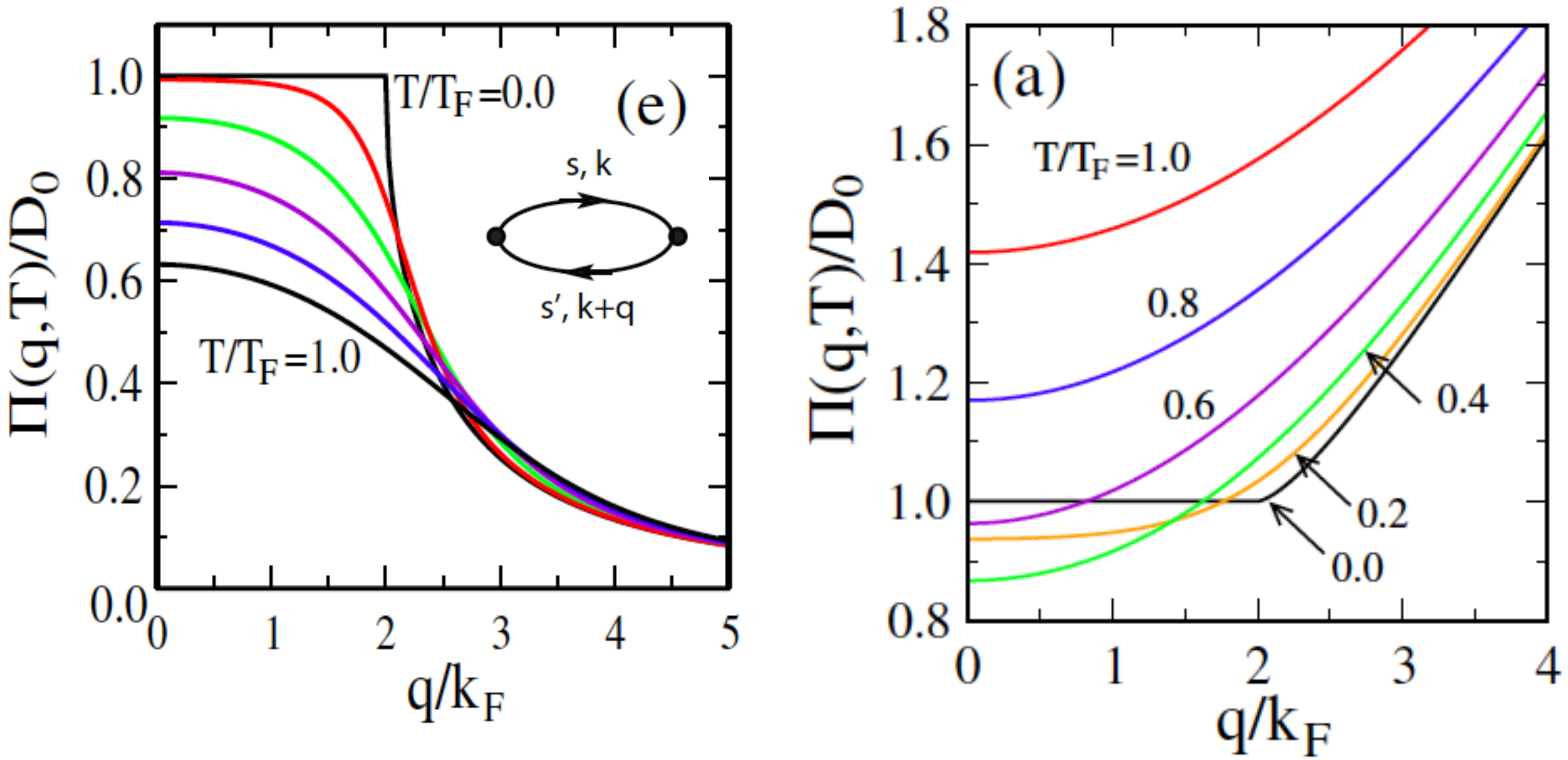




C. Juang, S. Adam, J-H. Chen, E. D. Williams, S. Das Sarma, and M. S. Fuhrer, *Phys. Rev. Lett.* **101**, 146805 (2008).

Fermi liquid away from DP

Weak Interactions = Screening

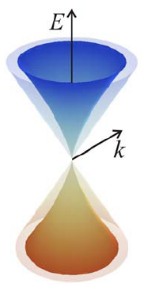


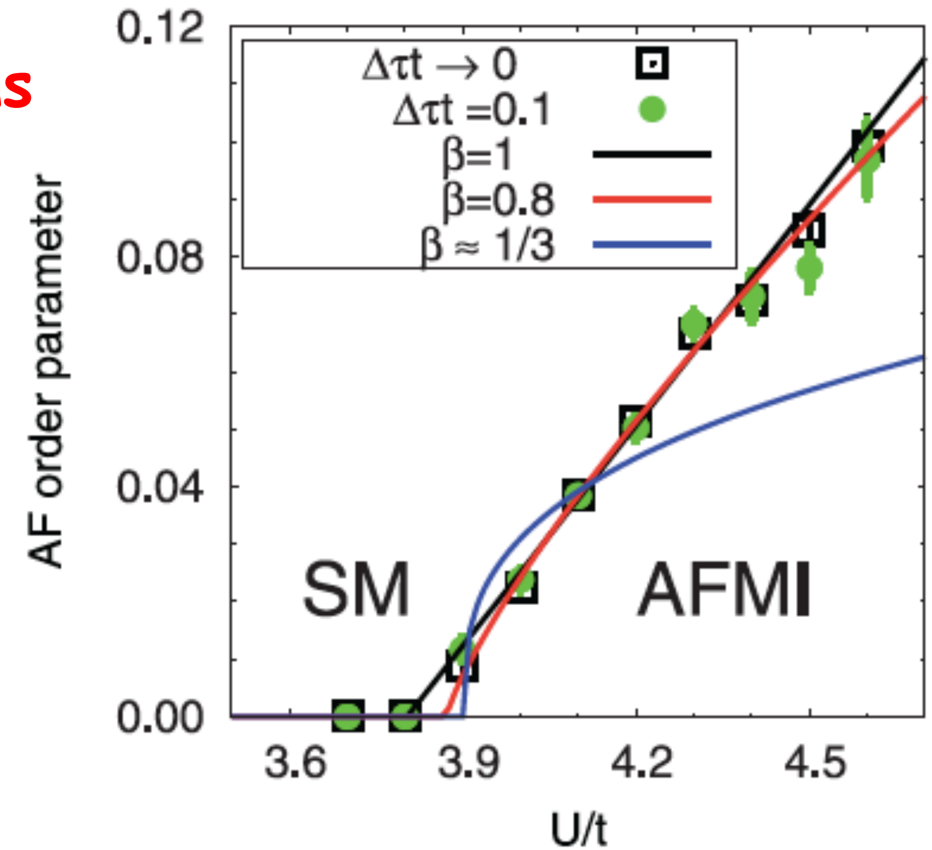
$$\varepsilon(q) = 1 + \frac{2\pi e^2}{\kappa q}\Pi(q)$$

- Screening is “metallic” on distances larger than the Fermi wavelength
- Screening is like a dielectric “insulator” on shorter distances
- Long-range nature of coulomb tail can not be screened

What about the Dirac point?

