Ground state of 2D Graphene in presence of Random Charged impurities

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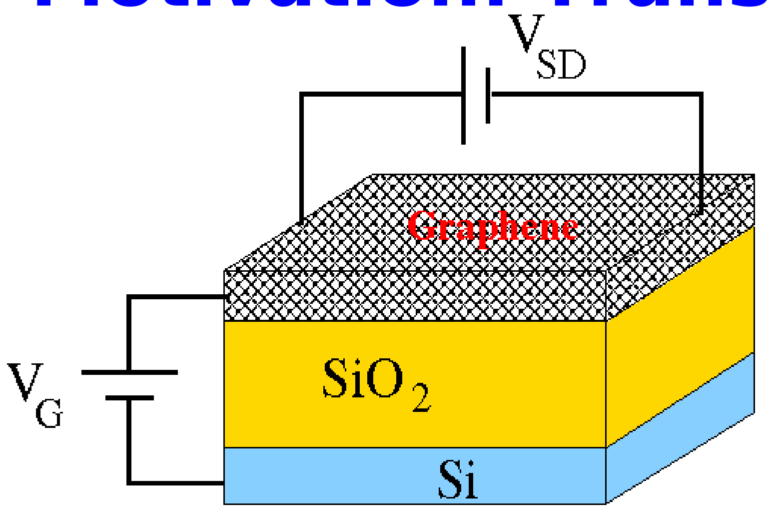
Work supported by:

NSF-NRI

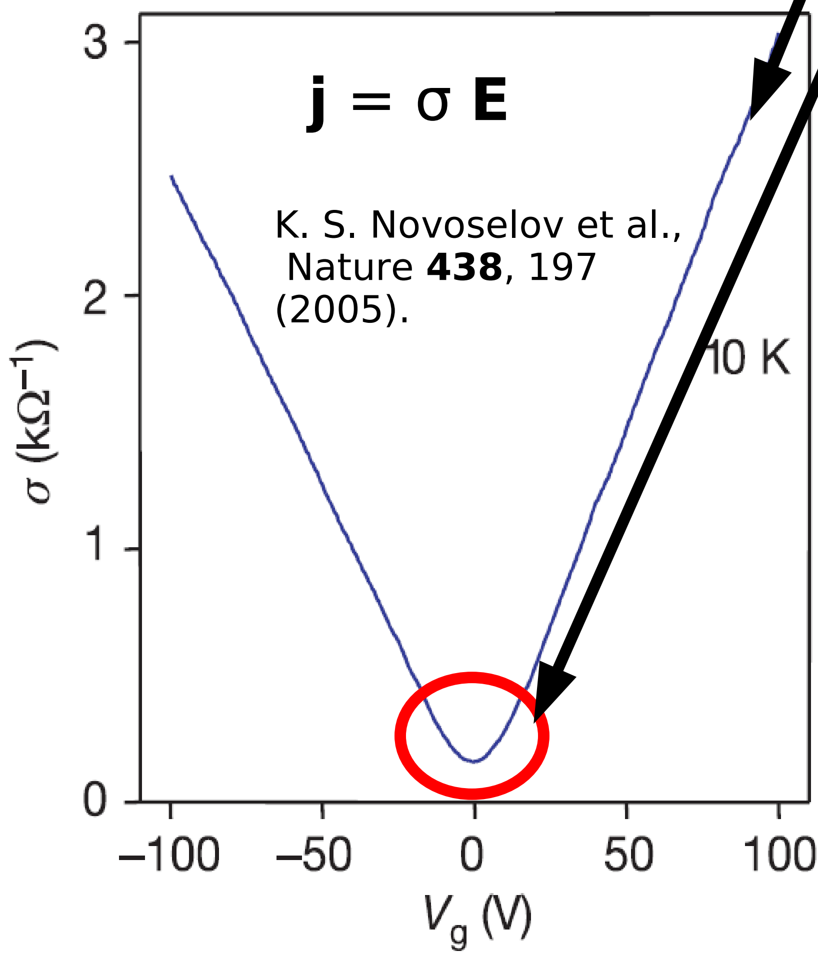
Motivation: Transport puzzles in graphene

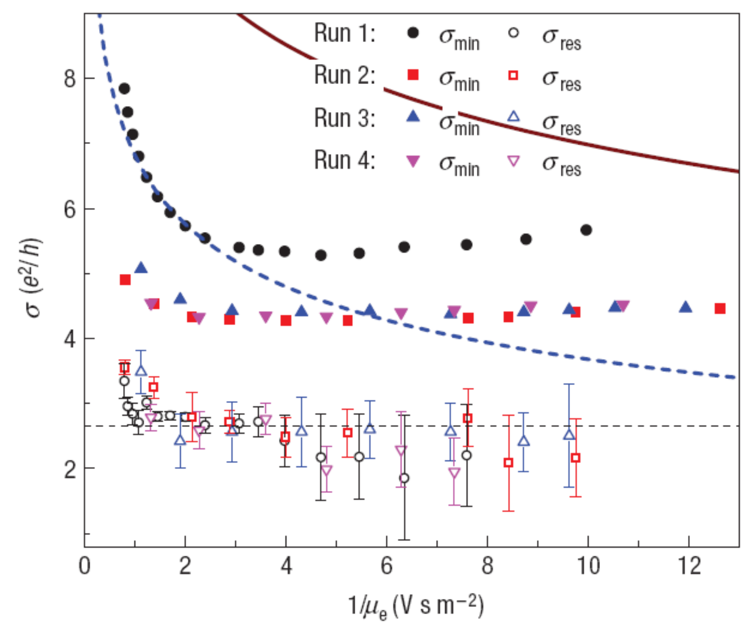


1) Linear scaling with doping: σ ~ n

2) Minimum of conductivity, σ_{min} , for n->0.

3) σ_{min} different from clean limit and depends on sample quality

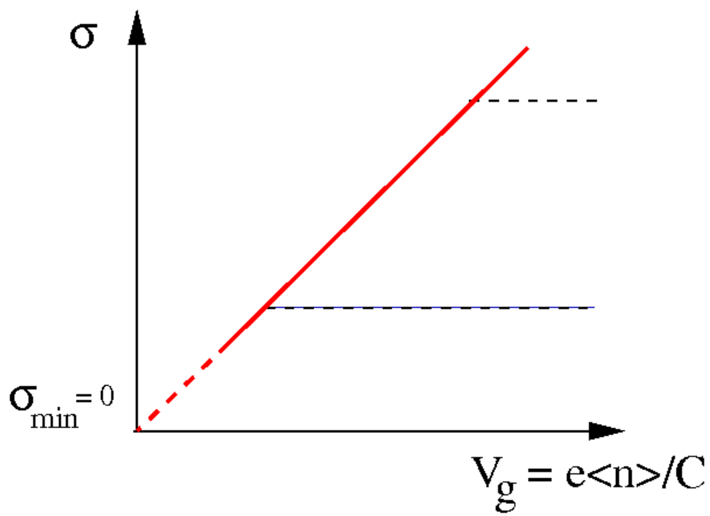


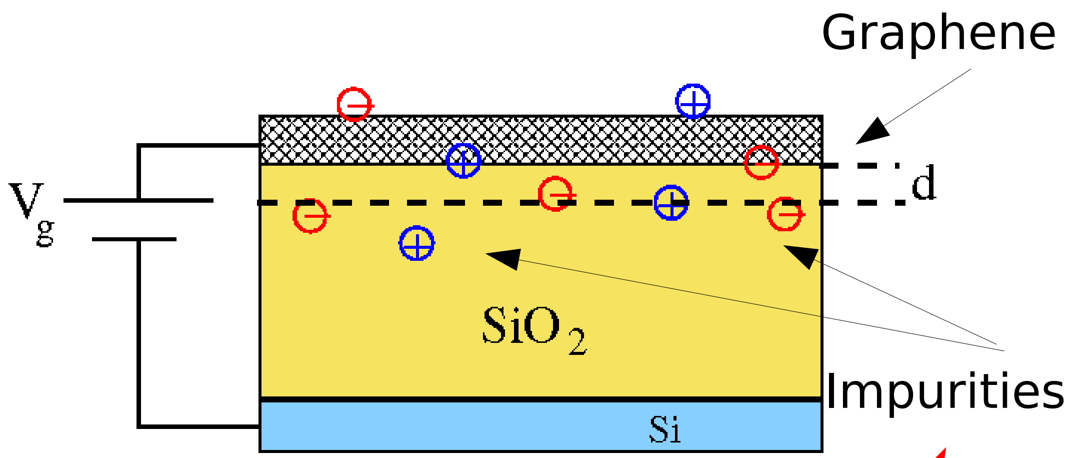


J.-H. Chen et al.
Nat. Phys. **4**, 377 (2008)

Y.-W. Tan et al. PRL **99**, 246803 (2007)

