Electronic structure and transport of disordered graphene

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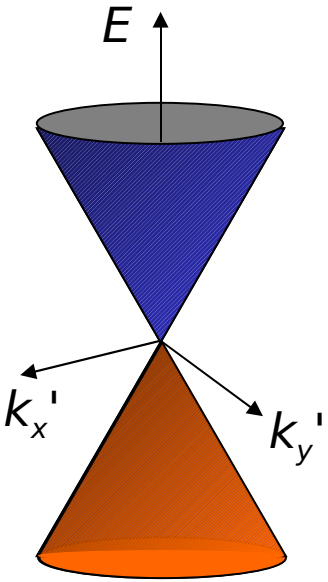
References:

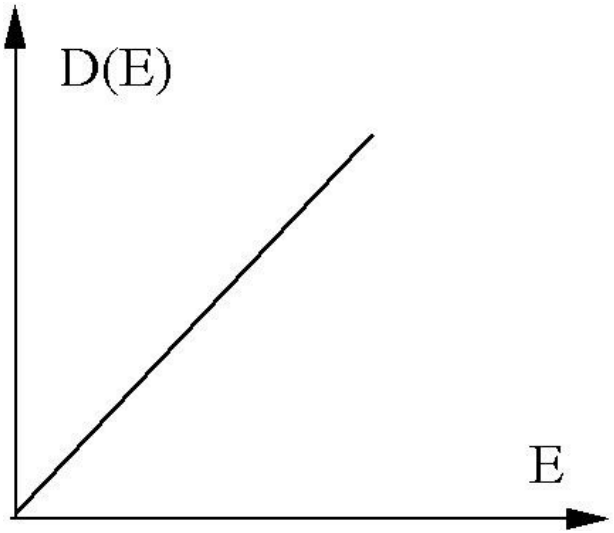
-) E. R. and S. Das Sarma, Phys. Rev. Lett **101**, 166803 (2008)

-) E. R., S. Adam and S. Das Sarma, arxiv:0809.1425.

Center for Nanoscale Science and Technology, NIST. Nov. 14th 2008

Problem: transport at the Dirac point



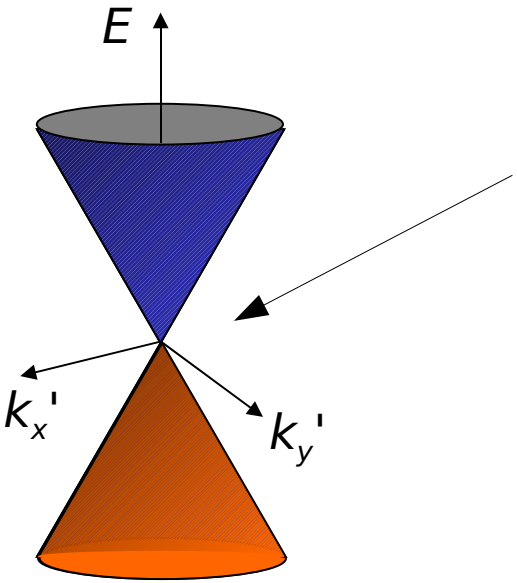


$$\sigma \propto D(E)\tau$$

$$\sigma = \begin{cases} 0 & \text{Intervalley scattering} \\ \infty & \text{Disorder that does not mix the valleys} \\ \dfrac{4e^2}{\pi h} & \text{In absence of any disorder} \end{cases}$$

Experimentally: σ is a sample dependent constant !

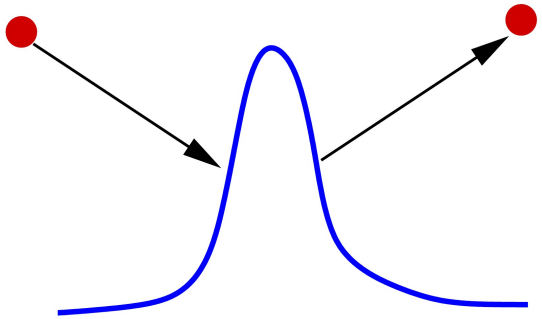
Density fluctuations

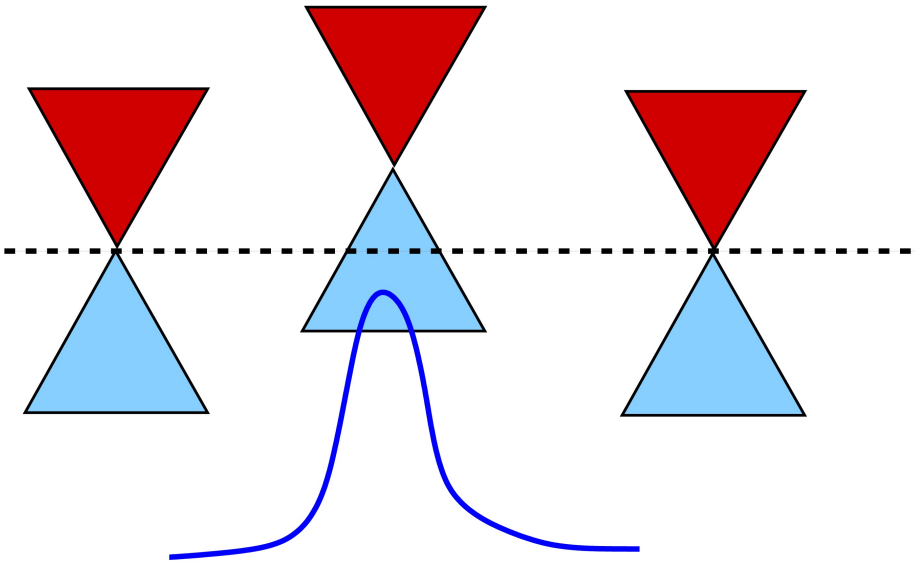


At the Dirac point the carrier density is zero

- Density fluctuations determine graphene physics close to the Dirac point;
- Linear screening breaks down.

Effect of disorder





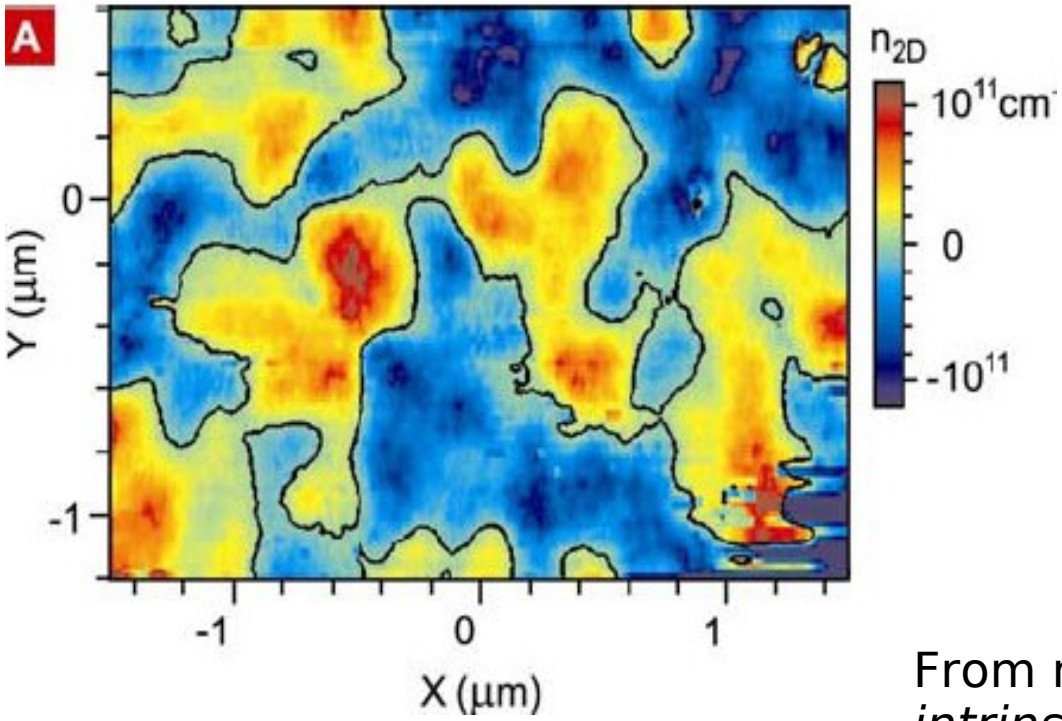
Scattering

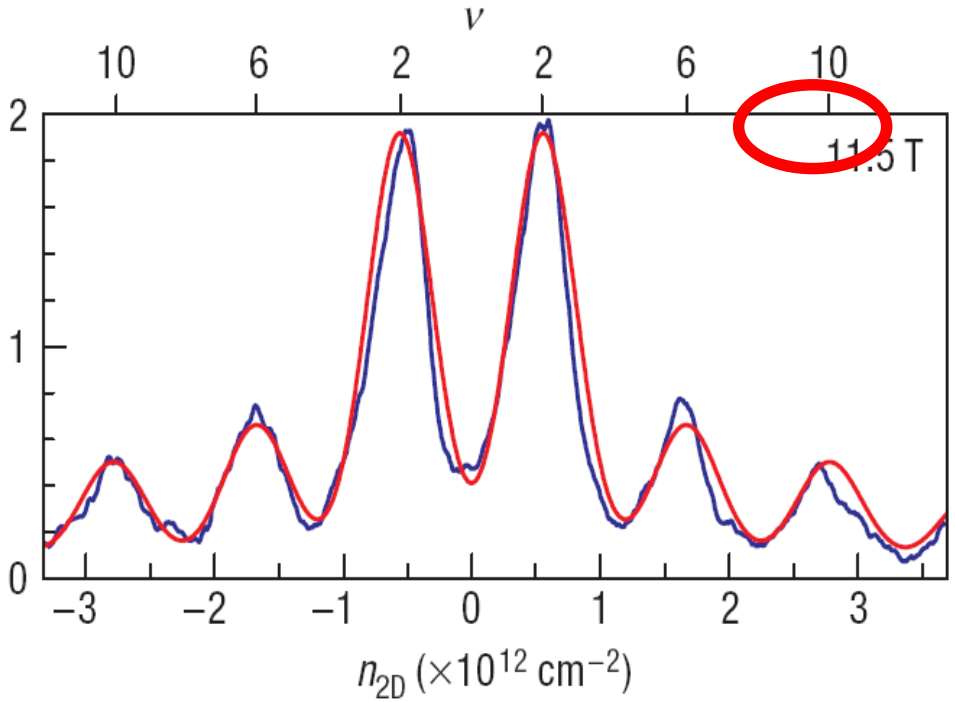
Shifts bottom of the band ⟷ shift of Fermi energy

At the Dirac point disorder induces electron-hole puddles

Suggested theoretically: E.H. Hwang, S. Adam, S. Das Sarma., PRL, **98**, 186806 (2007).

Electron-hole puddles.