Strong Interactions

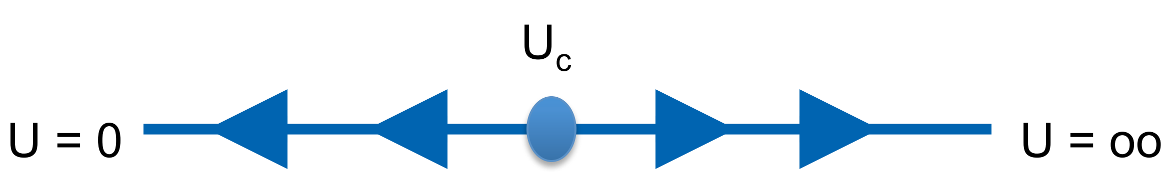




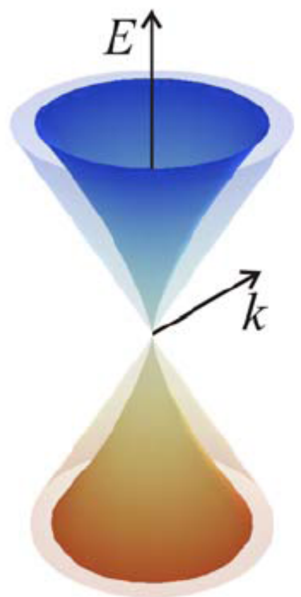
e.g. Sorella et al. Sci. Rep. (2012)
F. Assaad (2012-2014)

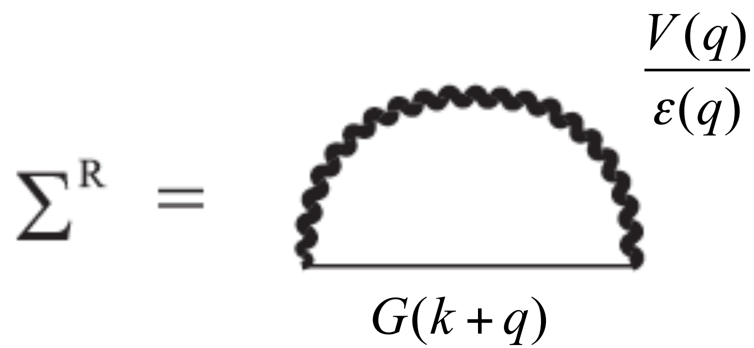
Semi-metal to AFM phase transition consistent with SU(2) SU(2) Heisenberg Gross-Neveu universality class

For strong interactions, Monte Carlo reveals gapped phase (anti-ferromagnet)



Divergent Fermi velocity





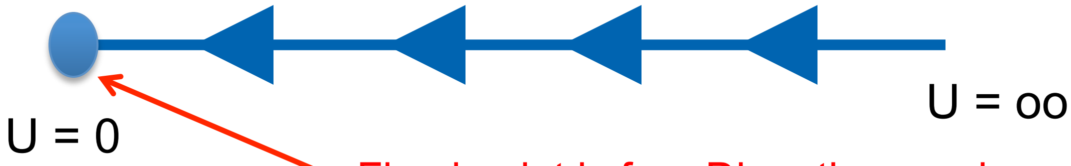
$$\frac{v_{\rm eff}}{v_0} = 1 + \frac{r_s}{4} \log\left[\frac{\sim 1}{ka}\right]$$

For weak interactions, perturbation theory reveals diverging Fermi velocity

V. Kotov, B. Uchoa, V. Pereira, A. H. Castro Neto and F. Guinea, *Rev. Mod. Phys.* (2012)

No consistent picture at DP

1. Renormalization Group [e.g. Sachdev (1998) / Guinea (1997)]



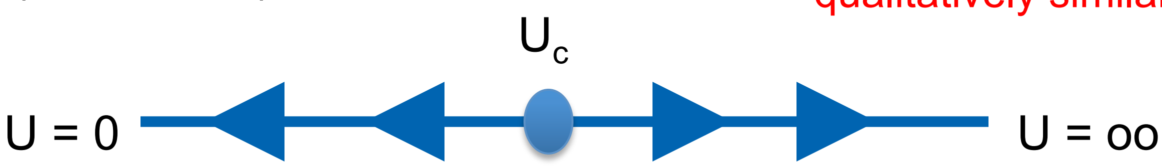
Fixed point is free Dirac theory where interactions are "dangerously irrelevant"

2. Diagrammatic perturbation approaches [e.g. Das Sarma et al. (2007)]

"marginal Fermi liquid"

3. Hubbard model on a honeycomb lattice (semi-metal to AFM Mott transition occurs at interaction strengths outside the experimental window) e.g. Sorella, Assaad, Katsnelson (2012-2014).

"qualitatively similar to a Fermi liquid"

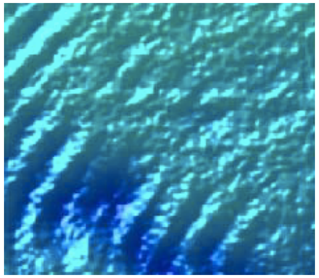


4. Lattice Monte Carlo applied to Dirac fermions with momentum cut-off e.g. Drut and Lahde (2009-2014).

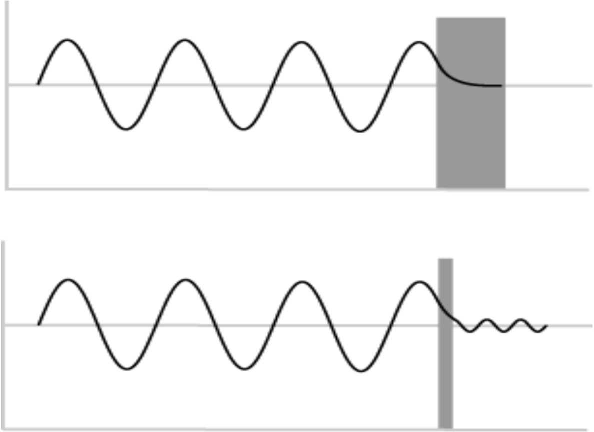
"chiral symmetry breaking insulating state for suspended graphene"

Perfect transmission

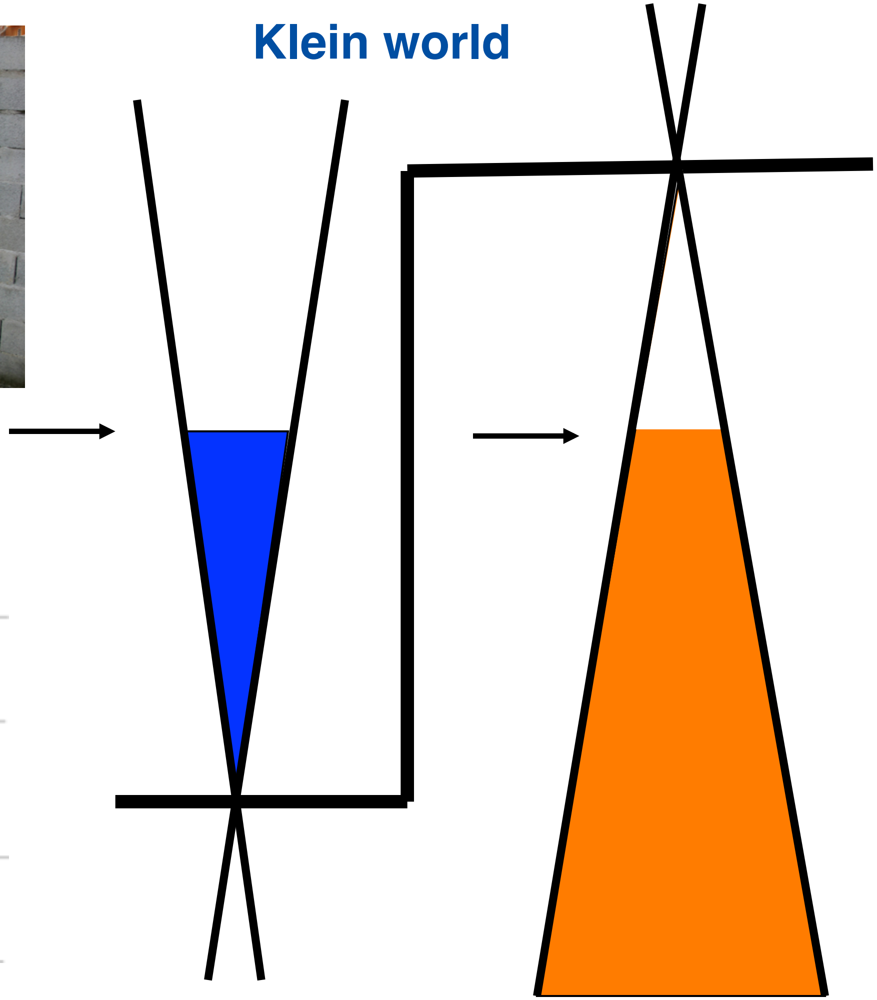
Quantum Interference



Classical world



Quantum world



Klein world

P-N junctions are completely transparent for direct incidence. Results in beam collimation.