Source of disorder





$V_{DIS}(q) = V_0$ → σ ~ const

Quasiparticle scattering is enhanced at low densities

$V_{DIS}(q) = 1/q$ → σ ~ n

Charge impurities

Screening

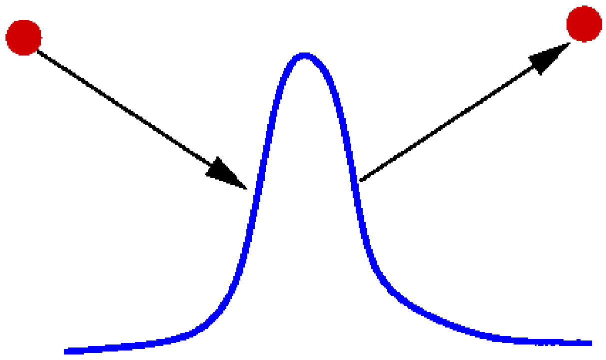
$$V_{\rm DIS} = \frac{2\pi e^2}{q + 2\pi e^2 \Pi(q)}$$

$$\Pi(k_F) \propto D(\epsilon_F) \propto k_F$$

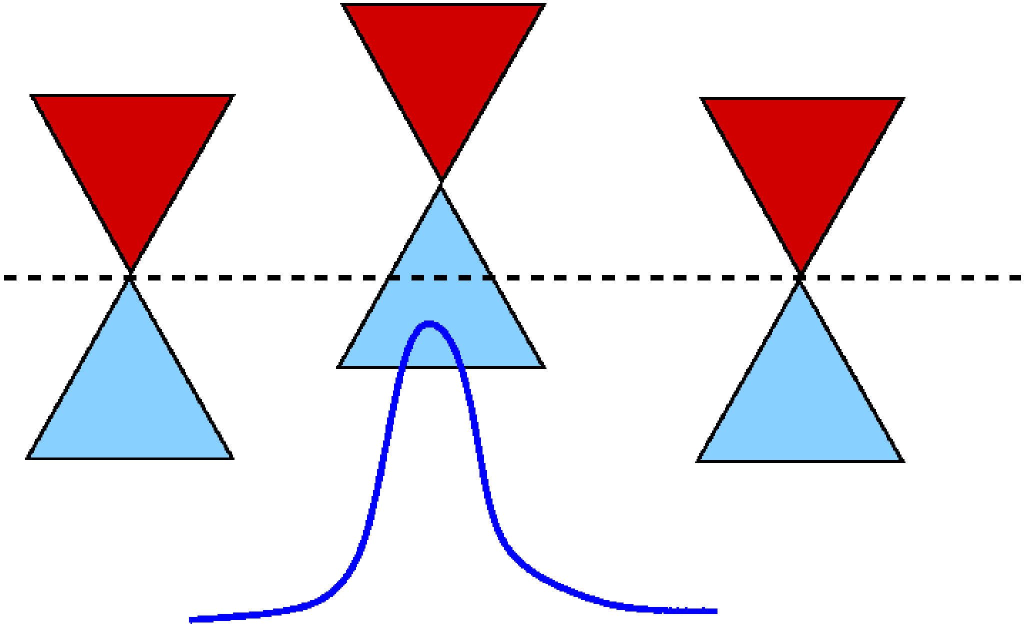
Screening does not change the density dependence of the conductivity!

K. Nomura & A.H. MacDonald PRL **96** 256602 (2006);
T. Ando, J. Phys. Soc. Jpn **75** 74716 (2006);
Hwang et al. PRL **99** 226801 (2007)

Effect of disorder



Scattering



Shifts bottom of the band $\leftrightarrow$ shift of Fermi energy

$\delta n(r)$

$$n(r) = <n> + \delta n(r)$$

At the Dirac point
$<n> = 0$

density fluctuations $\delta n(r)$ dominate the physics

Non-linear screening

Thomas-Fermi-Dirac theory

Developed a theory that is:

- **Microscopic**
- **Nonperturbative**

$$r_s = \frac{e^2}{\hbar v_F \bar{\epsilon}} \sim 1$$

It includes:

- **Disorder potential due to charge impurities;**
- **Nonlinear screening;**
- **Exchange and correlation effects;**

Build the energy functional E[n], n(**r**) is the carrier density .

$$E[n] = E_{kin}[n(\mathbf{r})] + E_H[n(\mathbf{r})] + E_{exch}[n(\mathbf{r})] - \int_A \mathbf{V_D} n(\mathbf{r}) d^2 r - \mu \int_A n(\mathbf{r}) d^2 r$$

V_D is the disorder potential generated by charge impurities .

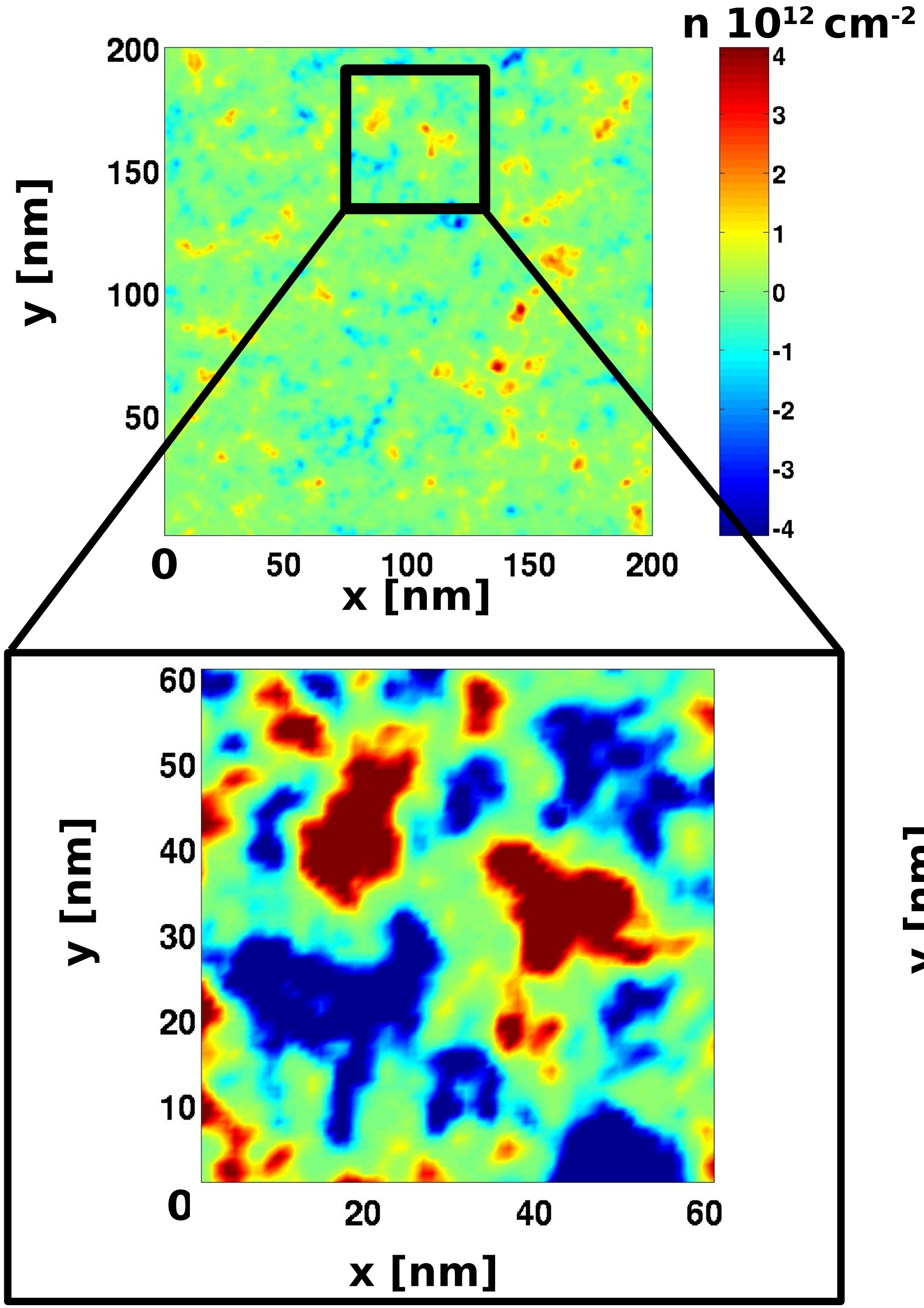
$$\frac{\delta E_{exch}}{\delta n} = \Sigma \approx -|C_1|\sqrt{n} - |C_2|\sqrt{n}\ln(|n|)$$

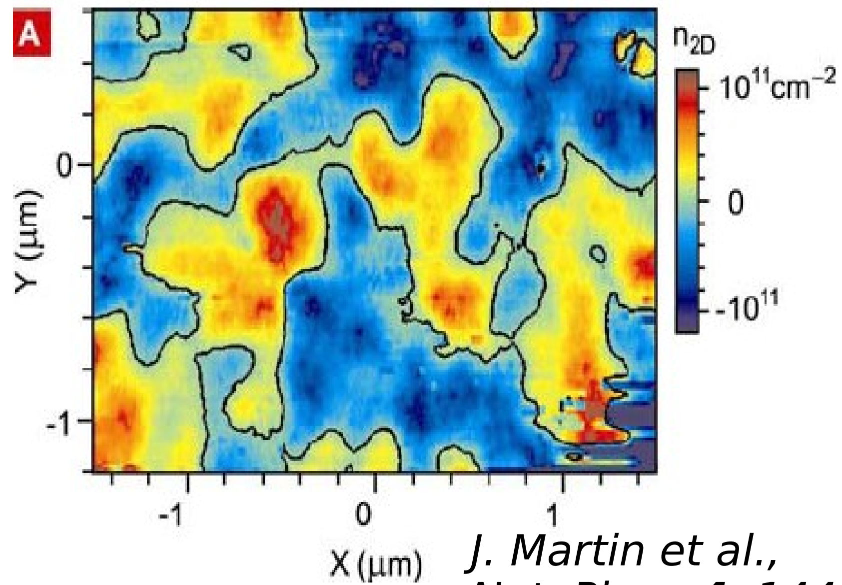
*Barlas et al. PRL **98** 236601(2007),*
*Hwang et al. PRL **98** 226801(2007),*
*Polini et al PRB **78** 115426 (2008).*

Correlation simply renormalizes the numerical factor C_2 .