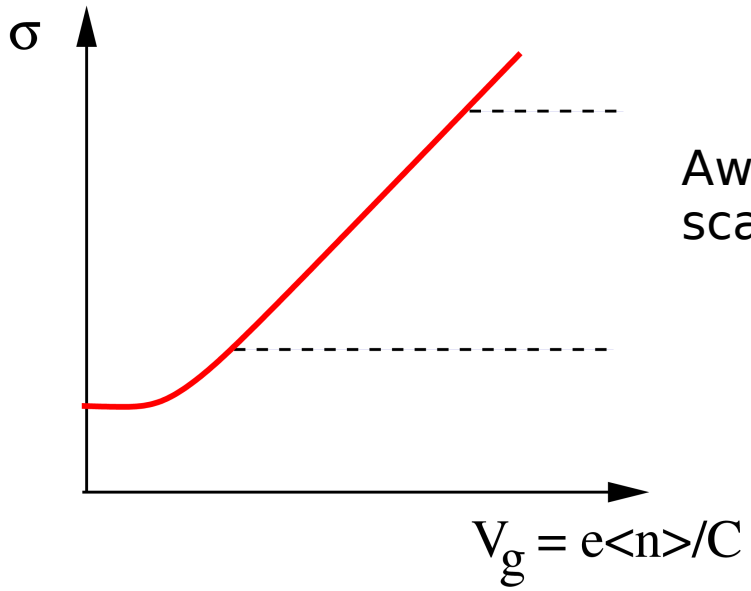
From measurements in high magnetic field the *intrinsic* density fluctuations are characterized by:

Correlation $\xi < 30$ nm

$n_{rms} \sim 2.3 \times 10^{11}$ cm^{-2}

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

Source of disorder



Away from the Dirac point the conductivity scales linearly wit the average carrier density <n>

$V_{DIS}(q) = V_0$ → σ ~ const

Quasiparticle scattering is enhanced at low densities

$V_{DIS}(q) = 1/q$ → σ ~ n

Charge impurities

Screening

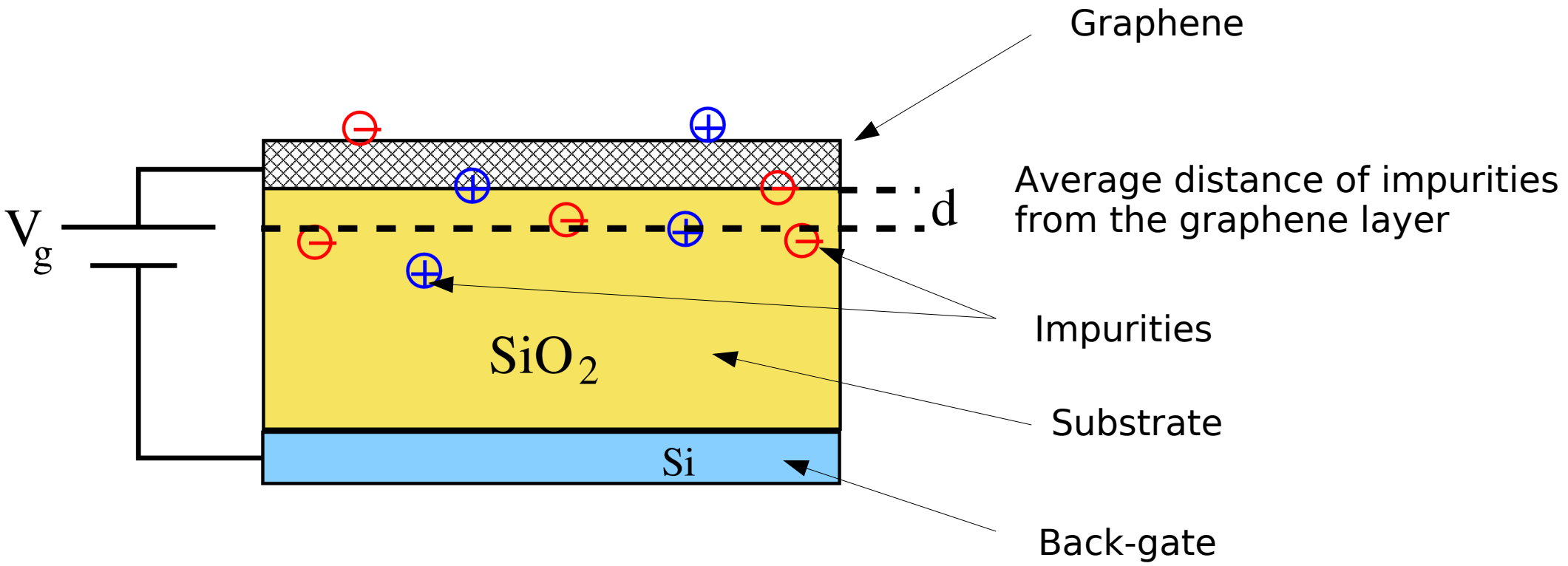
$$V_{\mathrm{DIS}} = \frac{2\pi e^2}{q + 2\pi e^2 \Pi(q)}$$

$$\Pi(q) \propto D(E_F)$$

Screening does not change the density dependence of the conductivity!

T. Ando J. Phys. Soc. Jpn (2006); Nomura & MacDonald PRL (2006); Hwang et al. PRL (2007)

System



From transport results at high doping we therefore assume that the main source of disorder are random charged impurities in the graphene environment. To minimize the number of parameters entering the theory we assume the charge impurity distribution to be 2D in a plane at distance ***d*** from the graphene layer.

Thomas-Fermi-Dirac theory

Start from the energy functional E[n] and then minimize it with respect to the electron density n. In presence of disorder for the total energy we have:

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

and then:

$$\frac{\delta E}{\delta n} = 0$$

$$\hbar v_F \mathrm{sign}(n)\sqrt{\pi n} + \frac{e^2}{2\epsilon_0}\int d^2r' \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + \Sigma(n) - \mathbf{V_D} - \mu = 0$$

Where Σ is the exchange self energy:

$$\Sigma \approx r_s \sqrt{|n|}\ln|n|\ ;$$

The correlation energy contribution is quite smaller and scales as the self energy :

$$\frac{\delta E_c}{\delta n} \approx F[r_s]\sqrt{|n|}\ln|n|$$

$$F[r_s] < r_s$$

and of opposite sign

Barlas et al. PRL (2007), Hwang et al. PRL (2007), Polini et al PRB (2008).

Construction of disorder potential

- We assume charge distribution with zero average. A nonzero average it simply translates in a voltage gate off-set.

$$\langle C(\mathbf{r}) \rangle = 0$$

- We assume the charge positions to be uncorrelated.

$$\langle C(\mathbf{r}_1) C(\mathbf{r}_2) \rangle = n_{\mathrm{imp}} \delta(\mathbf{r}_2 - \mathbf{r}_1)$$

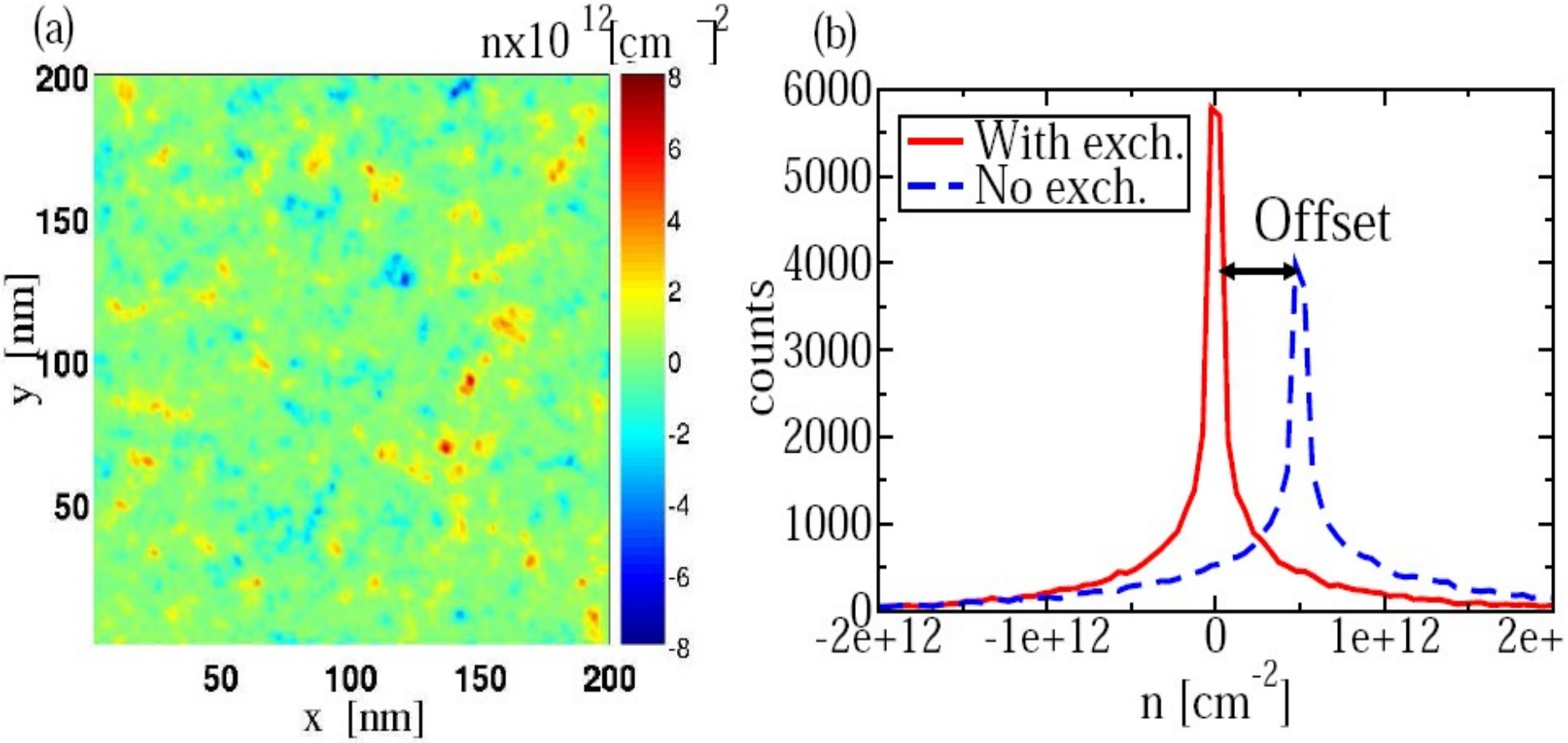
$$\langle C(\mathbf{q}) \rangle = 0$$
$$\langle C^2(\mathbf{q}) \rangle = n_{\mathrm{imp}}$$

- We then calculate C(q) using random number with Gaussian distribution and variance equal to impurity density.