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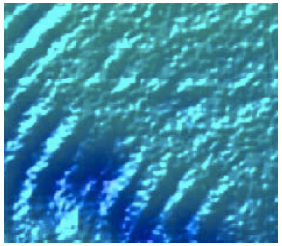
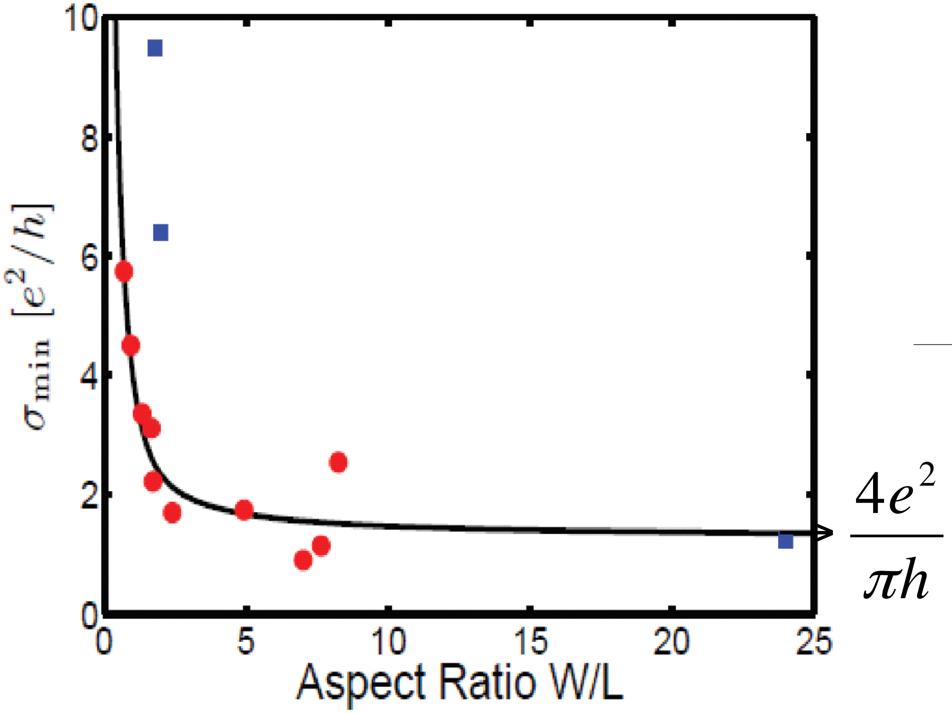
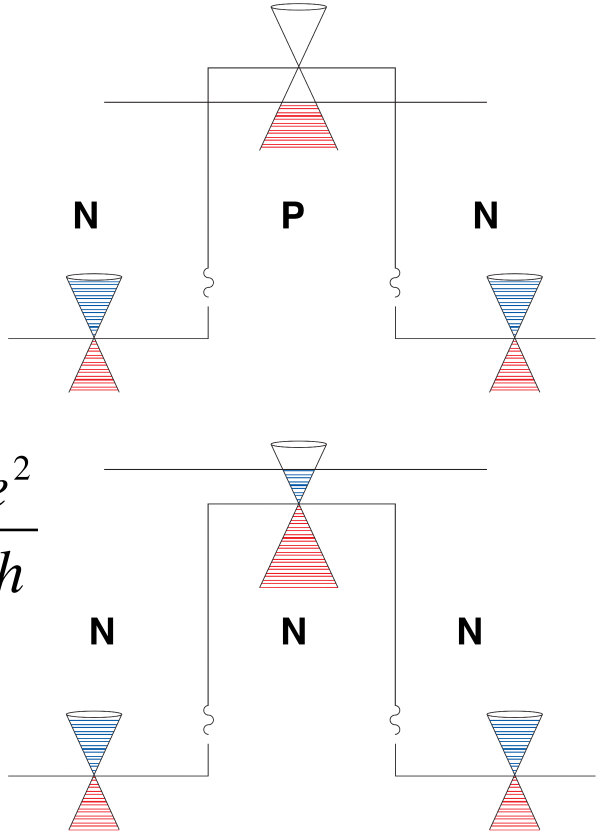
Universal ballistic σ_{min}

Quantum Interference





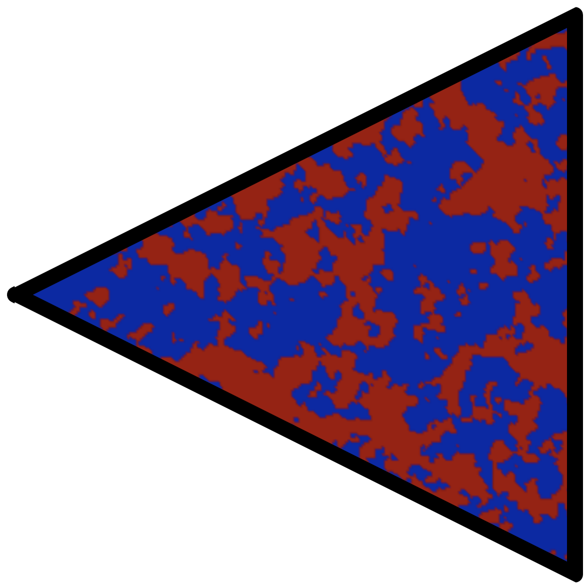


Without disorder and without interactions, both Kubo and Landauer formalisms give a universal ballistic minimum conductivity at the Dirac point.

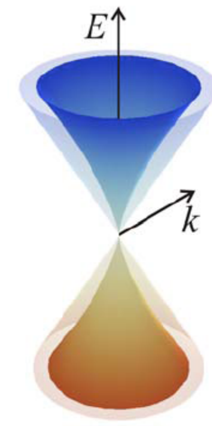
M. Katsnelson (2006);
C. Beenakker et al. (2006)

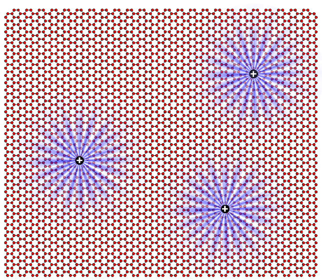
Delicate interplay between disorder, interactions and quantum effects

Most experiments are in the regime, where all these effects are relevant, but not dominant!