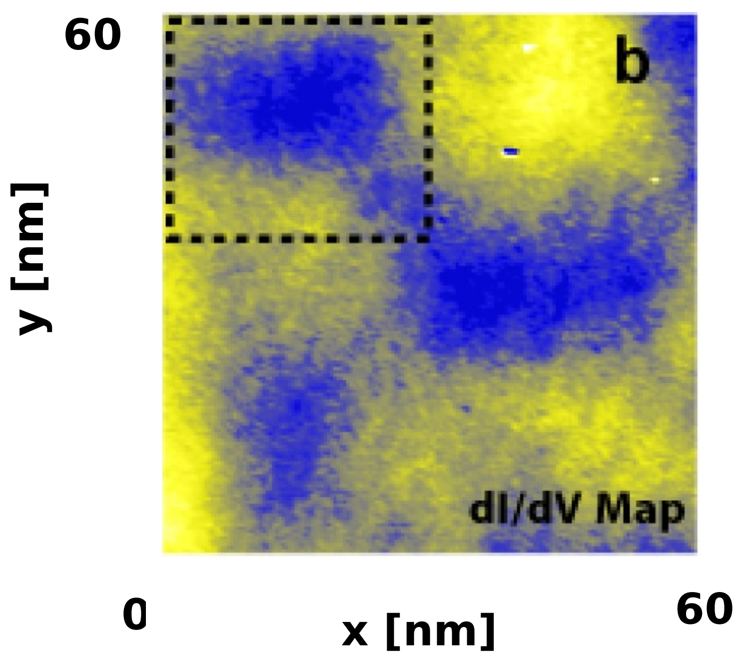
n_{imp} and *d*, reliably extracted from transport experiments at high doping.

Dirac point: single disorder realization





J. Martin et al., Nat. Phys. ***4****, 144 (2008)*



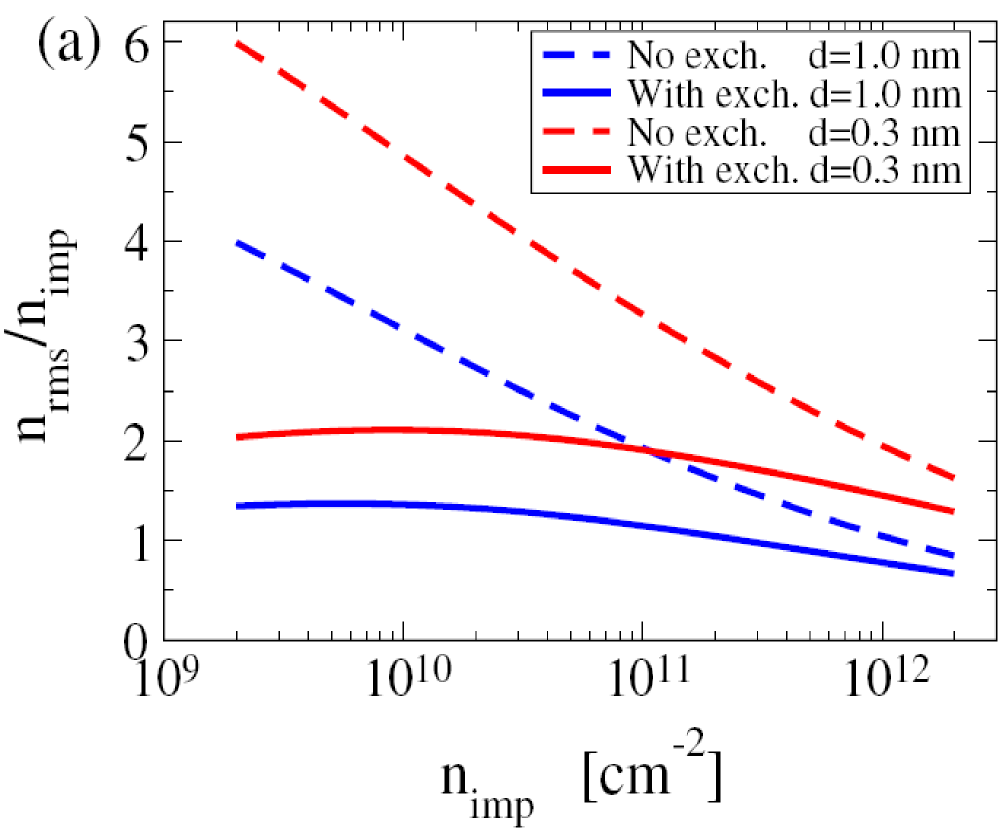
ER, S. Das Sarma, PRL ***101****, 166803 (2008)*

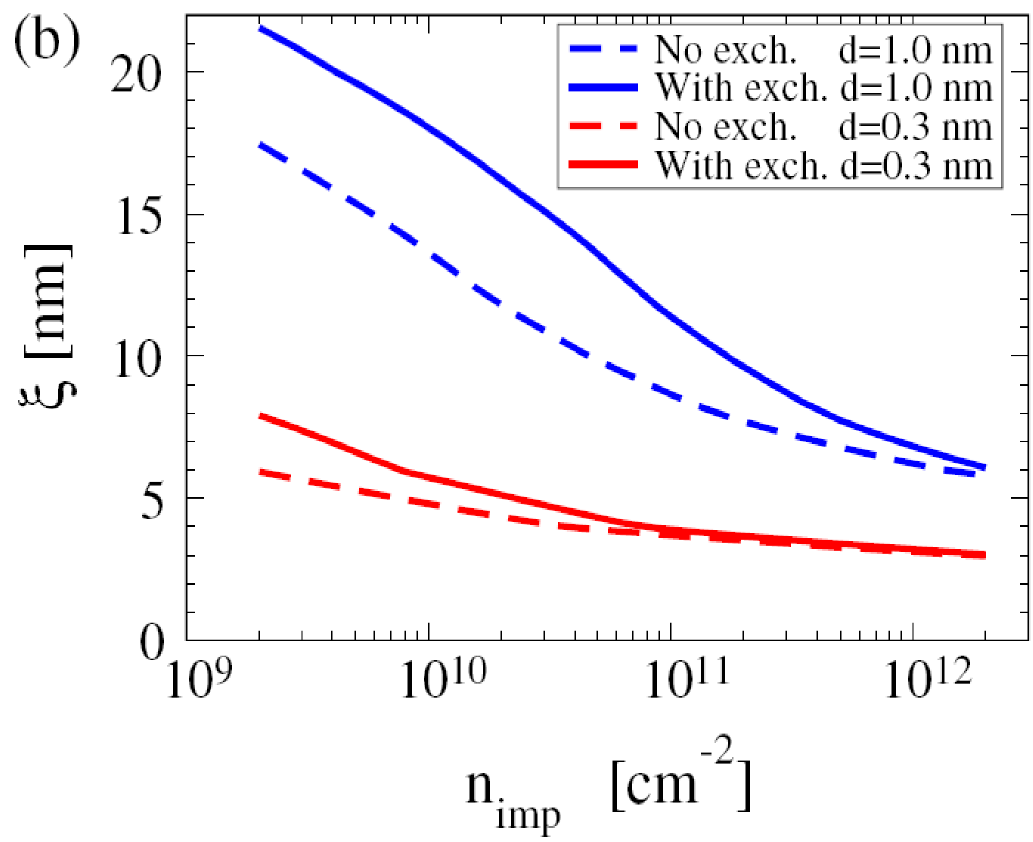
Y. Zhang et al. arXiv 0902.4793 (2009)