- Assuming the impurities to be in a layer at distance d we finally calculate V_D

$$V_D(\mathbf{q}) = 2\pi \frac{e^{-qd}}{q} C(q)$$

Dirac point: single disorder realization

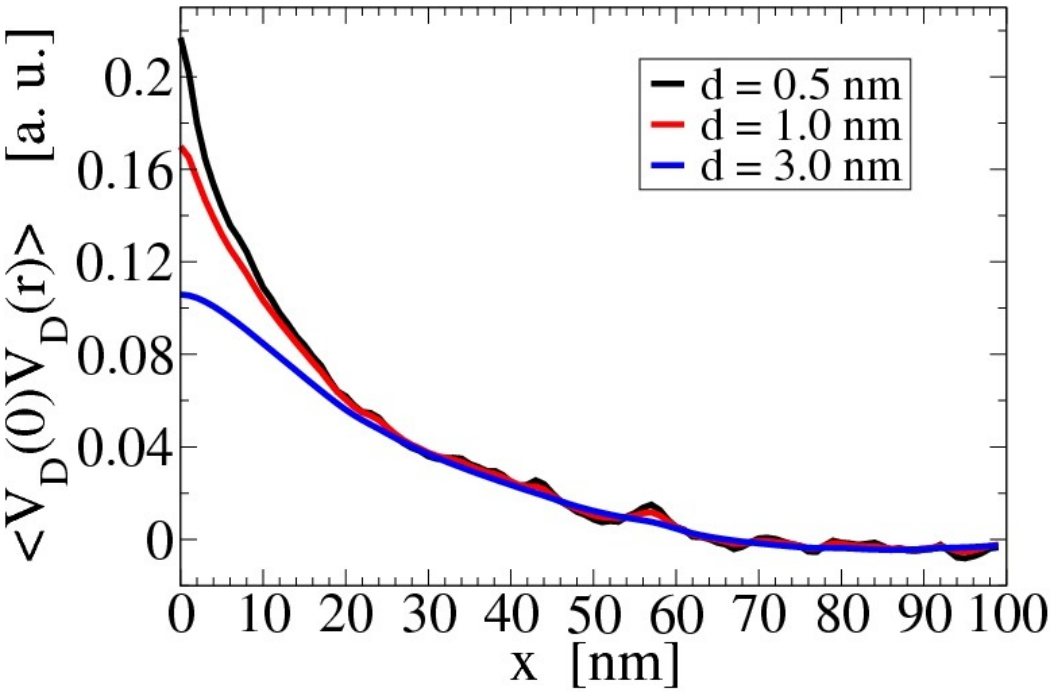


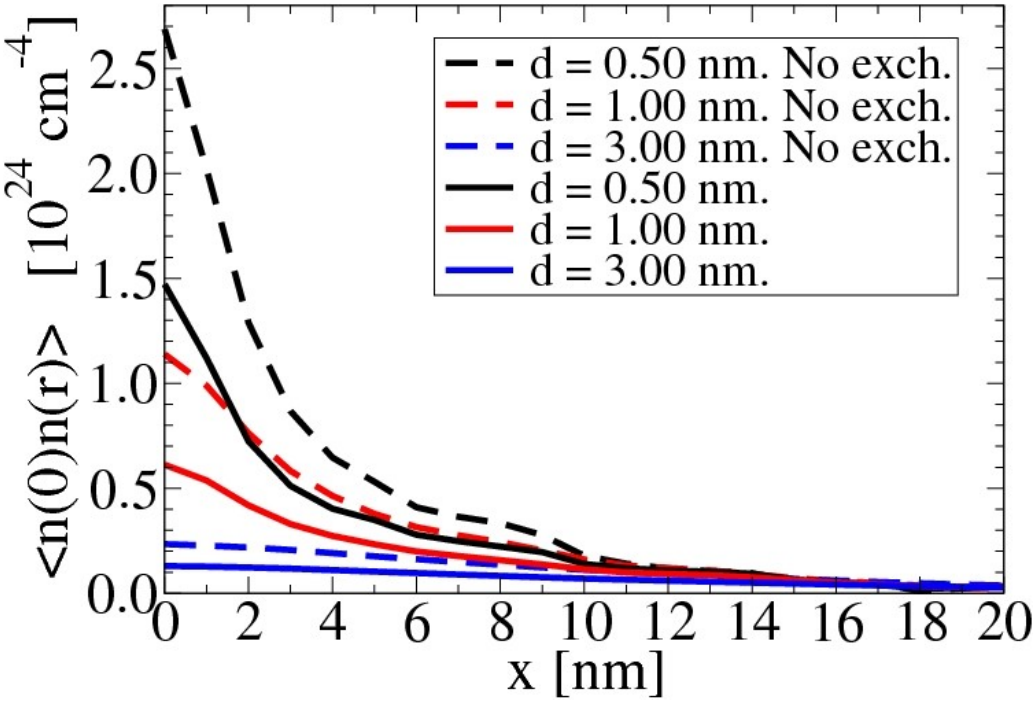
We can see that many-body effects, exchange, tend to suppress the density fluctuations as it can be seen from the “histogram” plot of the density distribution.

See also M. Polini et al. PRB (2008)

Disorder averaged correlation functions

By considering several disorder realizations we calculate the disorder averaged correlation functions:

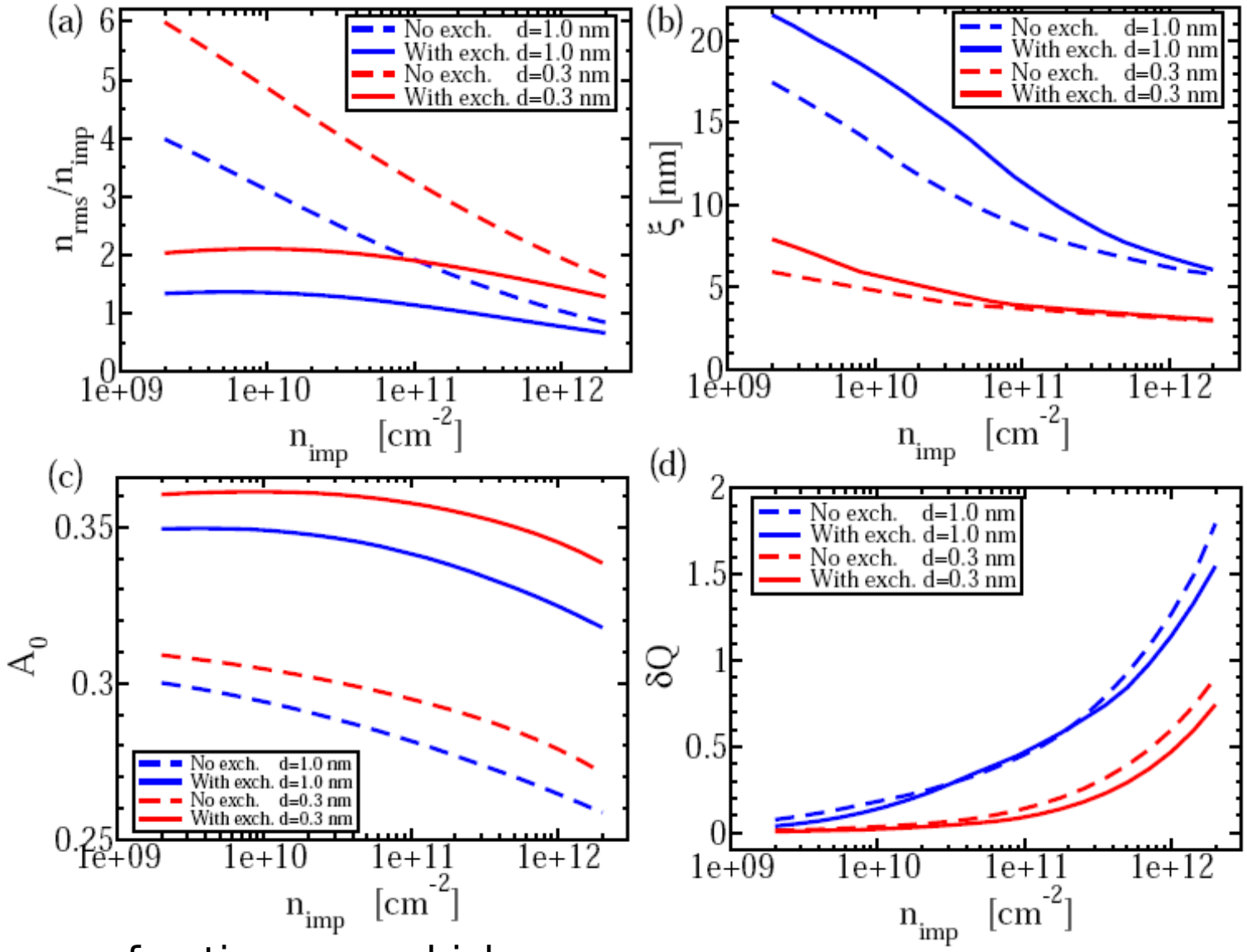




From the correlation functions we can calculate the fluctuations root mean square, rms, and their correlation length ξ estimated as the FWHM.

$$n_{\mathrm{rms}} \equiv \sqrt{\langle n(0)n(0)\rangle} \qquad \xi \equiv FWHM[\langle n(0)n(r)\rangle]$$