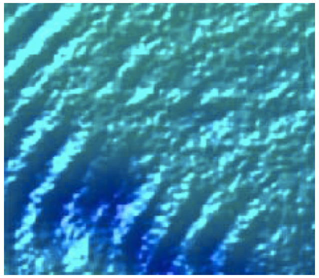


Electron Interactions



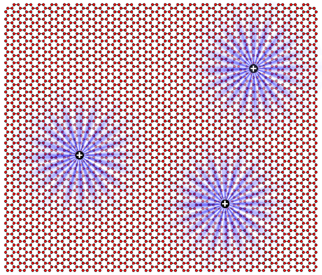


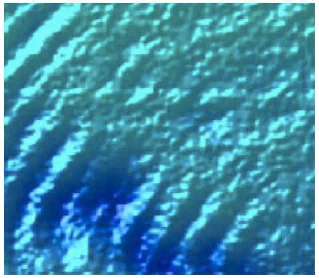
Disorder



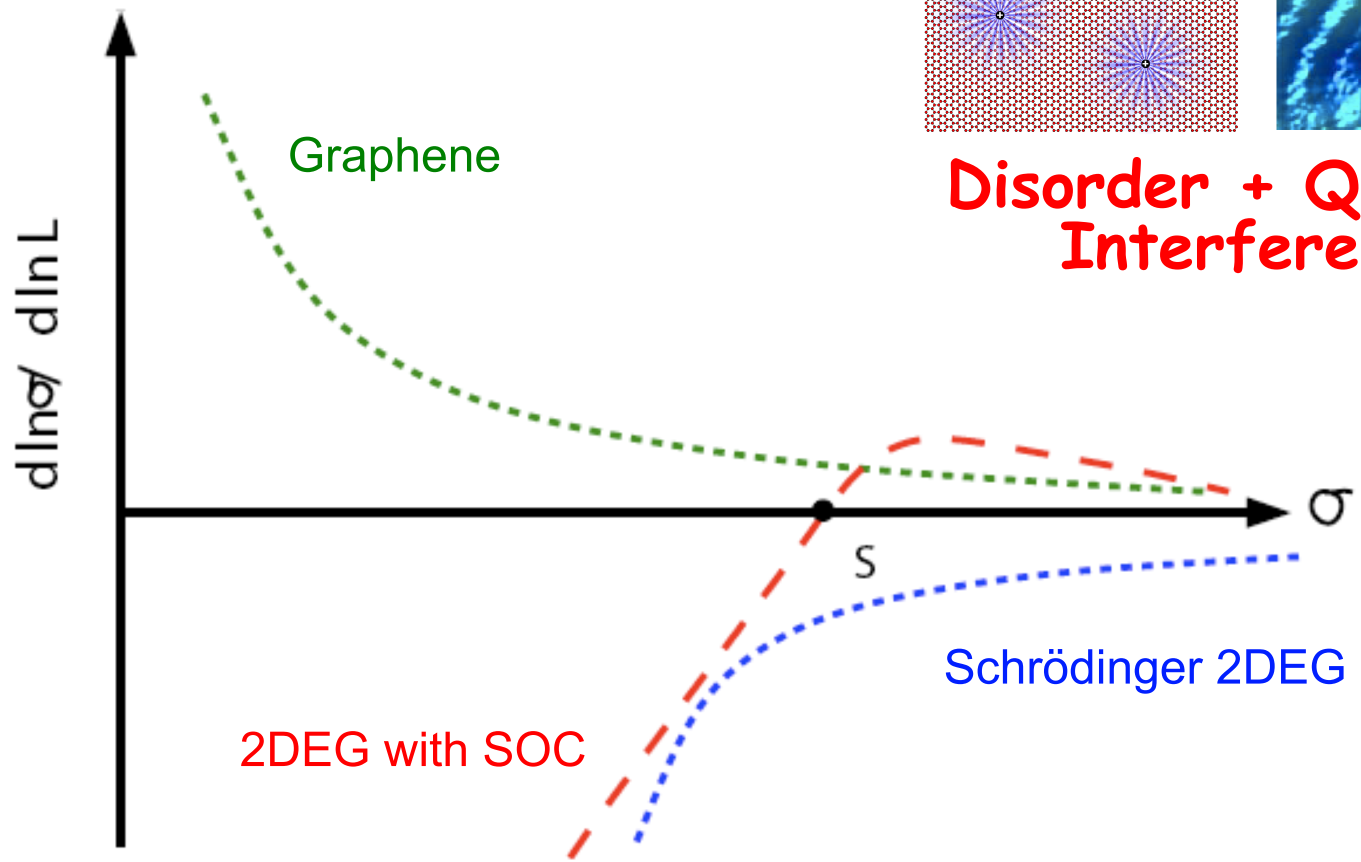
Quantum Interference

Scaling theory of localization





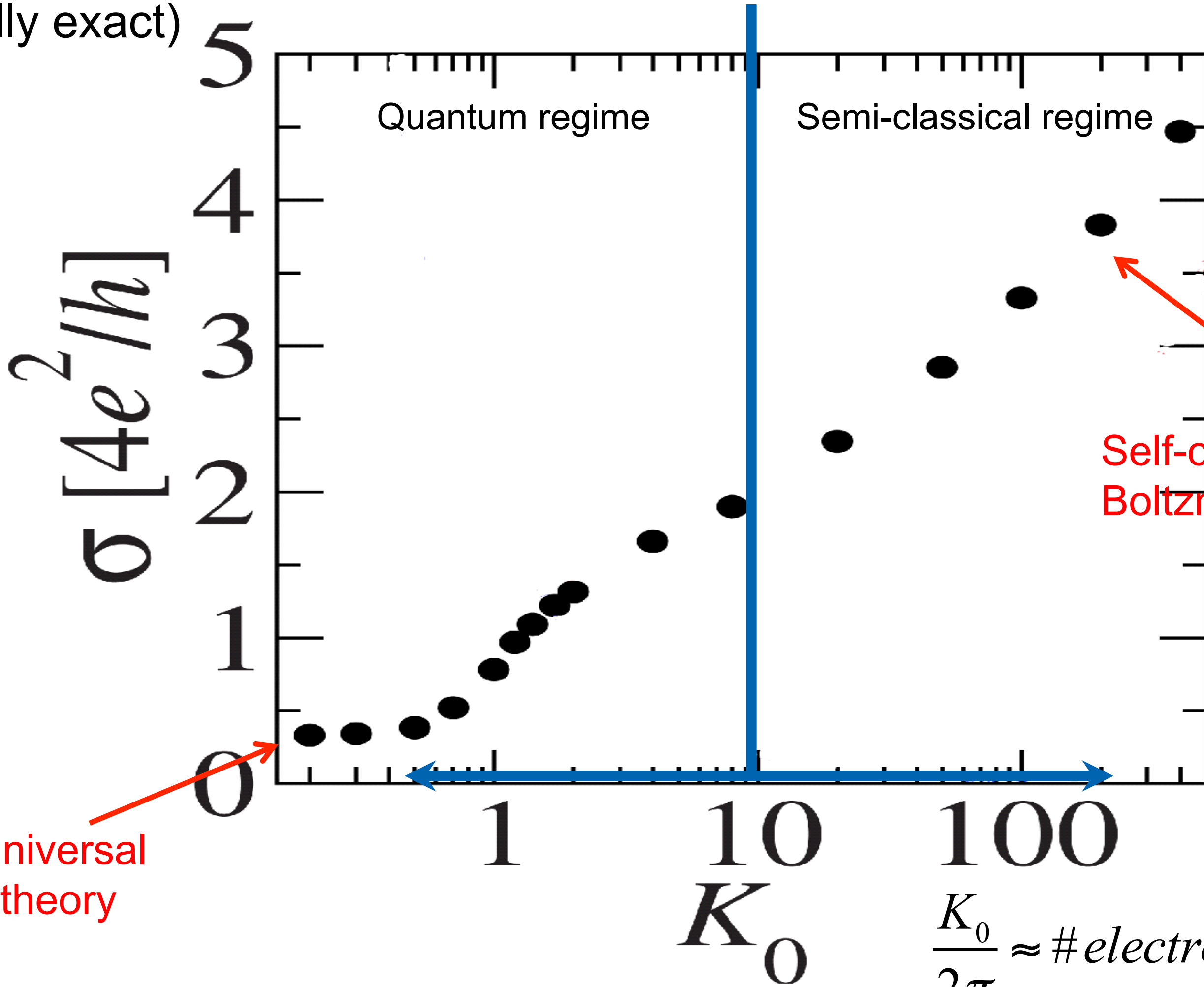
Disorder + Quantum Interference

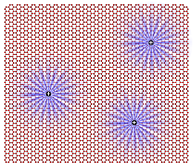


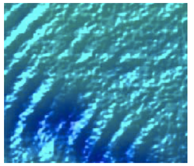
No Anderson localization

Dirac point conductivity (numerically exact)

S. Adam, P. W. Brouwer and S. Das Sarma, Phys. Rev. B ***R*** **79**, 201404 (2009)







$$\langle U(\mathbf{r})U(\mathbf{r}')\rangle = K_0 \frac{(\hbar v)^2}{2\pi\xi^2} e^{-|\mathbf{r}-\mathbf{r}'|^2/2\xi^2},$$

Self-consistent diffusive Boltzmann transport theory

Ballistic universal quantum theory

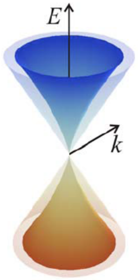
$$\frac{K_0}{2\pi} \approx \# electrons \text{ per puddle}$$

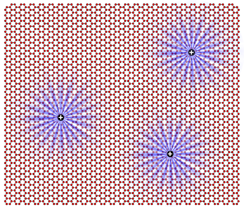
How does an inhomogeneous Fermi liquid screen external potentials?