Disorder averaged results at the Dirac point

Density fluctuations
root mean square: n_{rms}

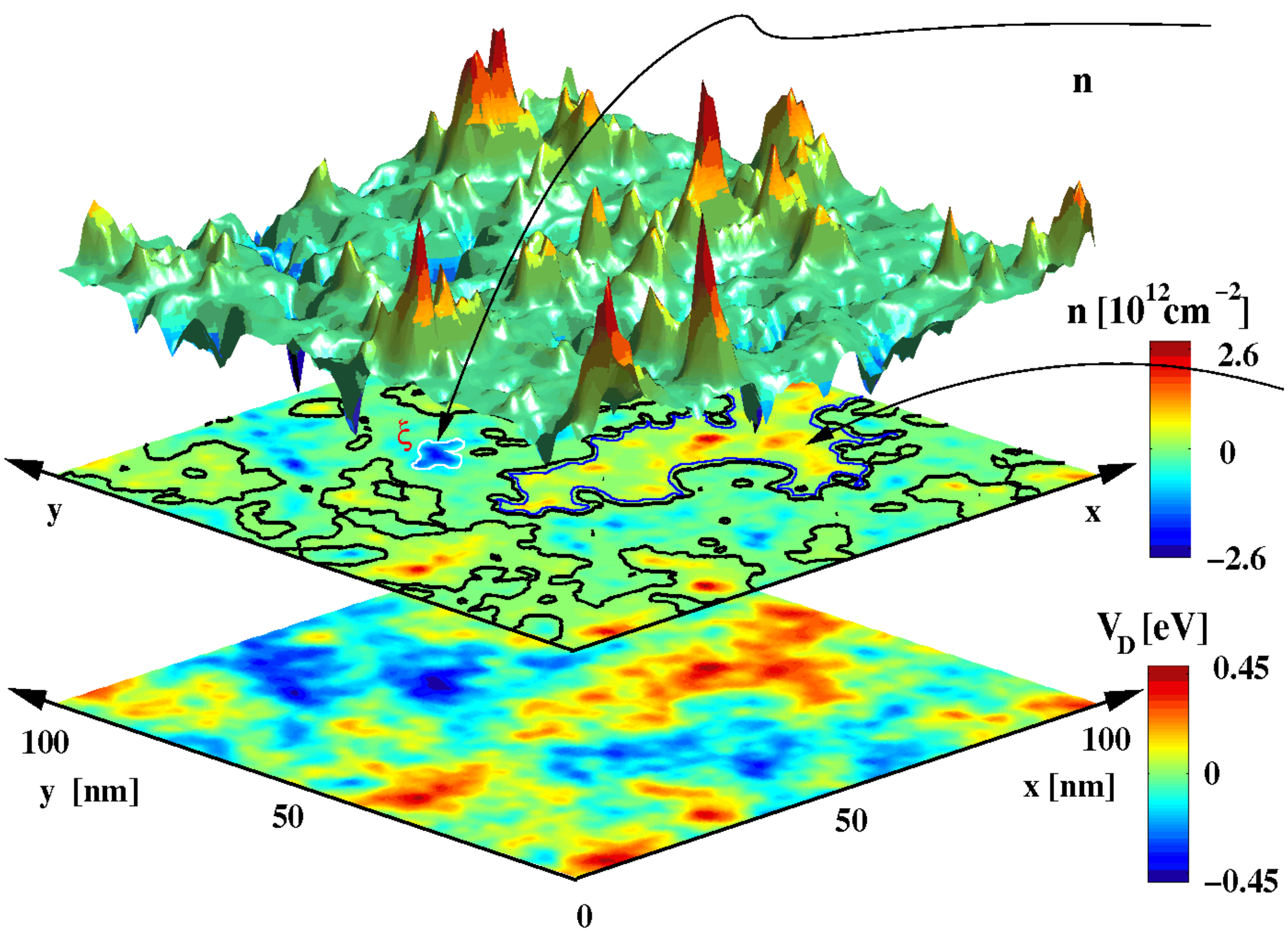
Correlation length: ξ





ER and S. Das Sarma,
Phys. Rev. Lett. ***101****, 166803 (2008)*

Carrier density properties

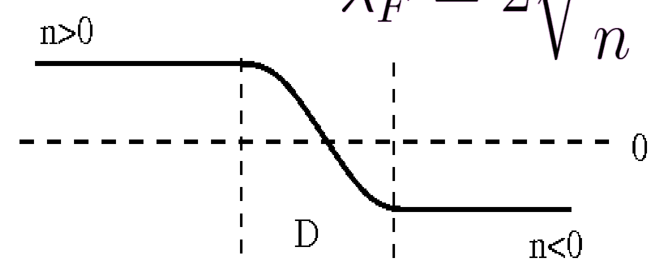


Small region of size ξ, ~10 nm, fixed by non-linear screening, and high density. δQ ~ 2e. Result in agreement with recent STM experiment [Zhang et al. arXiv:0902.4793]

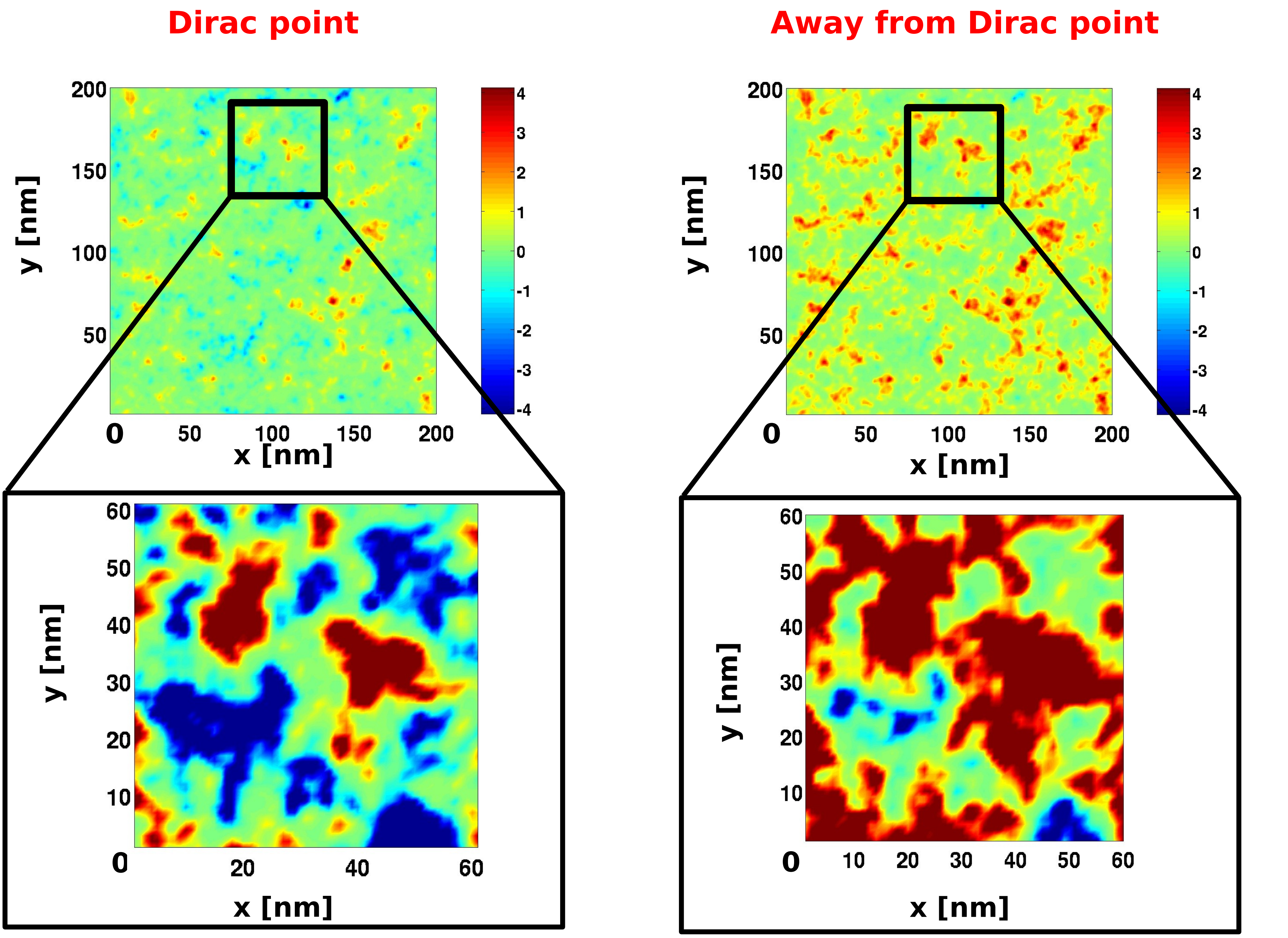
Wide regions of size ~ L (sample size) and low density. δQ ~ 10e.

The density across the electron-hole puddles boundaries (p-n junctions) varies on length scales, D, of the order of

$$\lambda_F = 2\sqrt{\frac{\pi}{n}}$$



Away from the Dirac point.