Density rms and correlation length, as function of impurity density



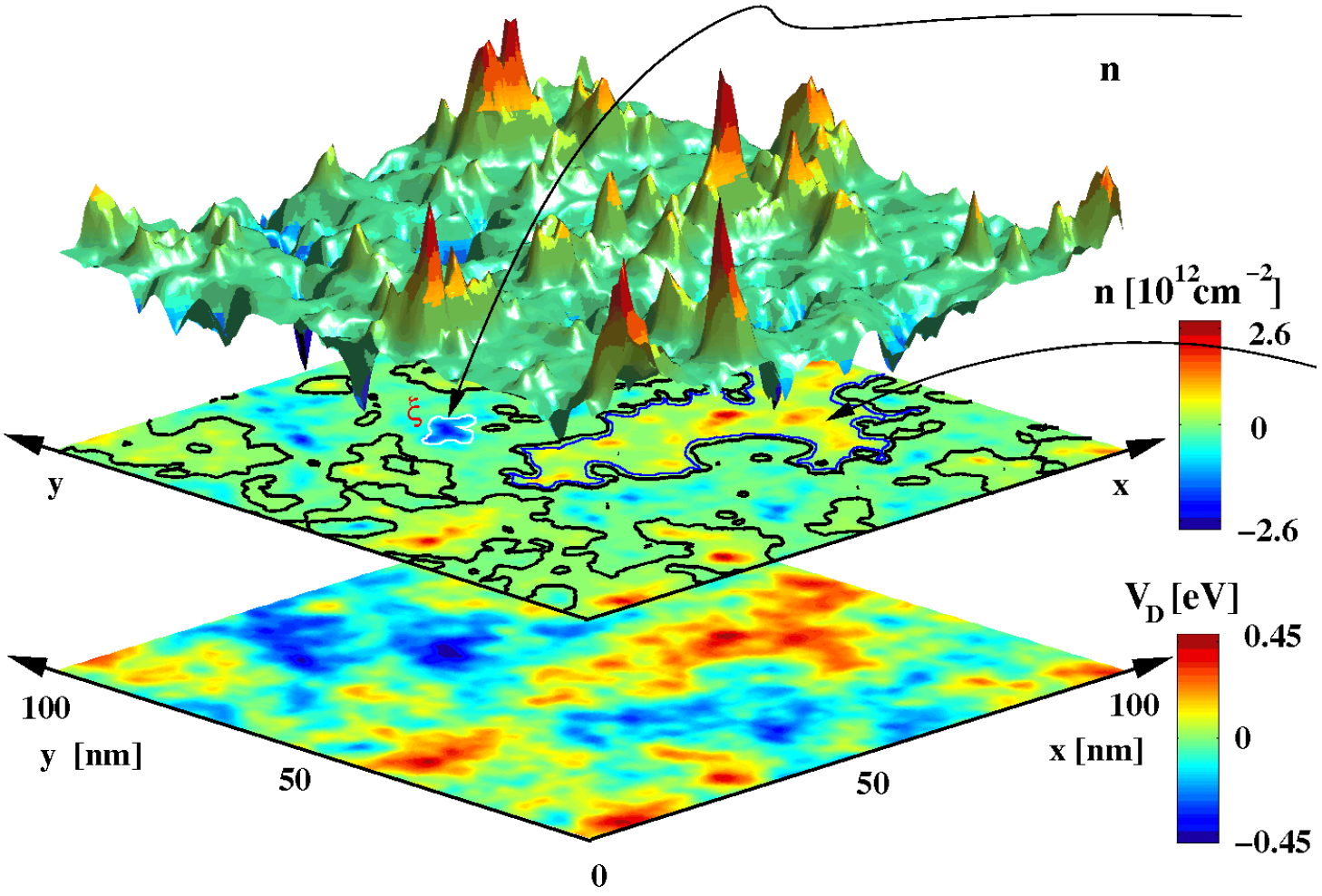
A_0 : area fraction over which

$|n(\mathbf{r}) - \langle n \rangle| < n_{rms}/10$

$$\delta Q \equiv n_{rms} \pi \xi^2$$

Compare well with S. Adam et al. PNAS (2007).

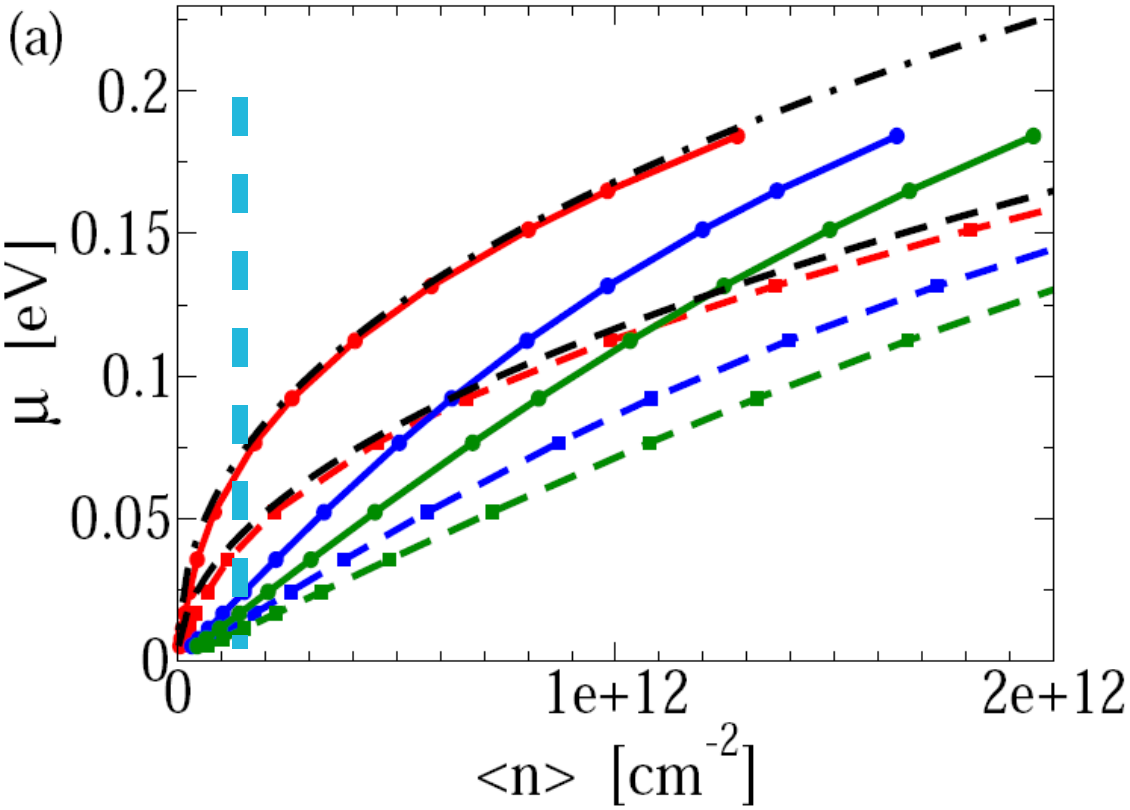
Carrier density properties

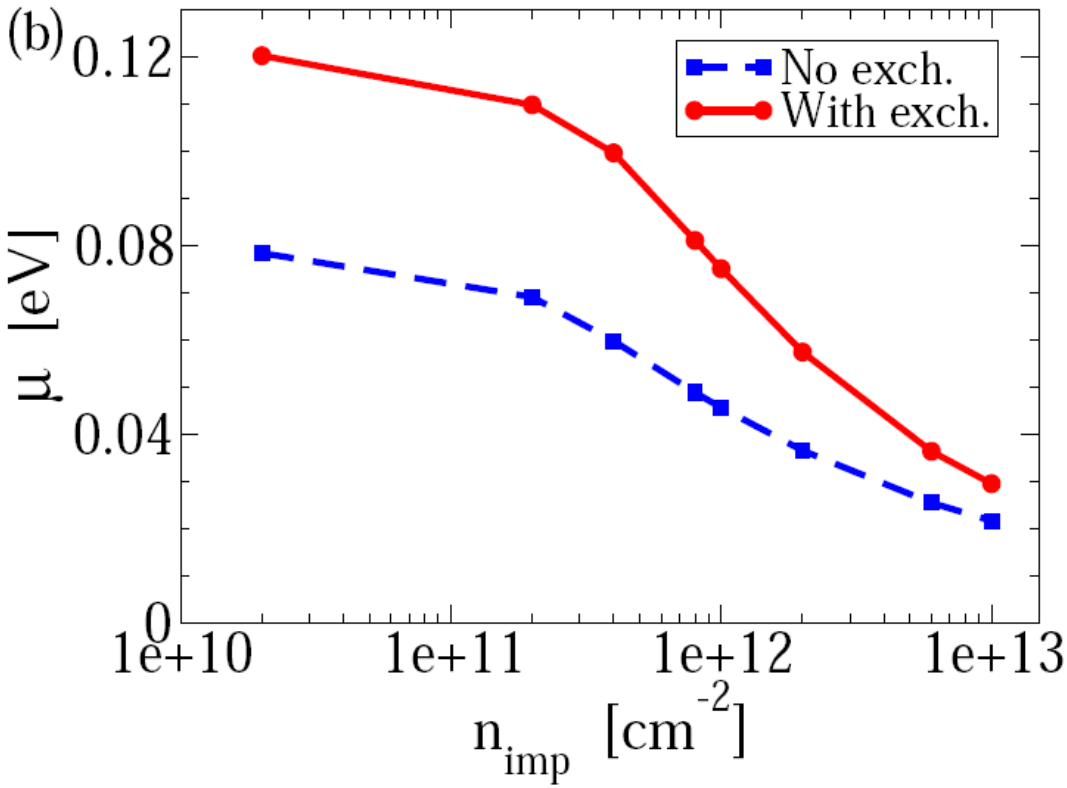


Small region of size ξ, ~10 nm, fixed by non-linear screening, and high density. δQ ~ 2e. Result in agreement with recent STM experiment [V. Brar et al. unpublished]