Example of Thomas-Fermi screening:

$$V_{screened} = \frac{V_{bare}}{\varepsilon[q]}$$

Interactions + Disorder





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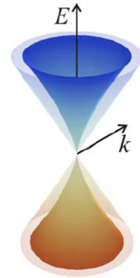

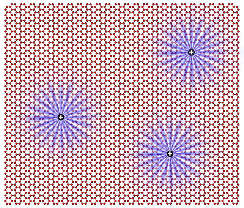

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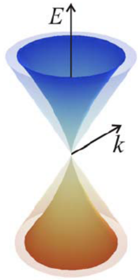
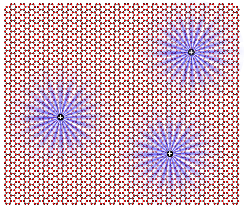
Interactions + Disorder





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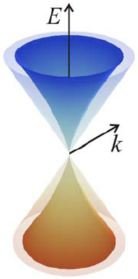

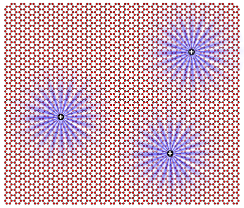

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$$v_{\mathrm{F}} \xrightarrow{\text{2DEG}} \frac{\hbar\sqrt{\pi n}}{2m}$$

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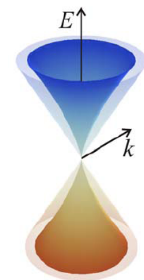
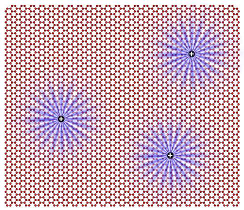
Example of Thomas-Fermi screening:

Interactions + Disorder





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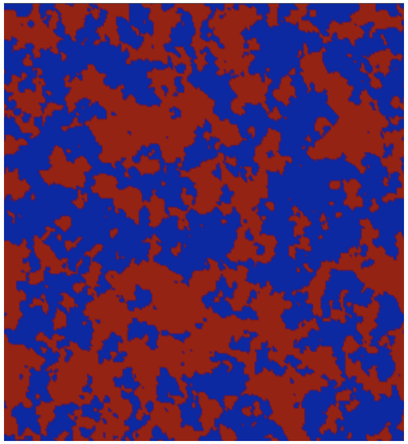
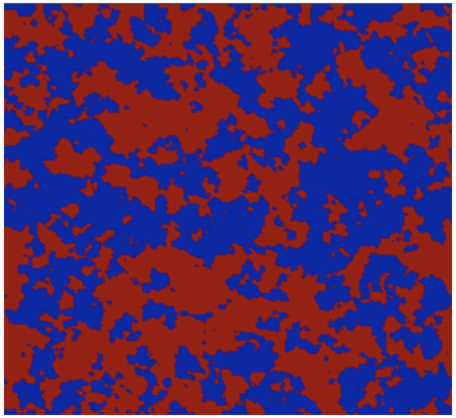
Inhomogeneous Dirac: $\epsilon(q) = 1 + \frac{e^2}{\hbar v_{\mathrm{F}}}\frac{\sqrt{\pi n_{\mathrm{rms}}}}{\sqrt{3}q}$



What is $n_{rms}(n_{imp})$?

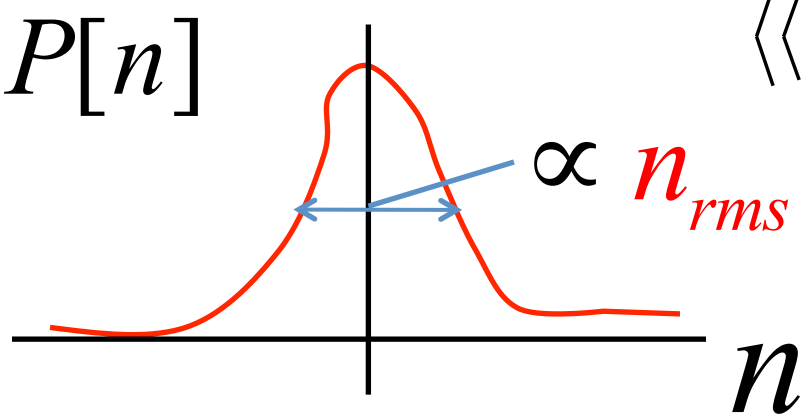


250 nm x 250 nm

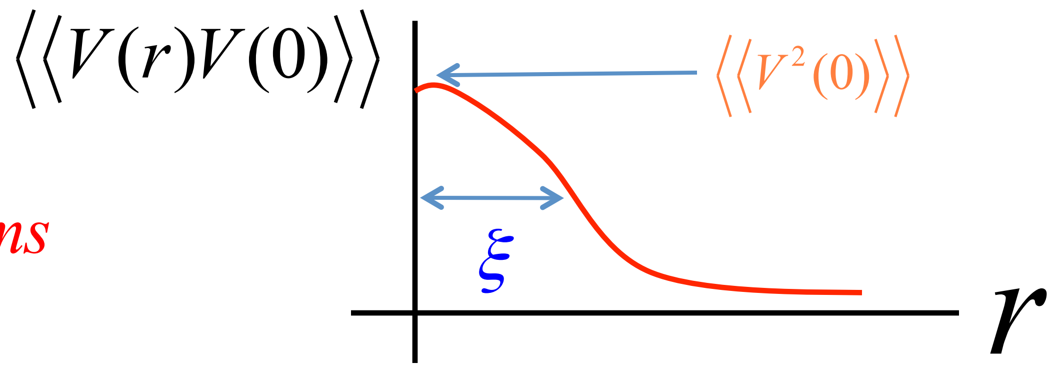
Statistical properties of density fluctuations and the Dirac point

Any physical observable could then be calculated

1. Histogram of the carrier density (distribution function):

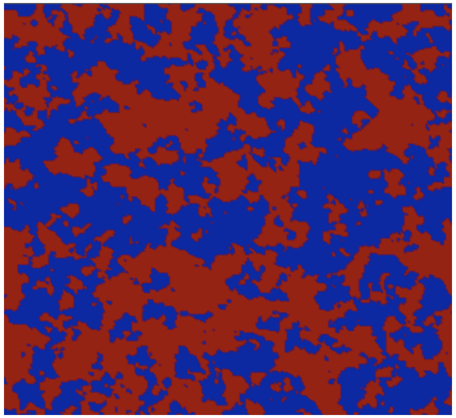


2. Screened potential correlation function:



Characterizes the puddle depth and length

What is $n_{rms}(n_{imp})$?