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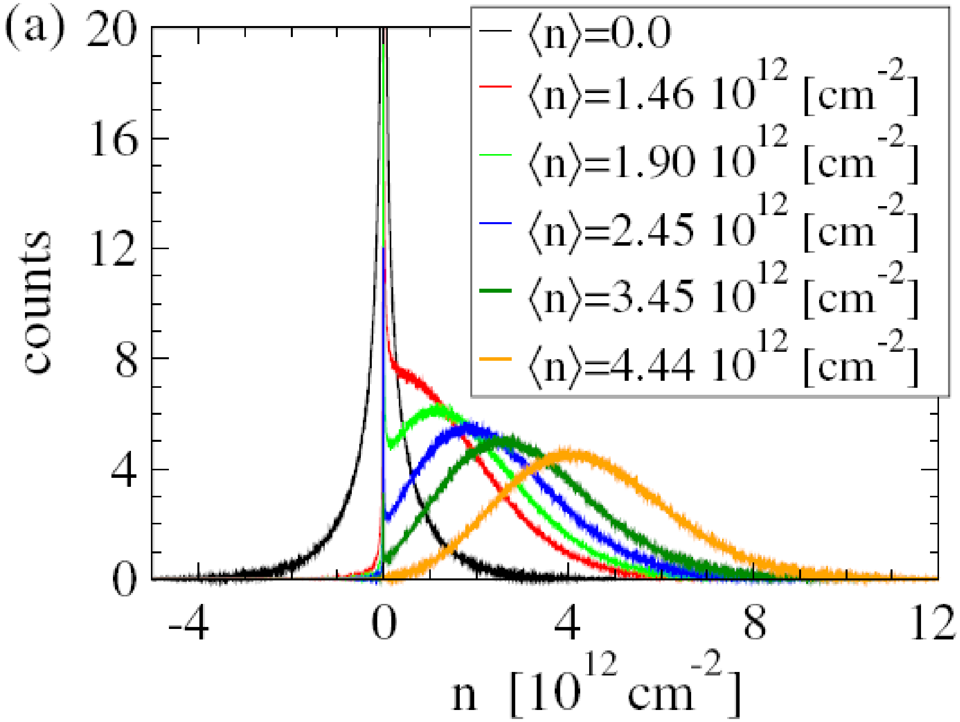
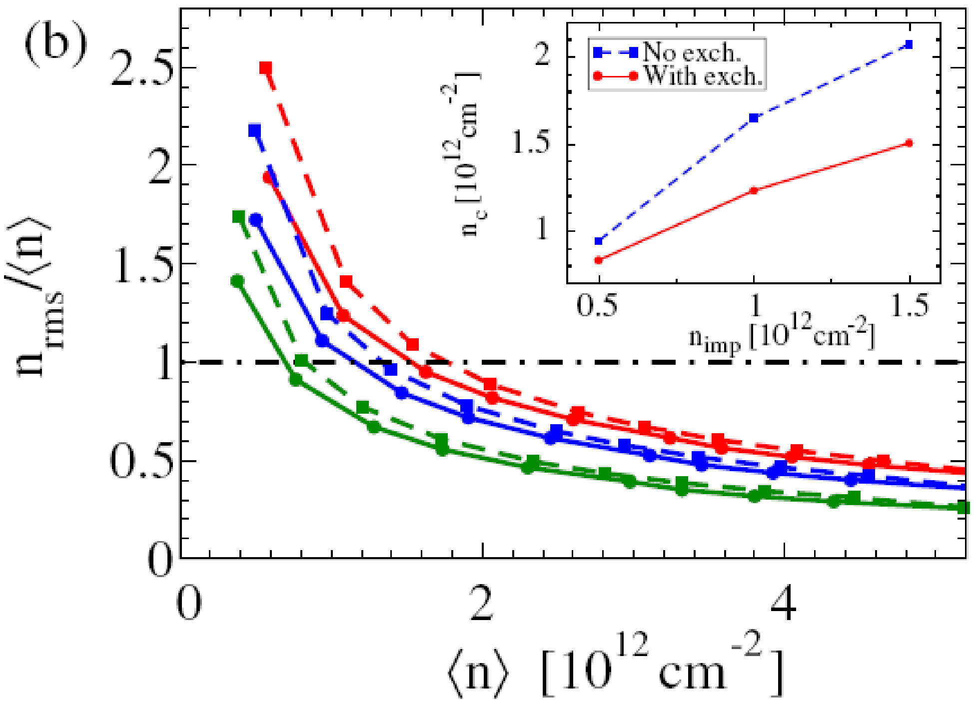




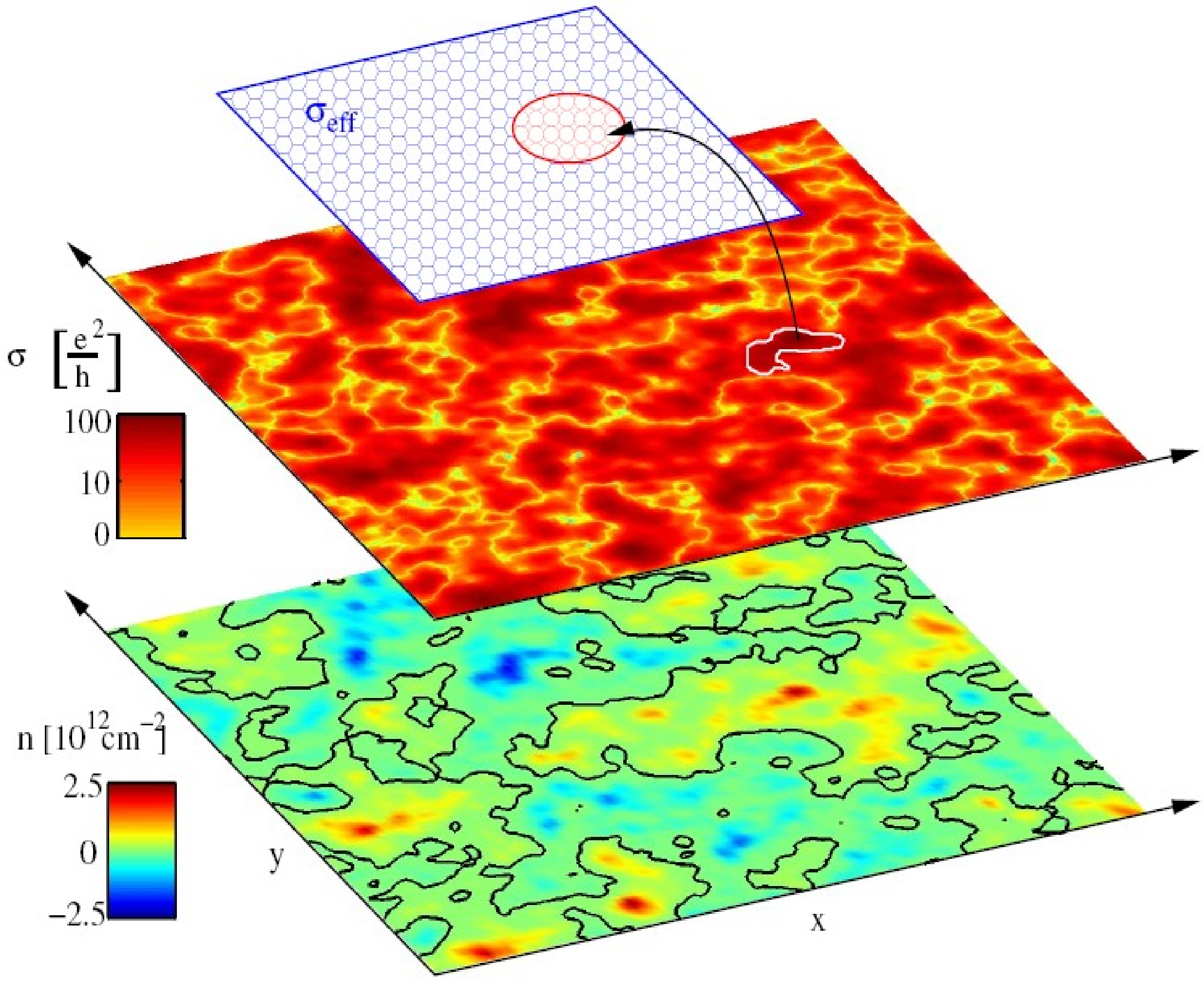
The density probability distribution has bimodal character

Up to high carrier densities densities fluctuations dominate

Dirac-point physics dominates over finite range of gate voltages

Inhomogeneous conductivity

The inhomogeneous character of the n will be reflected in inhomogeneous transport properties such as the conductivity, σ.



$$\sigma \propto \frac{|n|}{n_{\mathrm{imp}}}$$

Locally

Effective Medium Theory

In presence of strong inhomogeneities a natural approach is the Effective Medium Theory, EMT. Bruggeman Ann. Phys. (1935), Landauer (1952)

$$\mathbf{J}(\mathbf{r}) = -\sigma(\mathbf{r})\nabla V(\mathbf{r})$$

Average over position and disorder configurations:

$$\langle \mathbf{J}(\mathbf{r})\rangle = -\langle \sigma(\mathbf{r})\nabla V(\mathbf{r})\rangle$$

Define *effective medium* transport coefficient:

$$\langle \mathbf{J}(\mathbf{r})\rangle = -\sigma_{\mathrm{eff}}\langle \nabla V(\mathbf{r})\rangle$$

We find:

$$\left\langle \int d^2r \frac{\sigma(\mathbf{r}) - \sigma_{\mathrm{eff}}}{\sigma(\mathbf{r}) + \sigma_{\mathrm{eff}}} \right\rangle = 0 \quad \longleftrightarrow \quad \boxed{\int dn \frac{\sigma(n) - \sigma_{\mathrm{eff}}}{\sigma(n) + \sigma_{\mathrm{eff}}} P(n) = 0}$$

Can we use it in graphene?