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

Away from the Dirac point. I

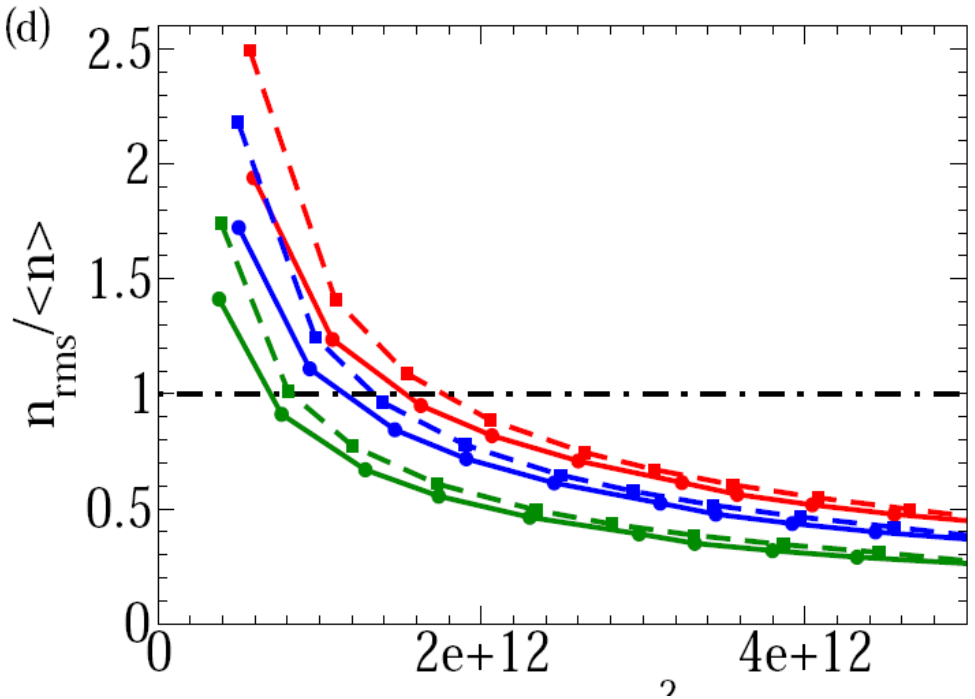


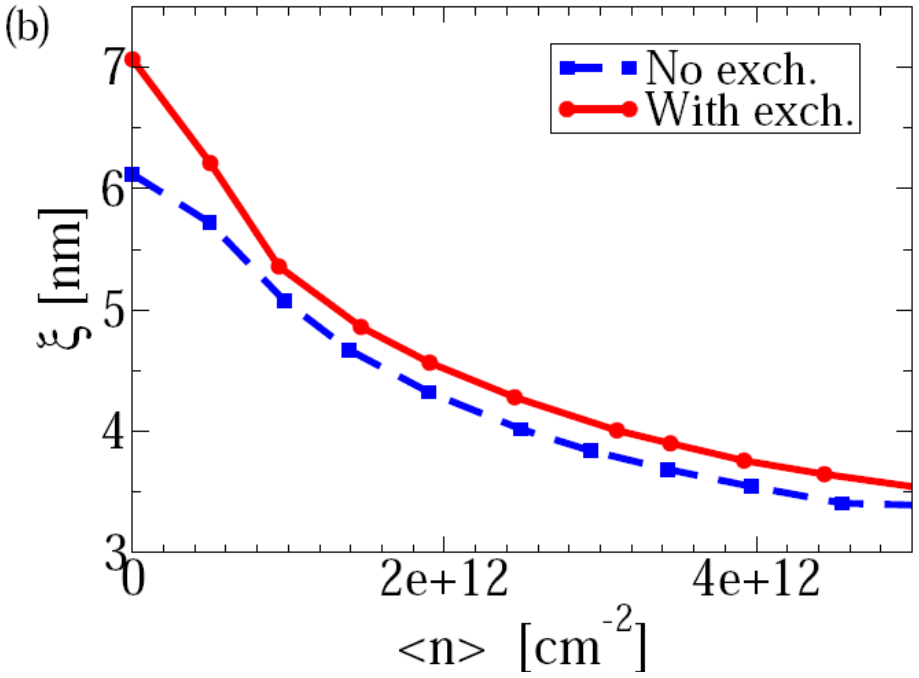


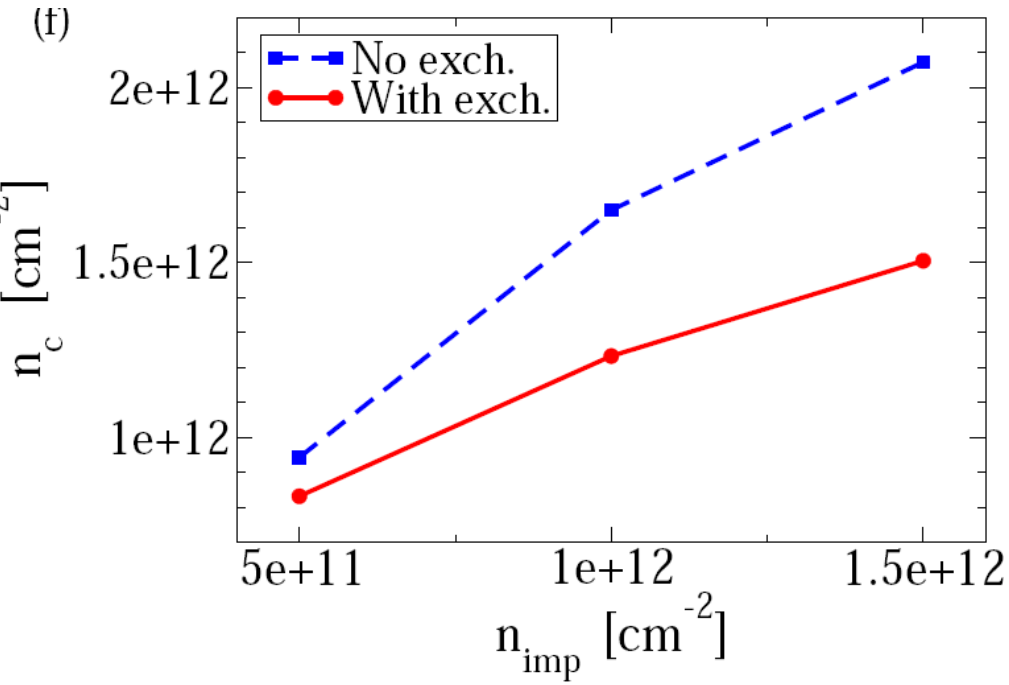
Because of the linear dispersion the relation between the chemical potential and the average density depends on disorder.

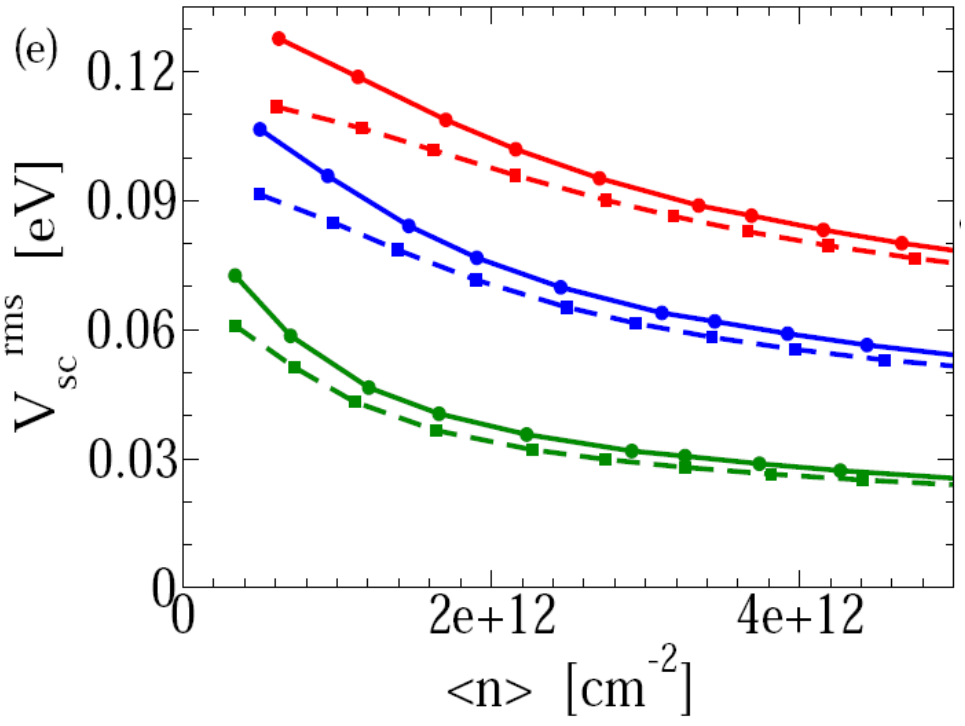
In addition, close to the Dirac point, many body effects strongly affect the μ(<n>) relation. Interplay of disorder and interaction is very important close to the Dirac point