250 nm x 250 nm

Statistical properties of density fluctuations and the Dirac point

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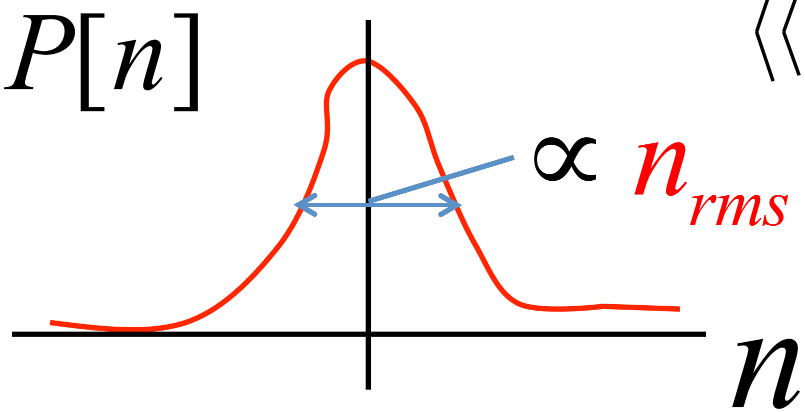
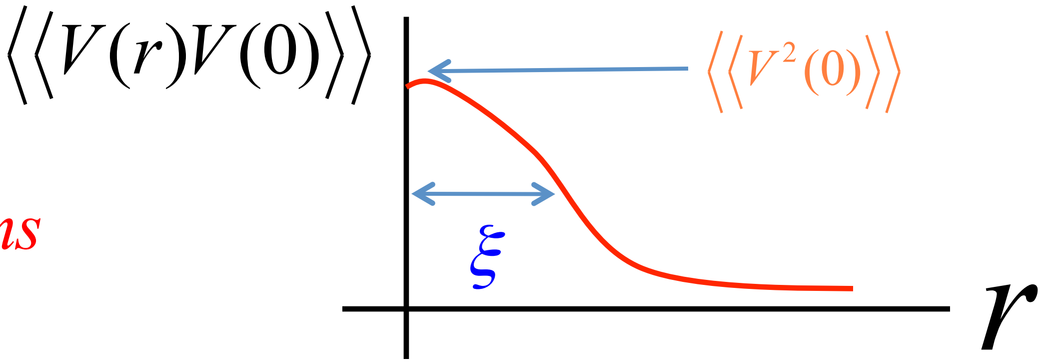
Calculate dimensionless quantity: $$\frac{n_{rms}}{n_{imp}} = ?$$

1. Histogram of the carrier density (distribution function):

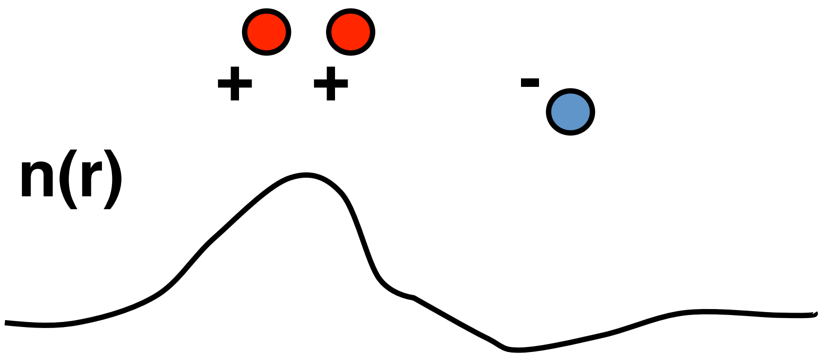


2. Screened potential correlation function:



Characterizes the puddle depth and length

Ansatz for Inhomogeneous screening



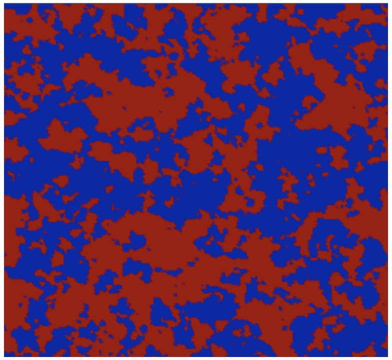
$$\phi_{scr}(q) = \frac{\phi_{bare}(q)}{\varepsilon(q, r_s, n)}$$

$$\varepsilon(q) = \text{const} \quad \text{(dielectric)}$$

$$\varepsilon(q) = 1 + \frac{\mathrm{q_{TF}}}{\mathrm{q}} \quad \text{(metal)}$$

$$\varepsilon(q, k_F, r_s) = \begin{cases} 1 + \dfrac{r_s \pi}{2}; & q << 2k_F \\ 1 + \dfrac{4k_F r_s}{q}; & \mathrm{q >> 2\,k_F} \end{cases} \quad \text{(Dirac)}$$

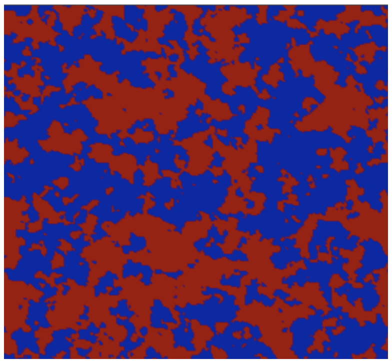
Ansatz for Inhomogeneous screening



$$\phi_{scr}(q) = \frac{\phi_{bare}(q)}{\varepsilon\left(q, r_s, \langle n \rangle = 0\right)}$$

$$\varepsilon(q, r_s, P[n]) \rightarrow \varepsilon\left(q, r_s, \langle n^2 \rangle, \langle n^3 \rangle, \ldots\right)$$

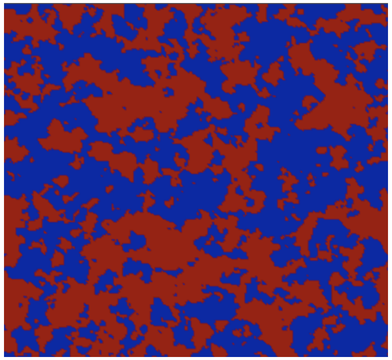
Ansatz for Inhomogeneous screening



$$\phi_{scr}(q) = \frac{\phi_{bare}(q)}{\varepsilon\left(q, r_s, \langle n \rangle = 0\right)}$$

$$\varepsilon(q, r_s, P[n]) \rightarrow \varepsilon\left(q, r_s, \langle n^2 \rangle, \langle \quad \rangle, \ldots\right)$$

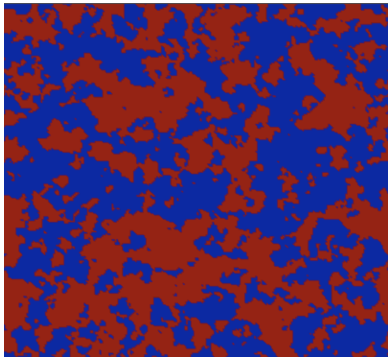
Ansatz for Inhomogeneous screening



$$\phi_{scr}(q) \approx \frac{\phi_{bare}(q)}{\varepsilon(q, r_s, n_{rms})}$$

$$\varepsilon(q, r_s, P[n]) \approx \varepsilon\left(q, r_s, \left\langle n^2 \right\rangle\right)$$