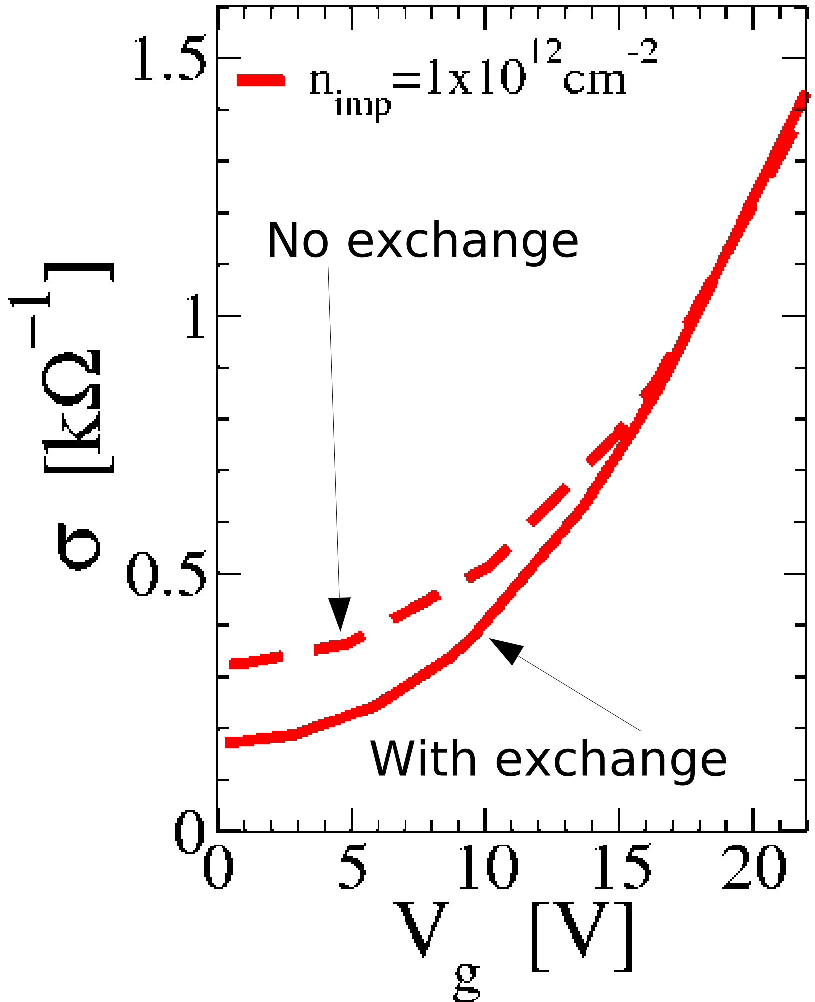
1) The mean free path, l, must be much smaller than the size of the homogeneous regions ✓

2) The resistance across the homogeneous regions must be much smaller than the resistance inside the regions. ✓

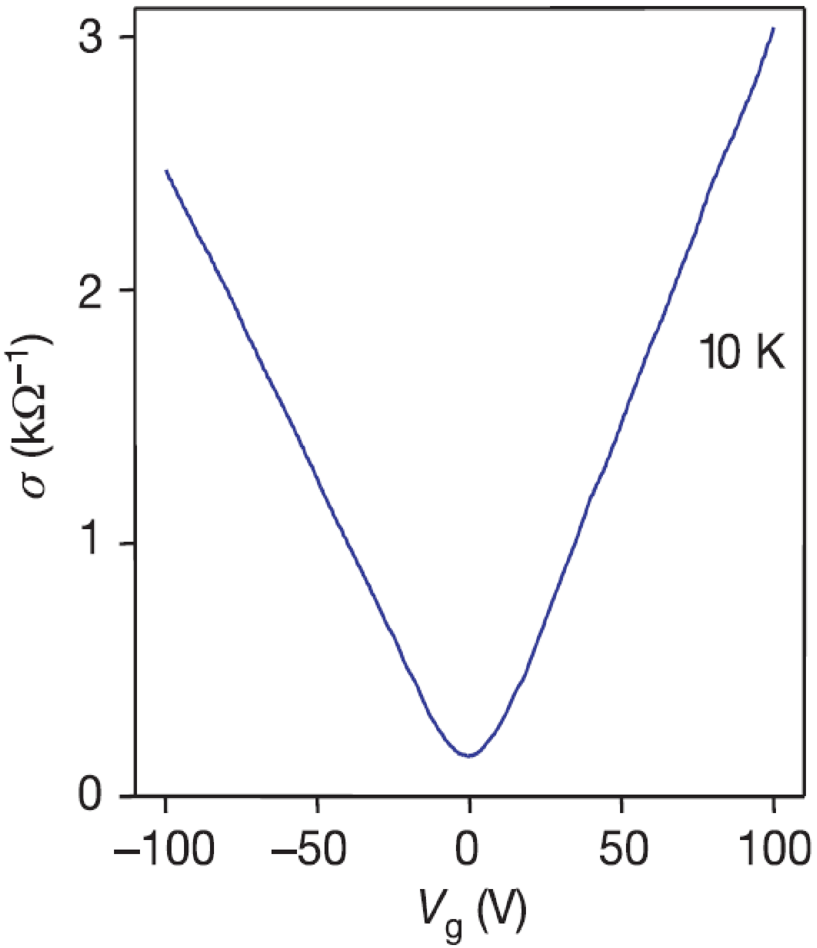
Cheianov & Falko, PRB (2006); Cheianov et al., PRL (2007); Fogler et al. PRB (2008)

In the limit $r_s = \alpha \rightarrow 0$ see also M.Fogler, arXiv:0810.1755 (2008). Talk J1-3

Conductivity vs. gate voltage



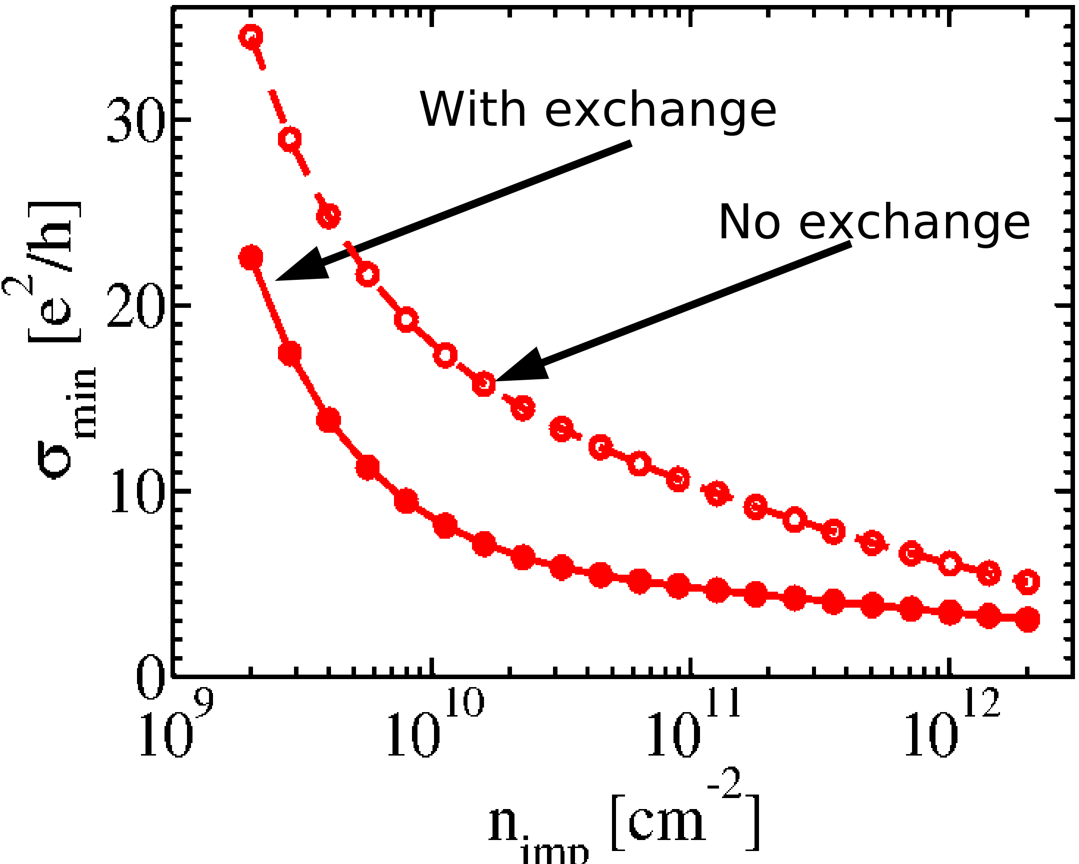
E.R. S. Adam, S. Das Sarma,
arxiv.0809.1425 (2008)



K. S. Novoselov et al.,
Nature **438**, 197 (2005).

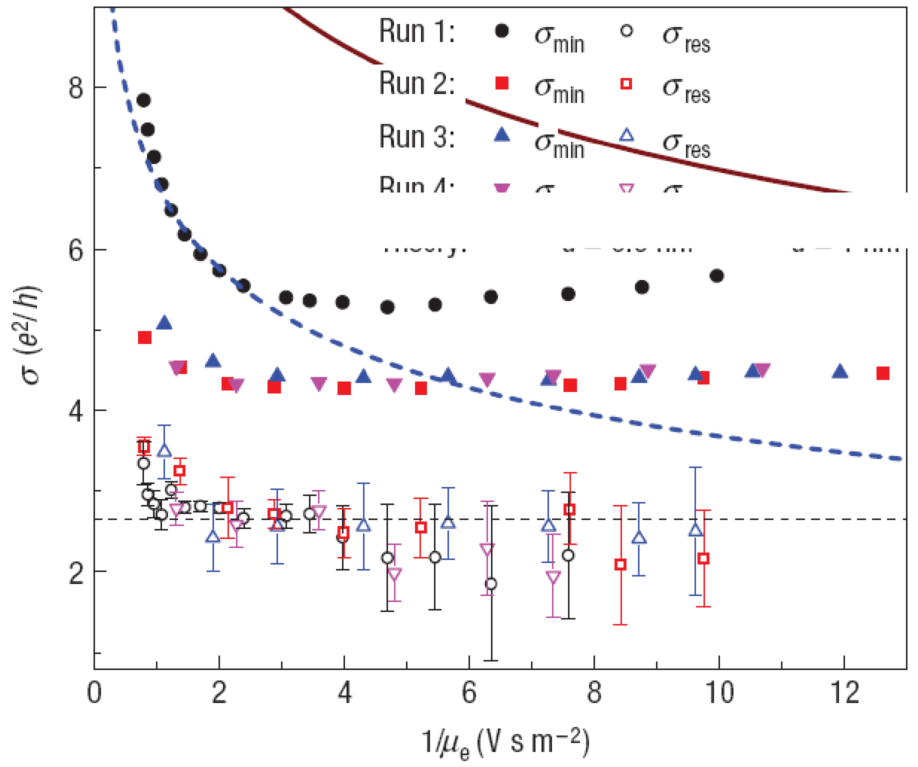
- Finite value of the conductivity at Dirac point;
- Recovers linear behavior at high gate voltages;
- Describes crossover;
- Shows importance of exchange-correlation at low voltages.