Away from the Dirac point. II

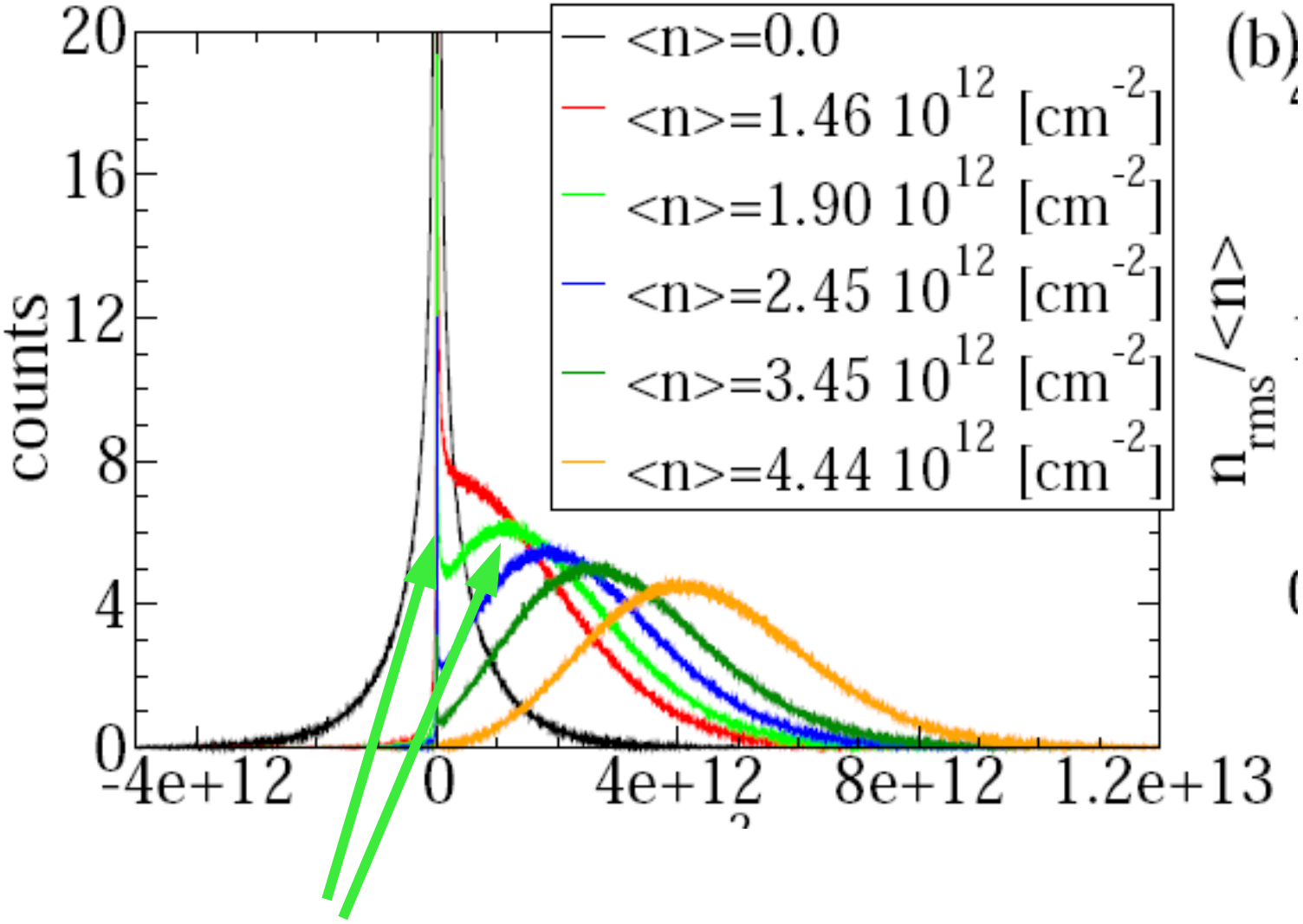








Density Probability Distribution

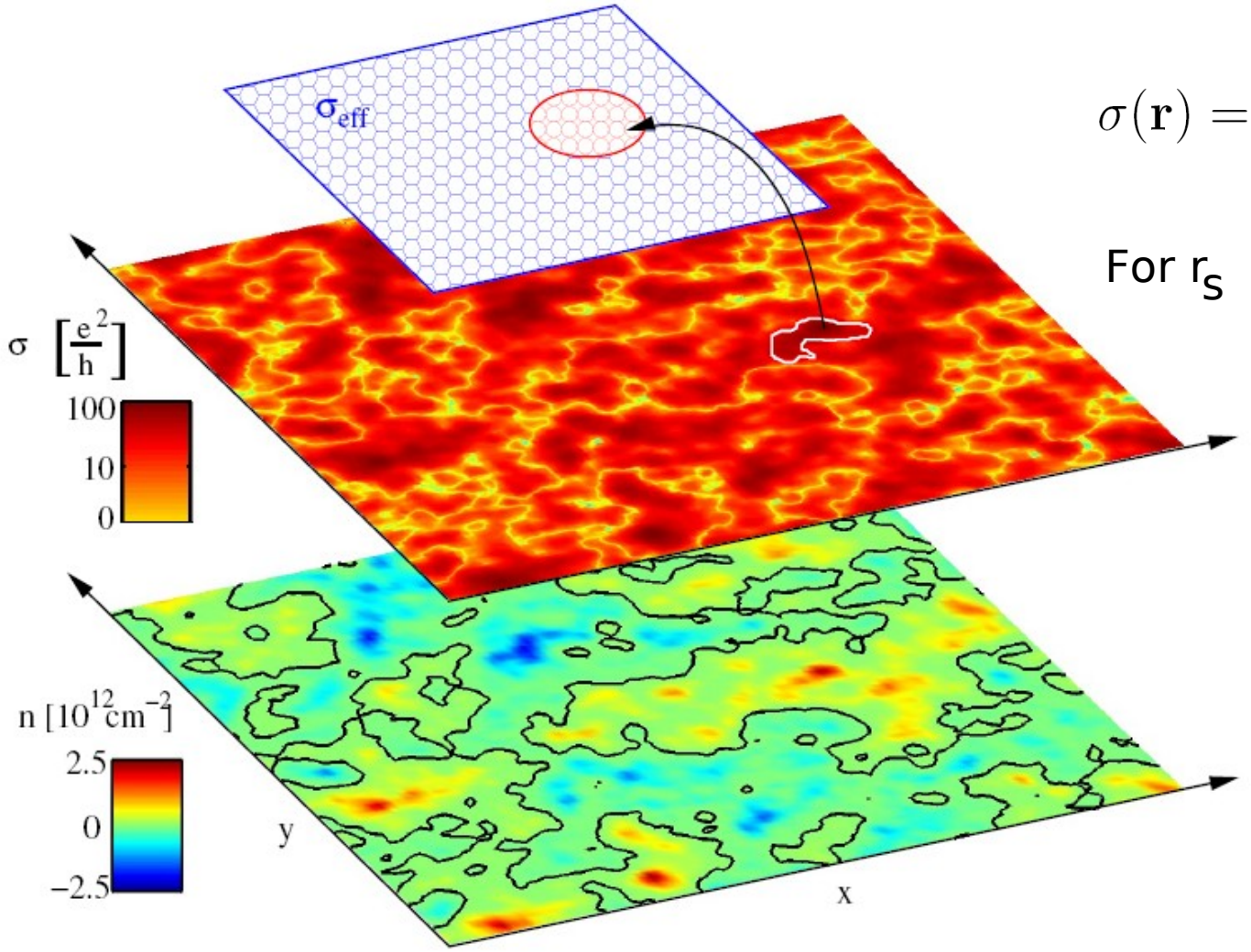


Bimodal Character

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, and the mean free path, l. Because in presence of disorder the density is strongly inhomogeneous, and different from zero almost everywhere, we assume the RPA-Boltzmann expression [Ando J. Phys. Soc. (2006); Nomura & MacDonald, PRL (2006); Hwang, Adam, Das Sarma, PRL (2007); Cheianov & Falko, PRL (2006), Adam et al. PNAS (2007)] to be valid locally also at the Dirac point:



$$\sigma(\mathbf{r}) = F(r_s)\frac{2e^2}{h}\frac{|n(\mathbf{r})|}{n_{imp}}$$

For r_s =0.8 is $F(r_s)$ = 10.

Effective medium theory

We use the Landauer-Bruggeman [Bruggeman Ann. Phys (1935), Landauer J. Appl. Phys. (1952)] Effective Medium Theory. In this approach an effective medium conductivity, σ_{eff} , is calculated requiring that the spatial average of the electric field fluctuations induced by the inhomogeneity of σ is equal to zero. In 2D this requirement translates into the equation:

$$\int d^2r \frac{\sigma(\mathbf{r}) - \sigma_{\text{eff}}}{\sigma(\mathbf{r}) + \sigma_{\text{eff}}} = 0$$

For graphene this equation, after disorder averaging, takes the form:

$$\left\langle \int d^2r \frac{\sigma(\mathbf{r}) - \sigma_{\text{eff}}}{\sigma(\mathbf{r}) + \sigma_{\text{eff}}} = 0 \right\rangle \Longleftrightarrow \int dn \frac{\sigma_0 \frac{|n|}{n_{imp}} - \sigma_{\text{eff}}}{\sigma_0 \frac{|n|}{n_{imp}} + \sigma_{\text{eff}}} P(n) = 0$$

$$\sigma(\mathbf{r}) = F(r_s) \frac{2e^2}{h} \frac{|n(\mathbf{r})|}{n_{imp}}$$

We know P(n): obtained using the Thomas-Fermi-Dirac approach.

Effective medium theory: regime of validity

The Effective Medium Theory is valid when:

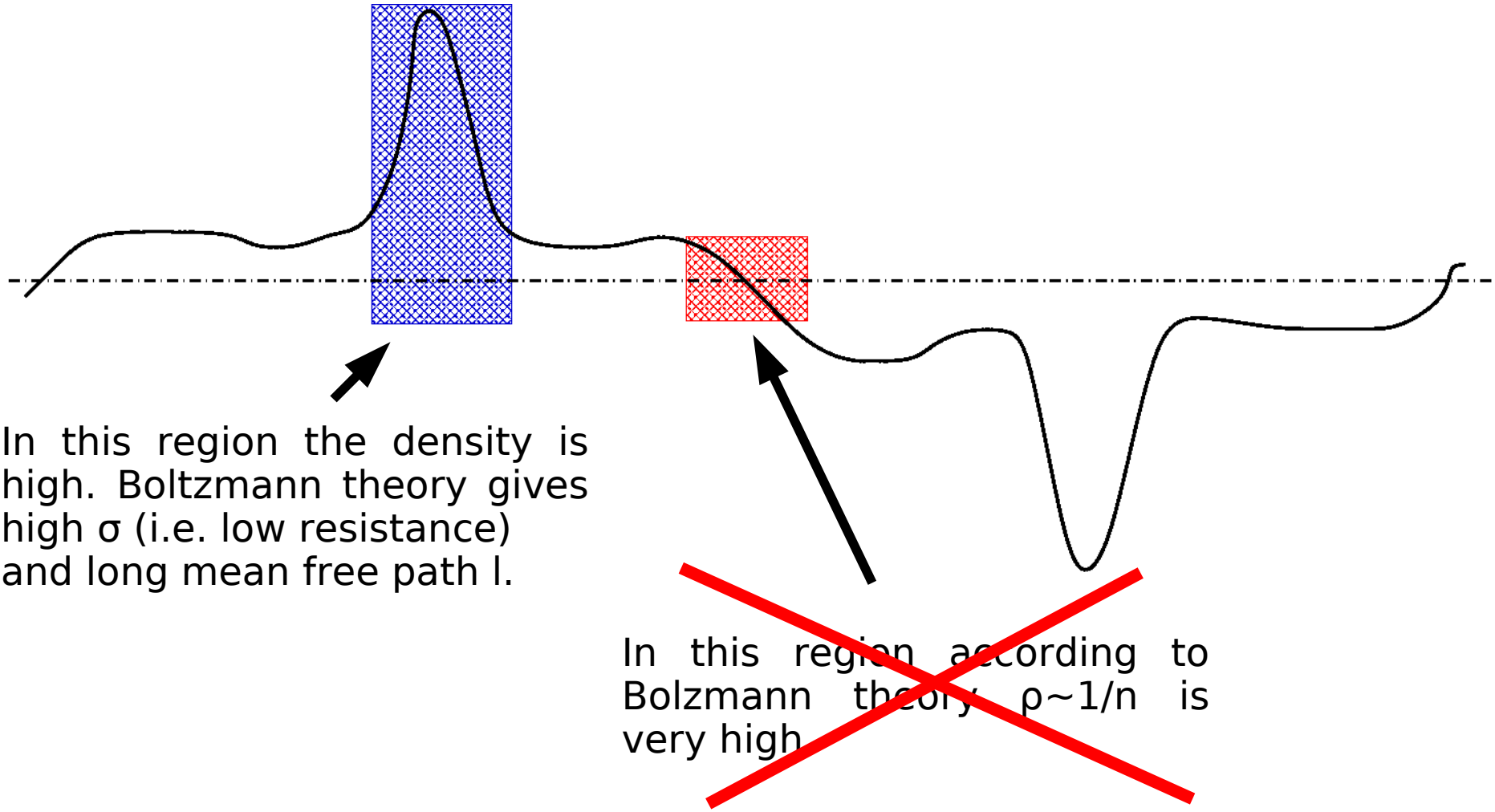
a)

$$l \ll \left[\frac{\nabla\sigma}{\sigma}\right]^{-1} \quad \longleftrightarrow \quad l \ll \left[\frac{\nabla n}{n}\right]^{-1}$$

From Boltzmann-RPA result

b) **Resistive contribution across p-n junctions between electron-hole puddles is small.**

Effective medium theory: why it works



In this region the density is high. Boltzmann theory gives high σ (i.e. low resistance) and long mean free path l.