Ansatz for Inhomogeneous screening

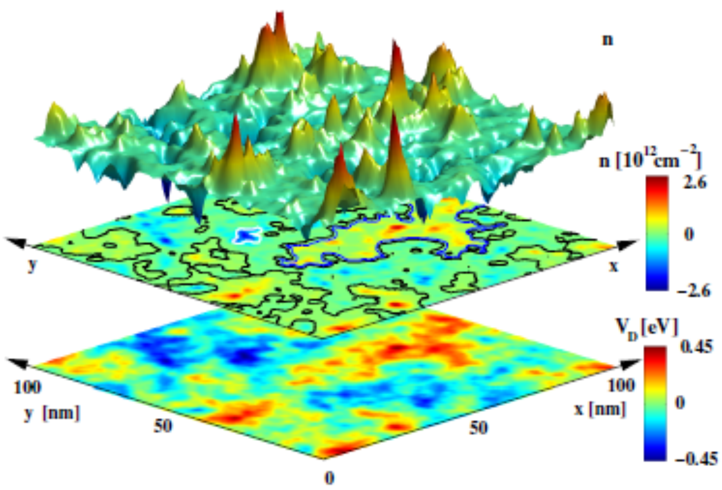


$$\phi_{scr}(q) \approx \frac{\phi_{bare}(q)}{\varepsilon(q, r_s, n_{rms})}$$

$$\frac{n_{rms}}{n_{imp}} = 2 r_s^2 C_0 \left[r_s, d\sqrt{n_{rms}} \right]$$

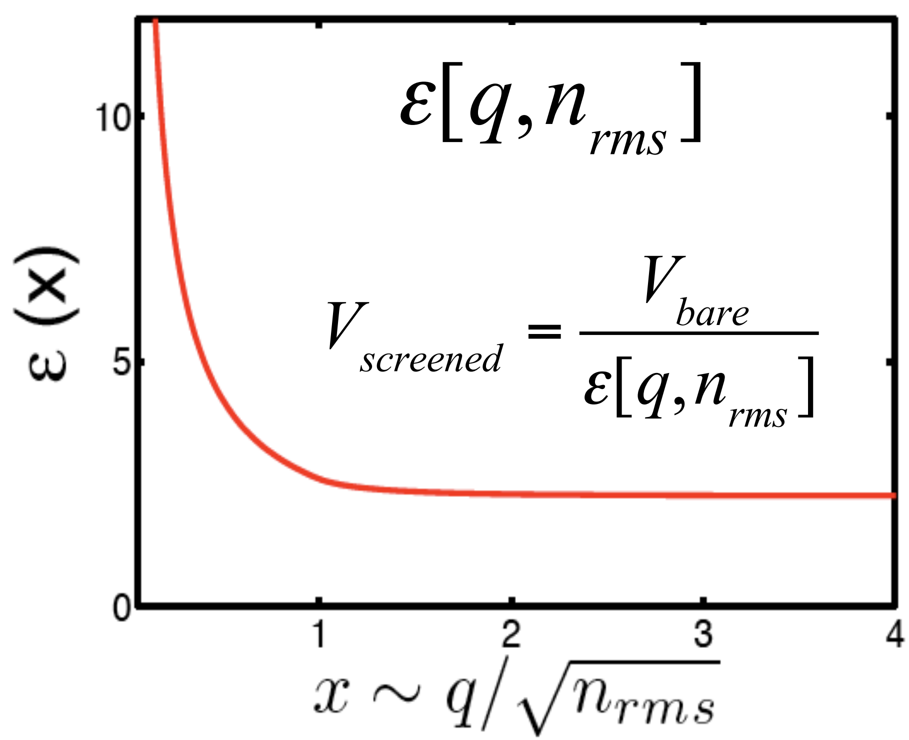
S. Adam, E. H. Hwang, V. M. Galitski and S. Das Sarma
Proc. Nat. Acad. Sci. USA **104**, 18392 (2007).

Local screening vs. global screening



E. Rossi and S. Das Sarma PRL **101**, *166803 (2008)*

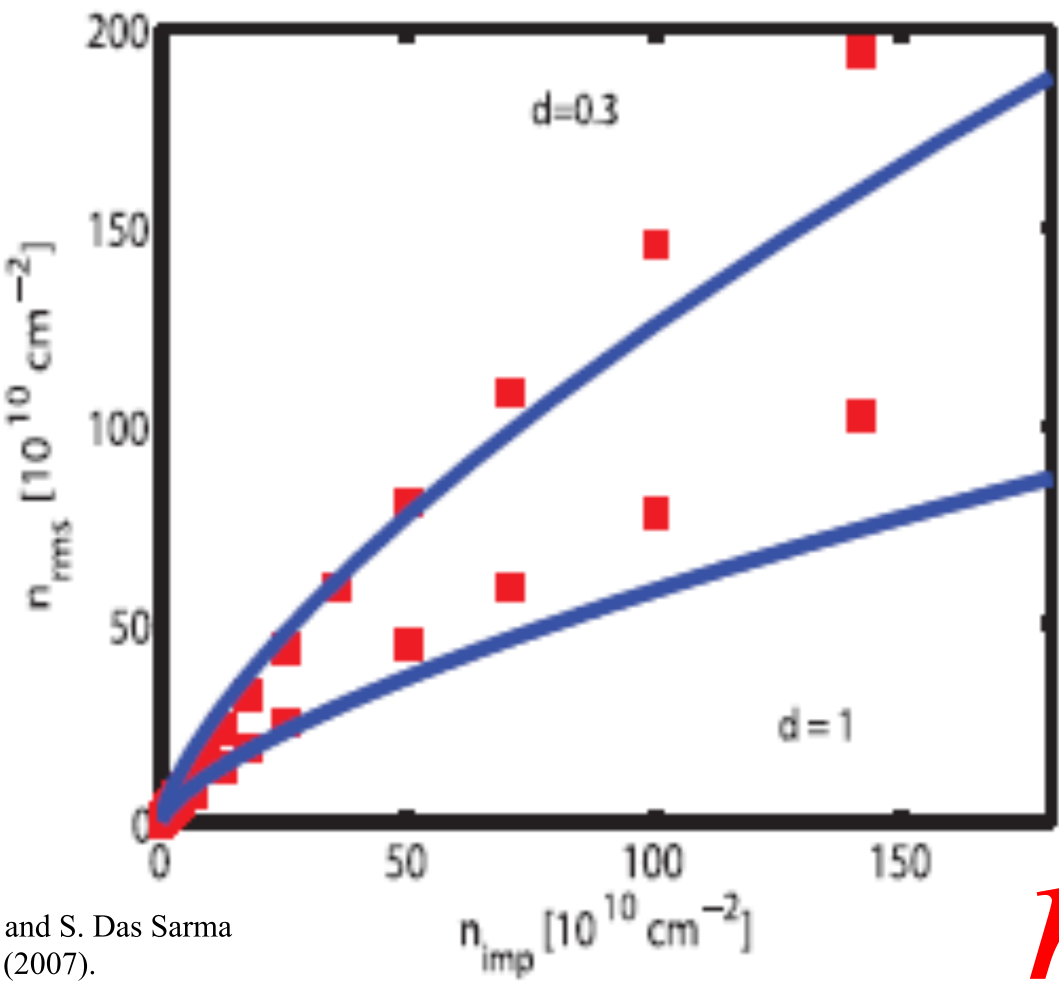
E. Rossi, S. Adam and S. Das Sarma, PRB **79**, *245423 (2009)*



S. Adam, E. H. Hwang, V. Galitski, S. Das Sarma, Proc. Nat. Acad. Sci. USA **104**, 18392 (2007).

Numerical verification

n_{rms}



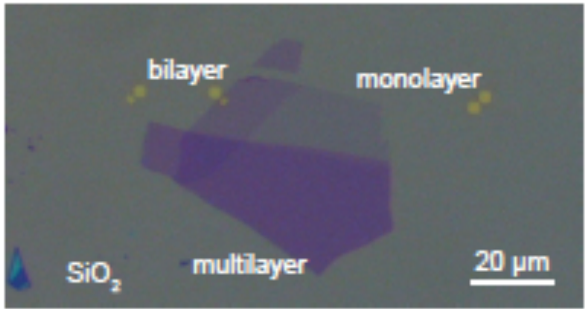
n_{imp}

S. Adam, E. H. Hwang, V. M. Galitski and S. Das Sarma
Proc. Nat. Acad. Sci. USA **104**, 18392 (2007).

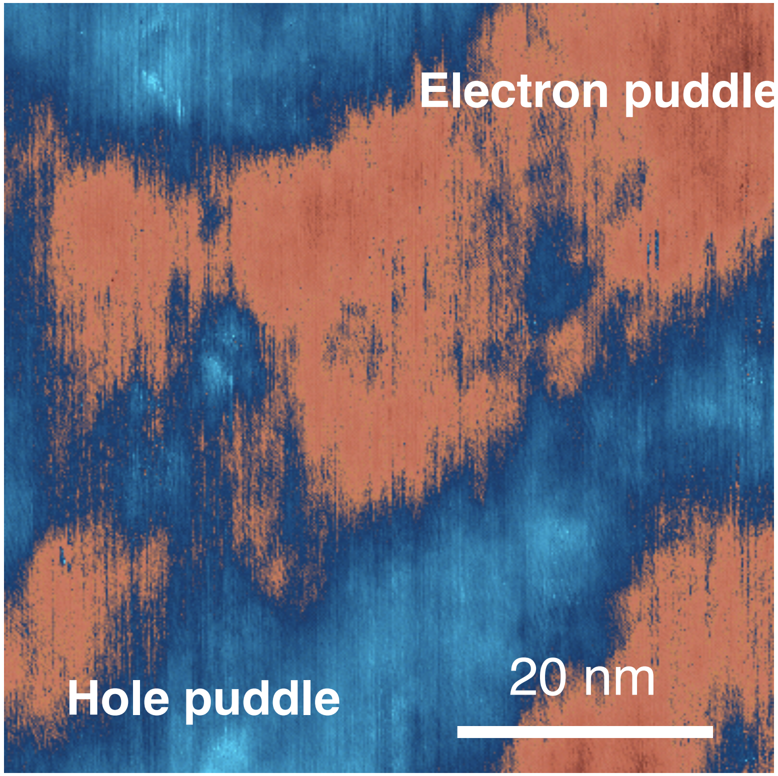
E. Rossi, S. Adam and S. Das Sarma
Phys. Rev. B **79**, 245423 (2009)