Minimum conductivity vs. impurity density



E.R., S. Adam, S. Das Sarma
arXiv.0809.1425 (2008)

also: S.Adam et al. PNAS **104**, 18392 (2007); Talk J1-2

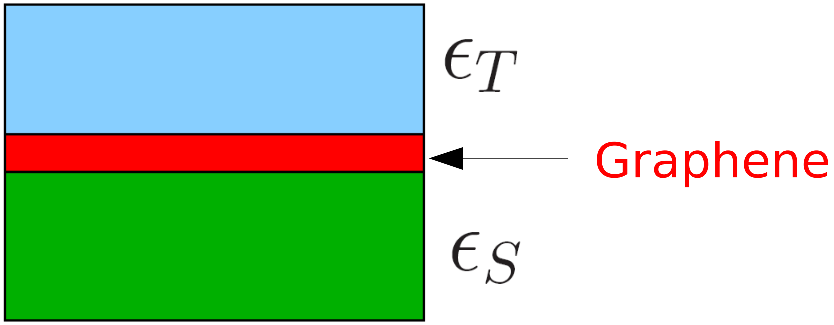


J.-H. Chen et al.
Nat. Phys. **4**, 377 (2008)

Dependence of conductivity on impurity density in qualitative and quantitative agreement with experiments.

Tuning the fine-structure constant, r_s

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



$$\bar{\epsilon} = \frac{\epsilon_T + \epsilon_S}{2}$$

r_s : 0.5 → 1

C. Jang et al.
Phys. Rev. Lett.
101, 146805 (2008)

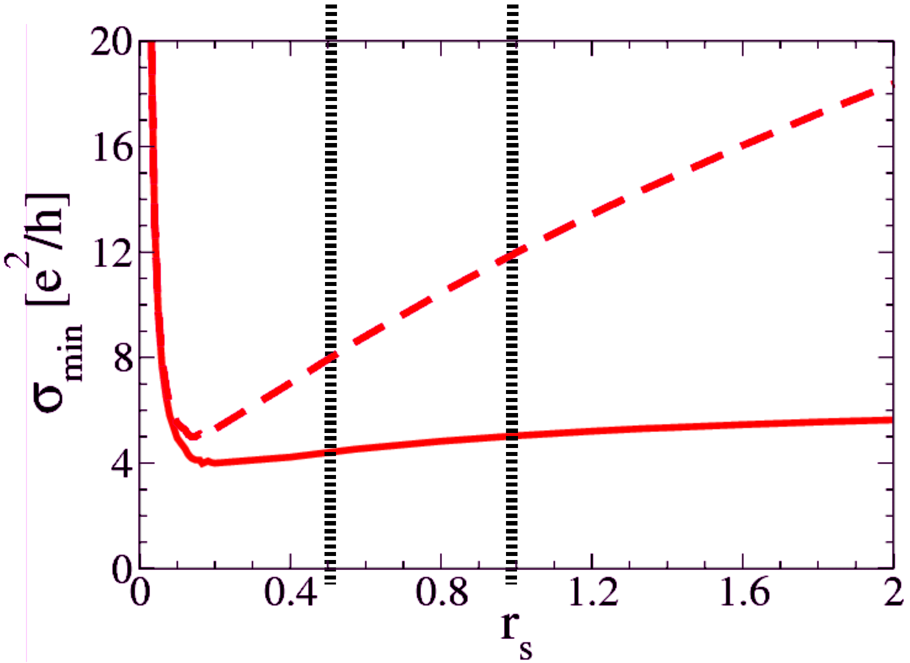
- r_s controls: **strength of disorder; strength of interaction, exchange.**

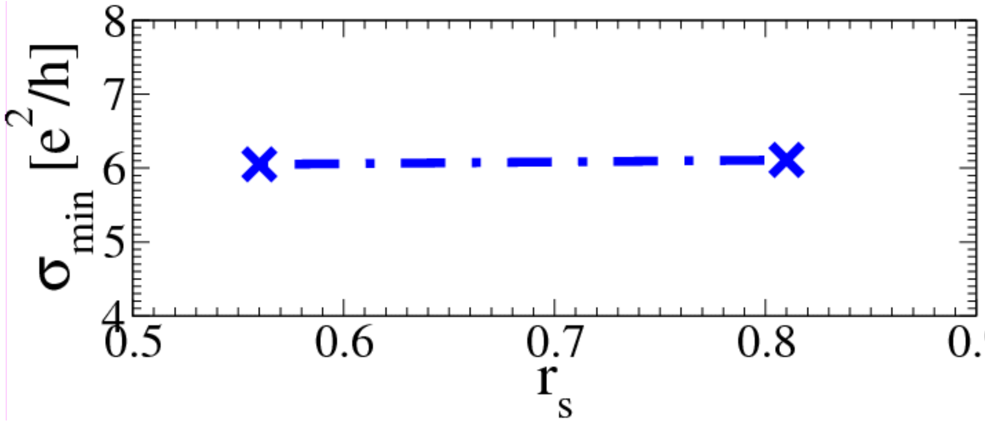
Strongly affects the density profile.

- r_s controls **strength of scattering**.

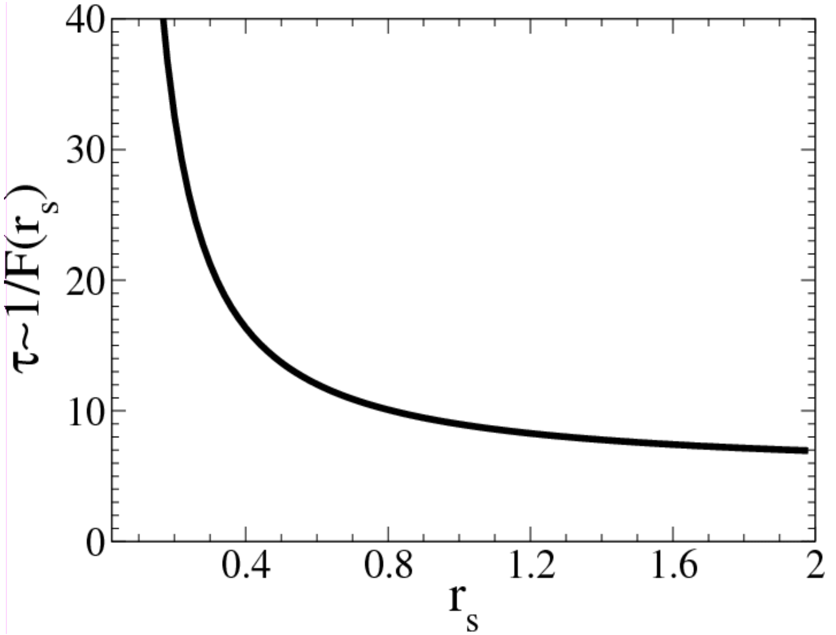
Affects scattering time

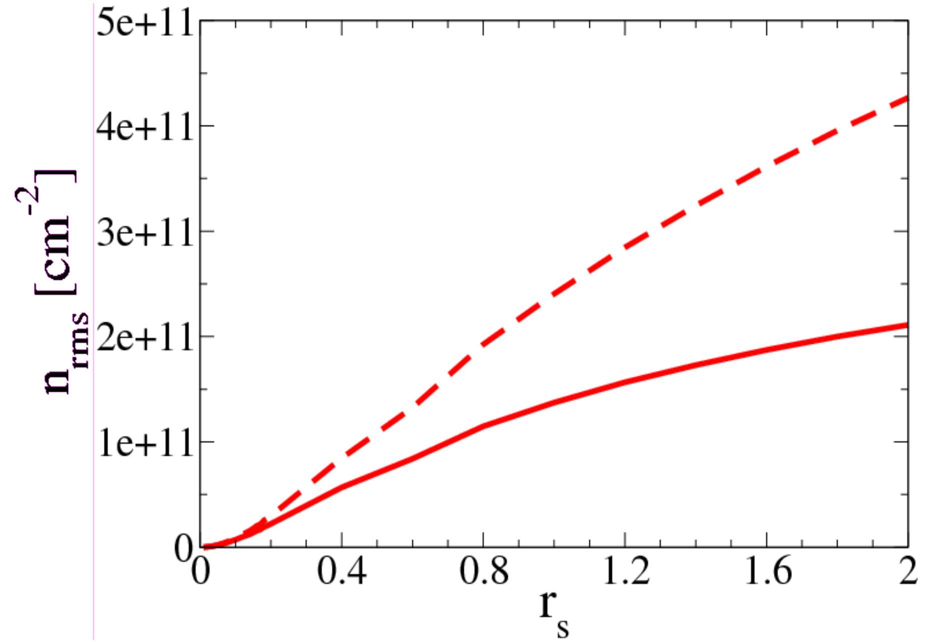
r_s dependence of the minimum conductivity