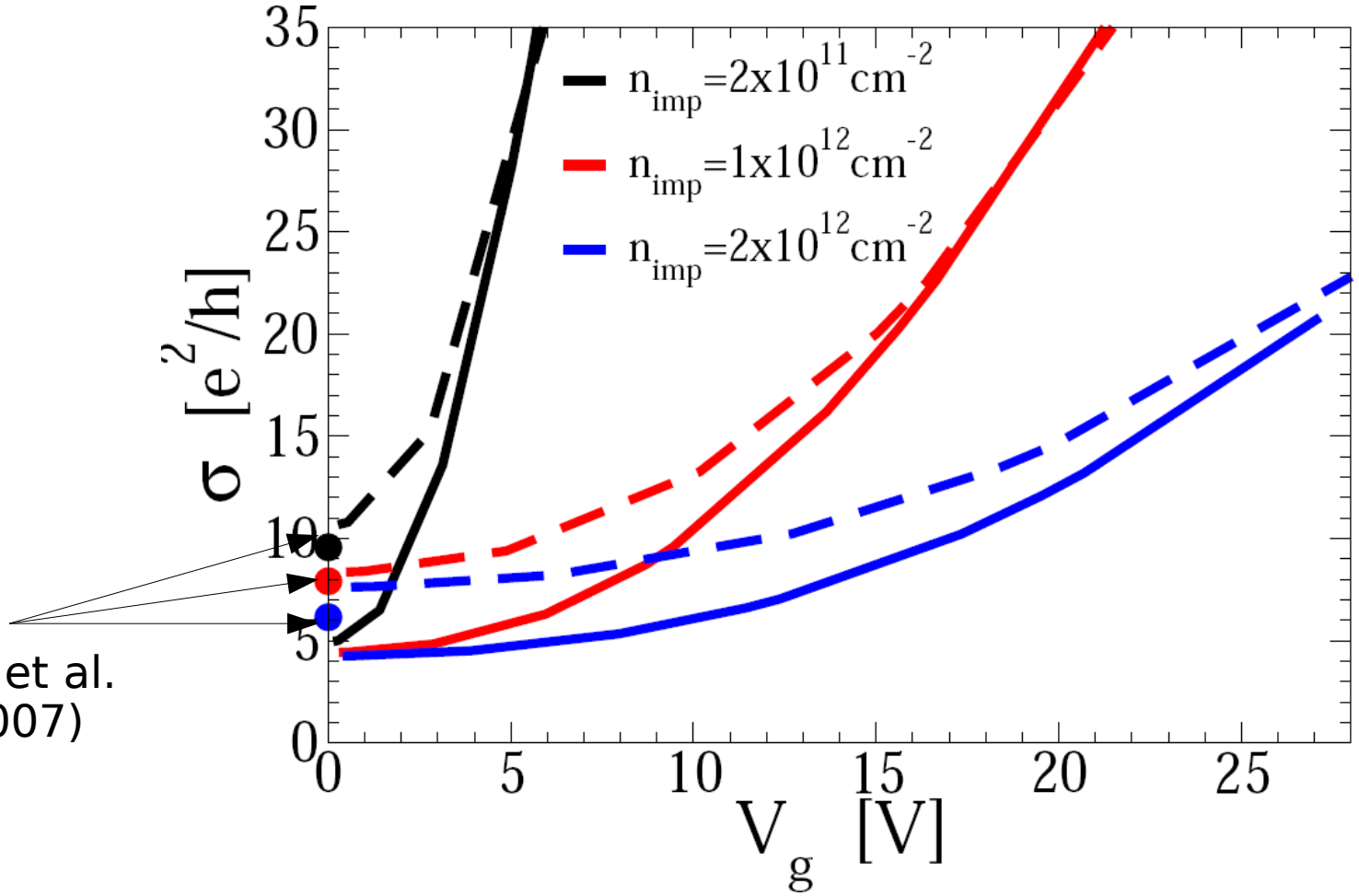
In this region according to Bolzmann theory ρ~1/n is very high

Boltzmann theory does not apply.

Klein Paradox => T~1 => Low resistance

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

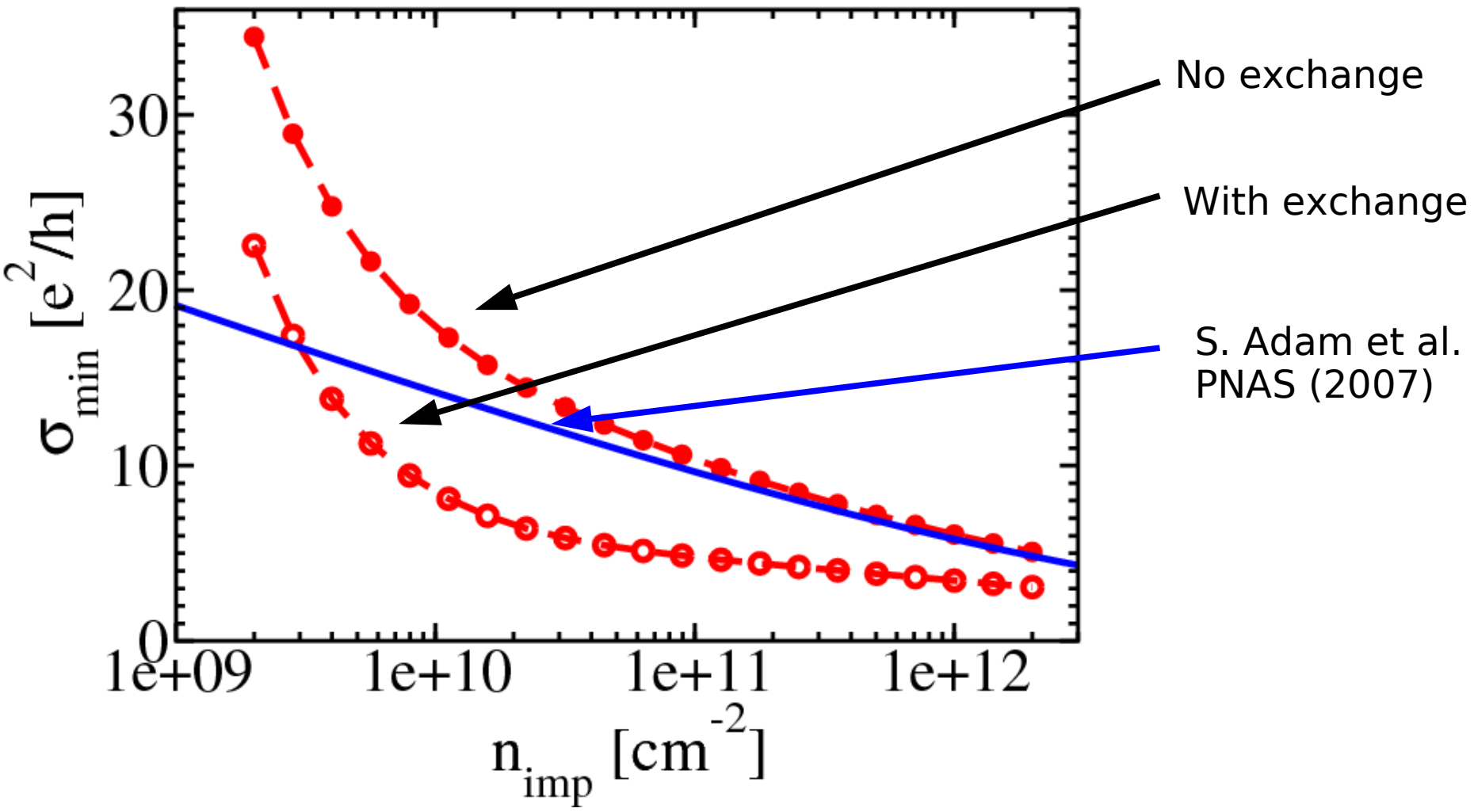
EMT: conductivity vs. gate voltage



S. Adam et al.
PNAS (2007)

- 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.

EMT: minimum conductivity vs. impurity density



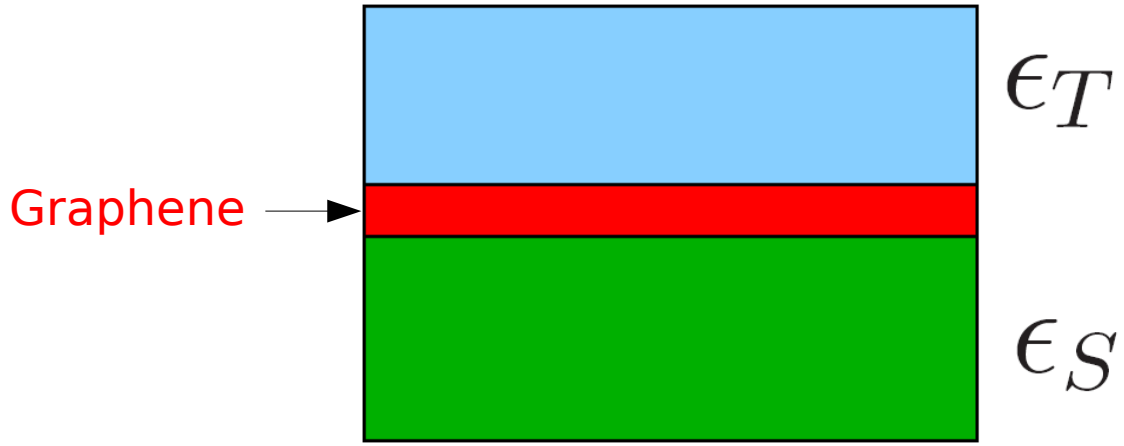
Dependence of conductivity on impurity density in qualitative and quantitative agreement with experiments.

Tuning r_s

C. Jang et al. PRL (2008)

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

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



$$\epsilon_S = 3.9$$

Vacuum

$$\epsilon_T = 1$$

$$r_s = 0.81$$

Ice

$$\epsilon_T = 3.2$$

$$r_s = 0.56$$

How r_s enters the theory

- r_s affects the ground-state carrier distribution:

$$\frac{1}{\hbar v_F}\frac{\delta E}{\delta n} = \mathrm{sign}(n)\sqrt{\pi n} + \mathbf{r_s}\int d^2r' \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + \mathbf{r_s}\hat{\Sigma}(n) - \mathbf{r_s}\hat{V}_D - \mu$$

- r_s controls the scattering time:

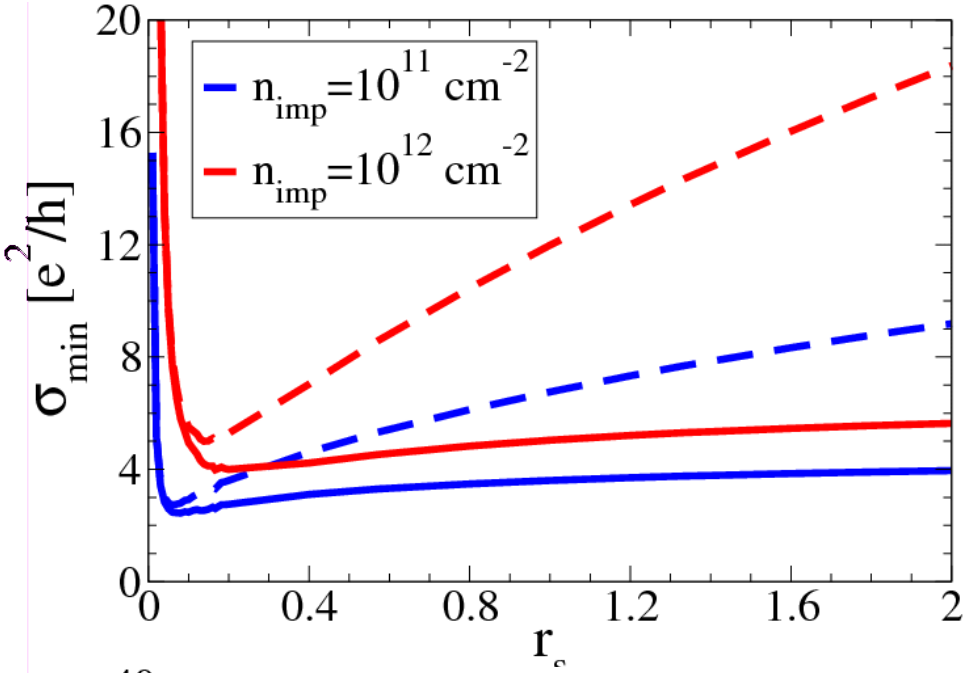
$$\frac{1}{\tau} = \frac{\sqrt{\pi} v_F n_{imp}}{\hbar\sqrt{n}} F(\mathbf{r_s})$$