Puddle Formation

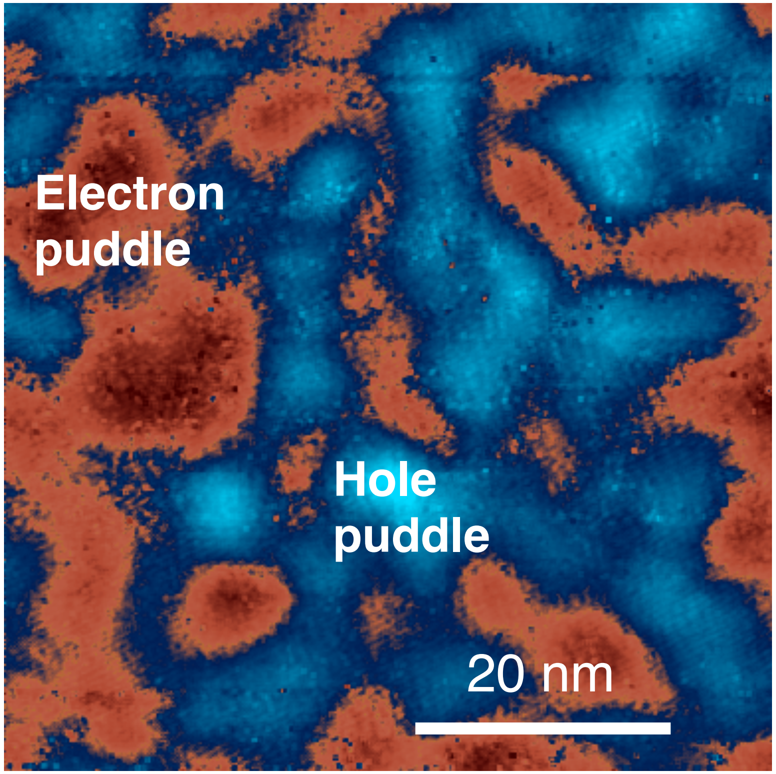
With J. A. Stroscio (NIST)
Phys. Rev. B 84, 235421 (2011)



Single Layer Graphene



Bilayer Graphene



Agreement with experiments [1]

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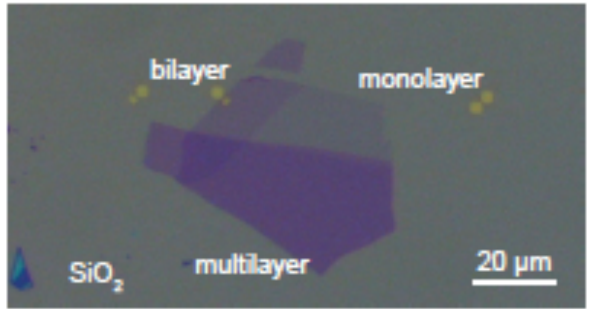
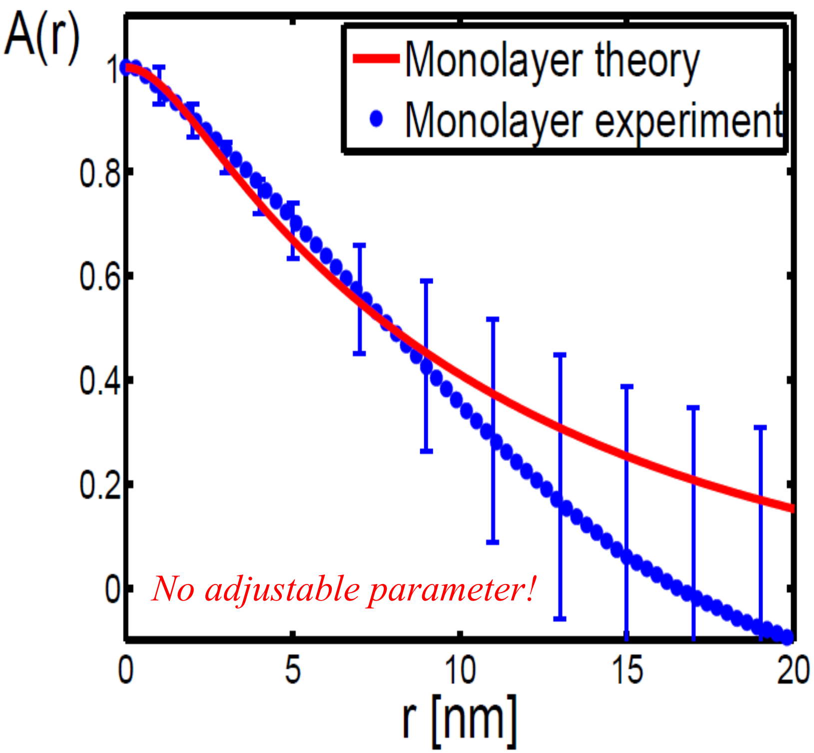
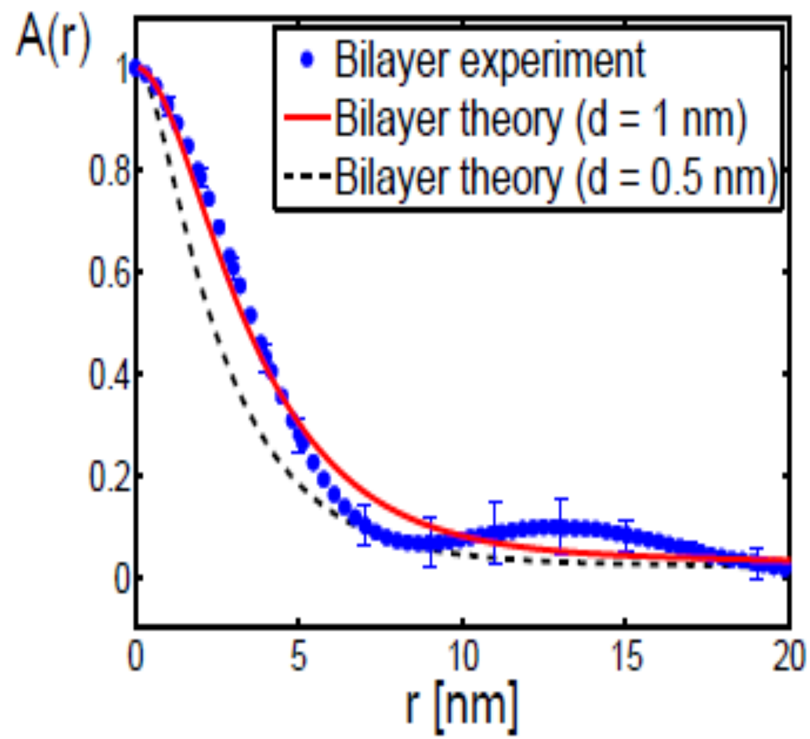
Collaboration with J. A. Stroscio (NIST)
Phys. Rev. B 84, 235421 (2011)



Single Layer Graphene



Bilayer Graphene



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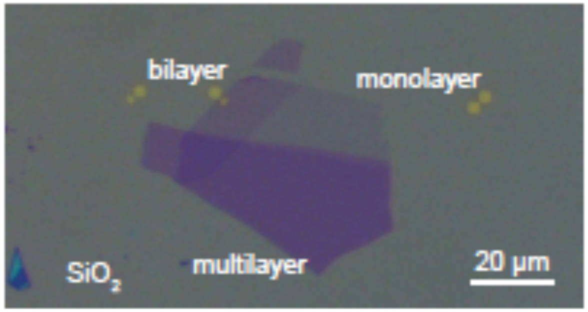

Monolayer graphene from a Brian LeRoy (Arizona)

Bilayer Graphene