C. Jang et al.
Phys. Rev. Lett. **101**, 146805 (2008)





Thermo-Transport

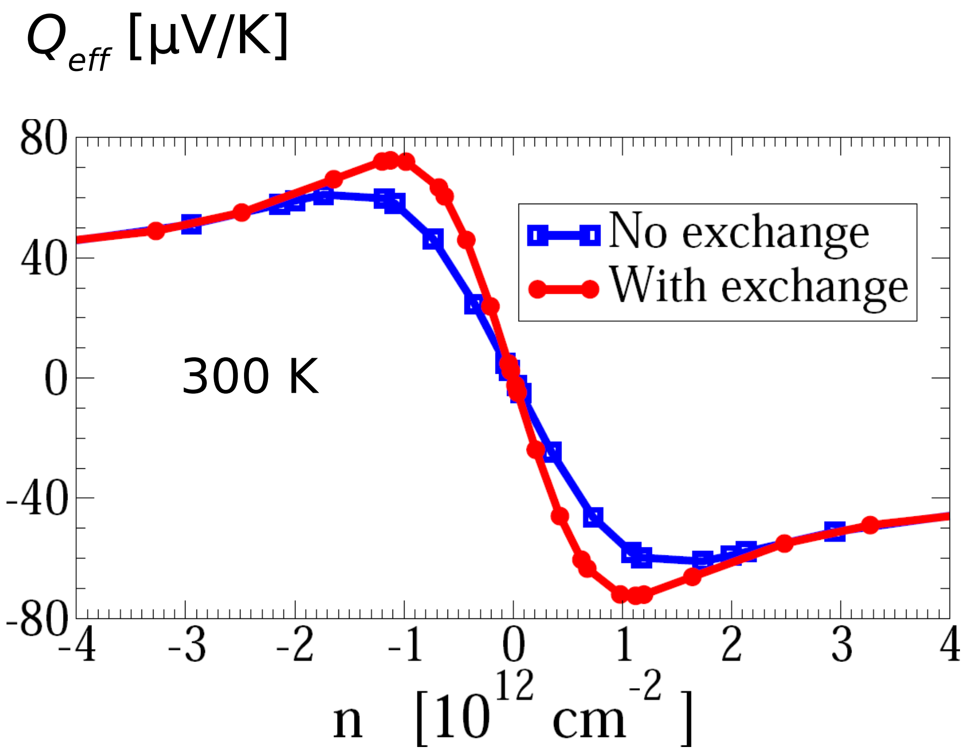
$$\mathbf{J} = -L^{11}\nabla V - L^{12}\nabla T$$
$$\mathbf{J}_Q = -L^{21}\nabla V - L^{22}\nabla T$$

Effective Medium

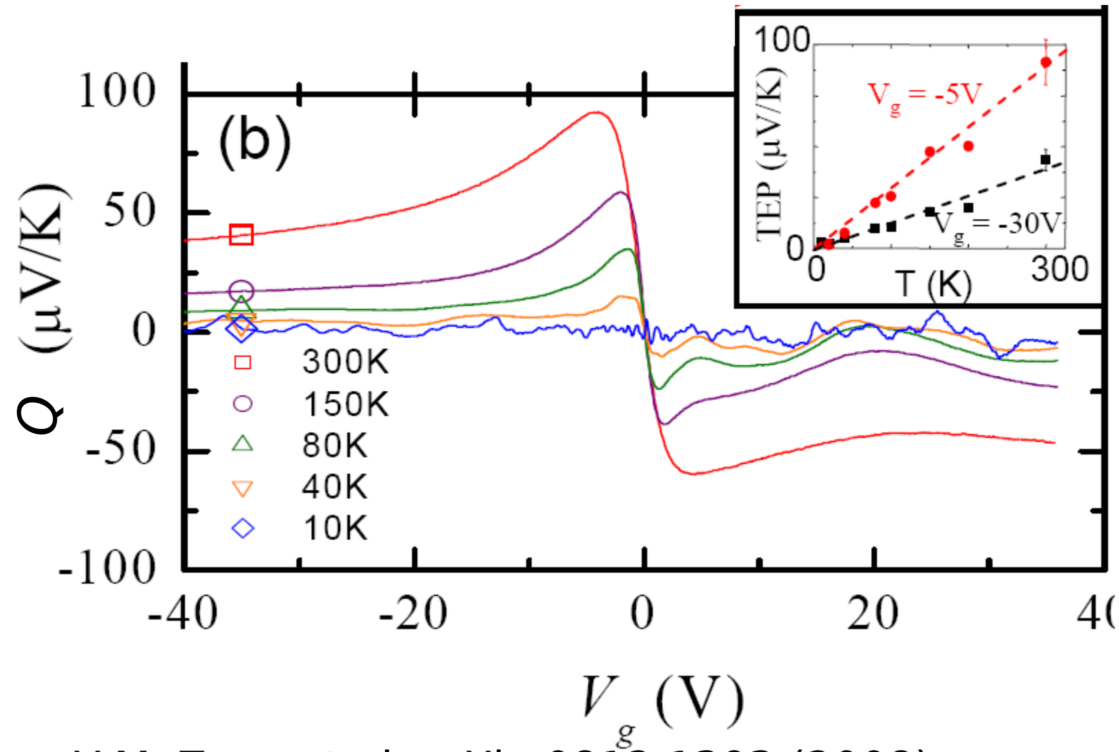
Average

$$\boxed{Q_{\text{eff}} = \frac{L^{12}_{\text{eff}}}{L^{11}_{\text{eff}}}}$$

Thermopower



E.H. Hwang, ER, S. Das Sarma
arXiv:0902.1749 (2009)



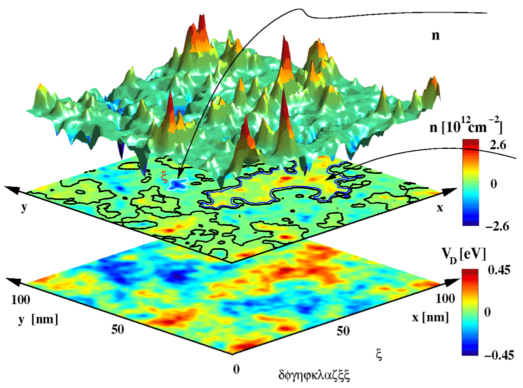
Y.M. Zuev et al. arXiv:0812.1393 (2008)

Also:

P. Wei et al. arXiv:0812.1411 (2008);
J.G. Checkelsky, N.P. Ong, arXiv:0812.2866 (2008)

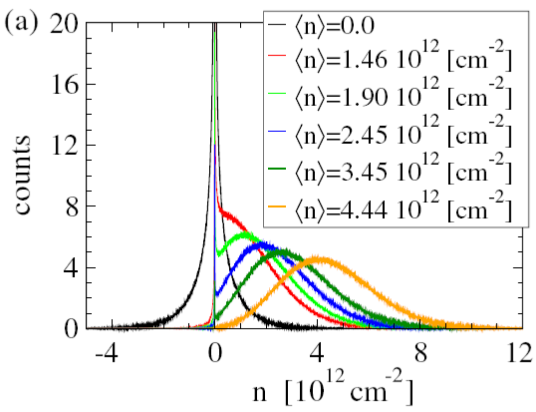
Conclusions

At the Dirac point:



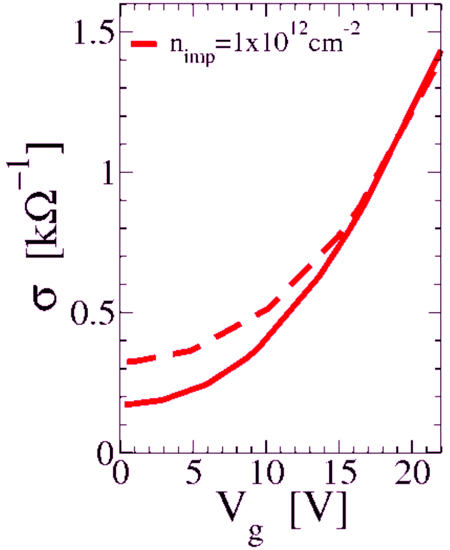
- Big puddles of size ~L and small density
- Small puddles of size ~ 10 nm and high density

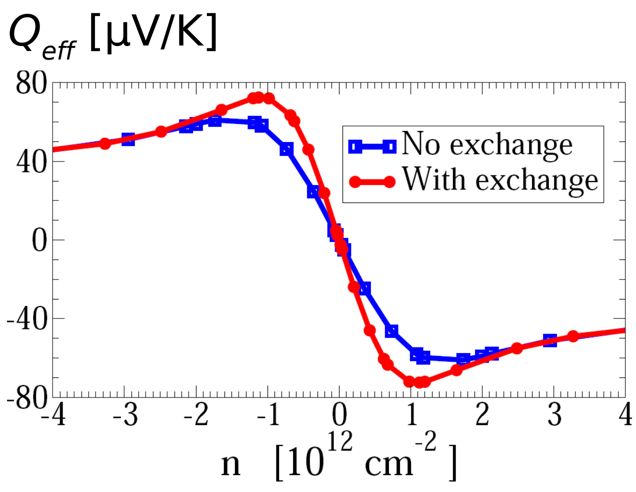
Away from the Dirac point:



- Dirac-point physics dominates over finite range of gate voltages
- n_{rms} >> <n> for dopings as high as 10^{12} cm^{-2}.

Effective medium theory





- Using detailed characterization of density landscape we can calculate transport properties via the EMT.