S. Adam et al. PNAS (2008).
E. Hwang et al. PRB (2008).

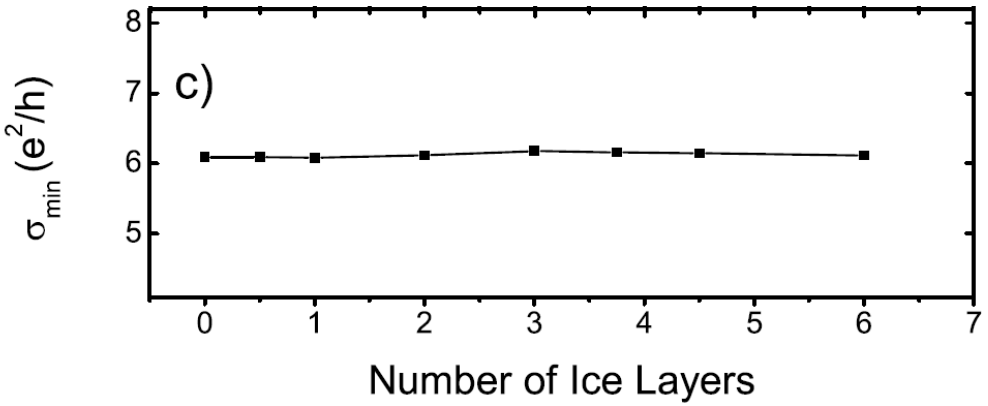
and therefore the local value of the conductivity

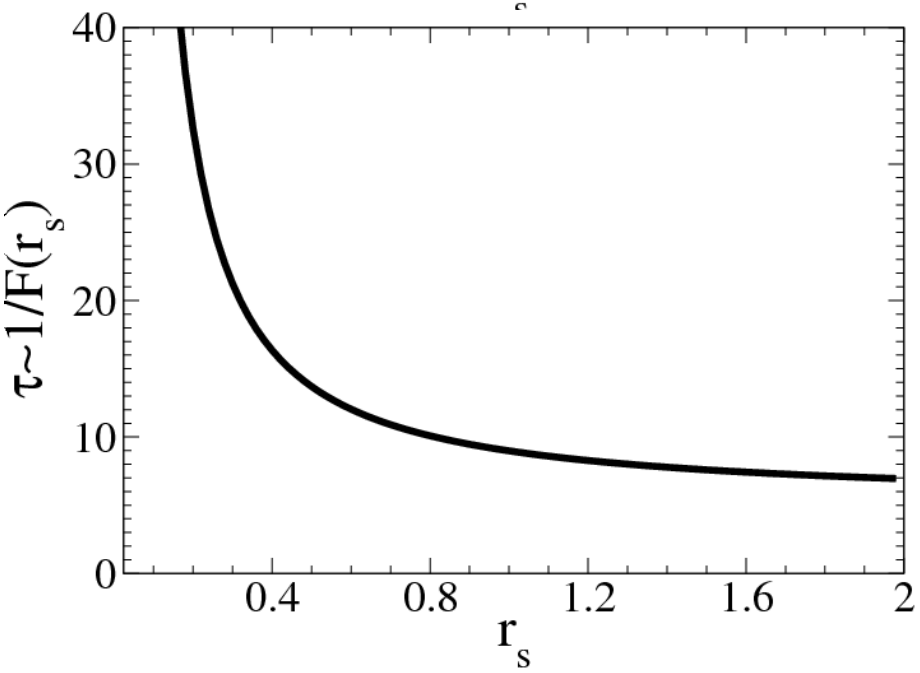
$$\sigma = 2\frac{e^2}{h}E_F\tau = 2\frac{e^2}{h}\frac{n}{n_{imp}}\frac{1}{F(\mathbf{r_s})}$$

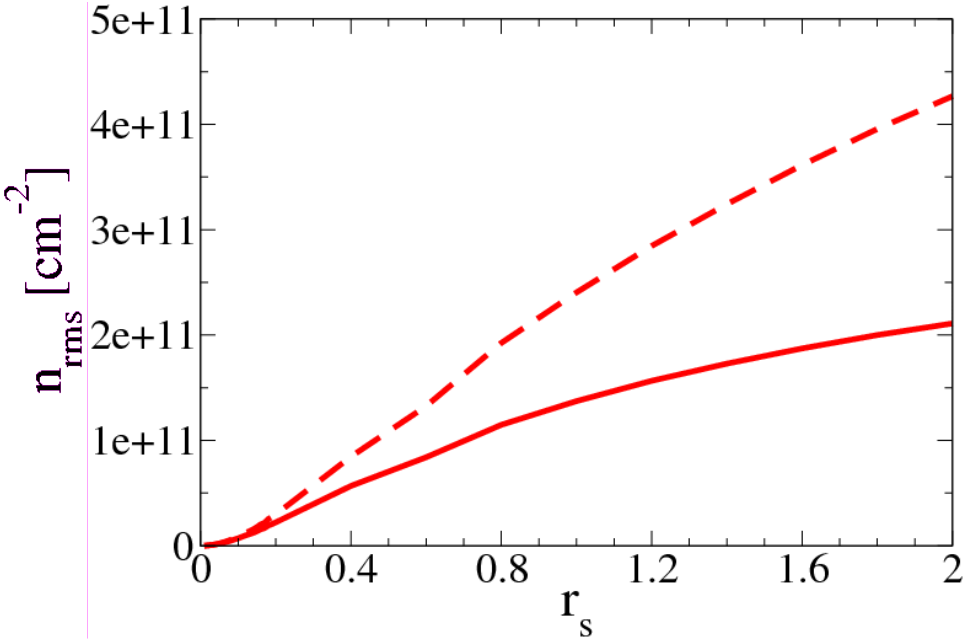
EMT: r_s dependence of the minimum conductivity



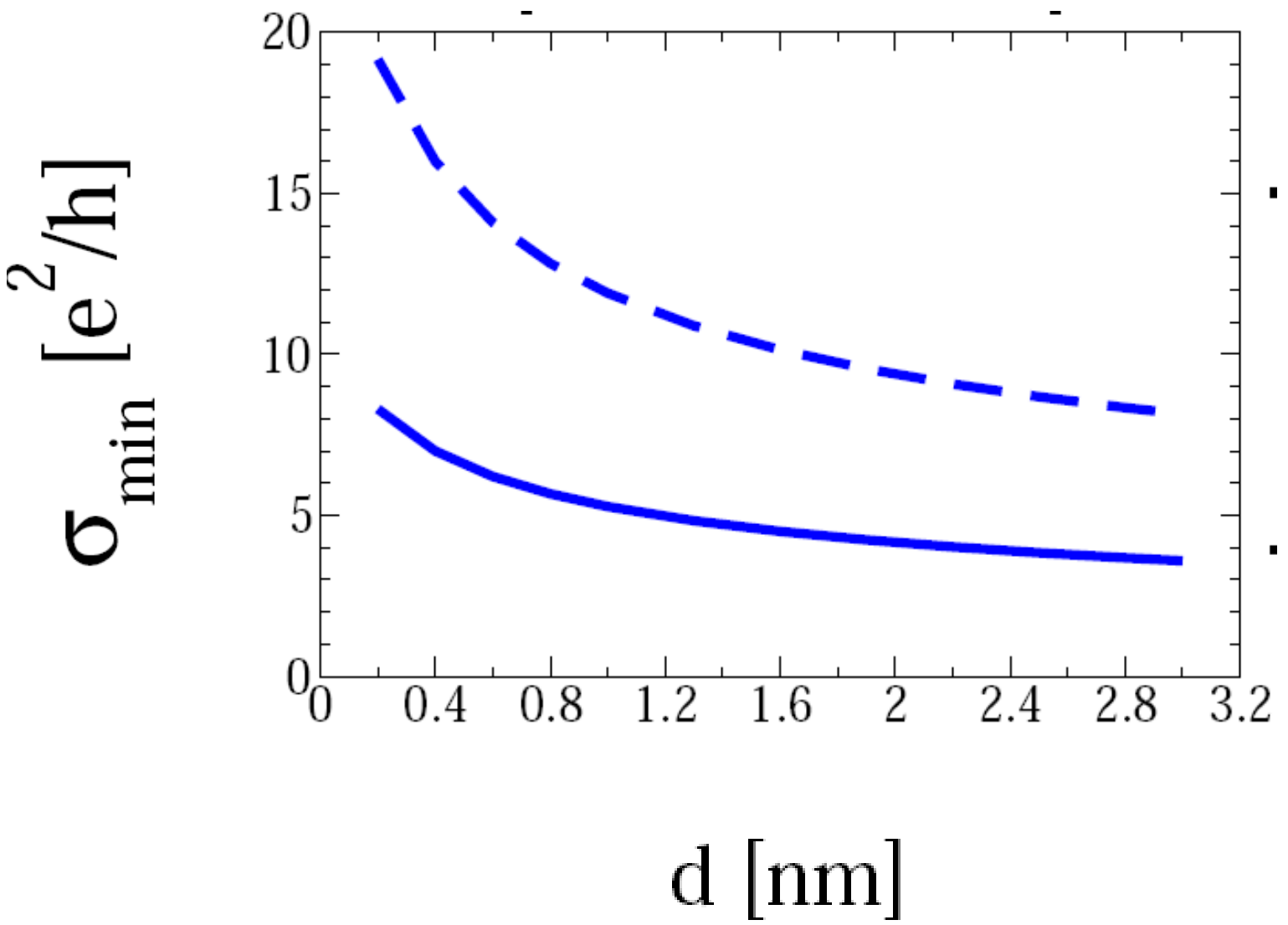
Experiment: C. Jang et al PRL (2008)







EMT: d dependence of the minimum conductivity



Conclusions

Close to the Dirac-point, disorder induced density inhomogeneities are extremely important to understand graphene properties, especially transport.

In presence of charged impurities we find:

- The carrier density is characterized by small regions with high density and big puddles. Non-linear screening and many body effects are essential to properly characterize the carrier density.
- $n_{rms} >> \langle n \rangle$ for gate voltages corresponding to average densities as high as 10^{12} cm^{-2}.
- The carrier density probability distribution close to the Dirac-point has bimodal character.
- Using effective medium theory we have shown how the density inhomogeneities explain the values of conductivity observed in current experiments and resolve the shortcomings of previous theories:
  - Finite value of σ at Dirac point and close to experimental values;
  - Crossover from Dirac point to high doping regime;
  - Interactions not strong enough to cause long-range order but essential to understand transport close to the Dirac point;