Graphene
From materials science to particle physics

Joaquín E. Drut
The Ohio State University

28th Lattice Symposium
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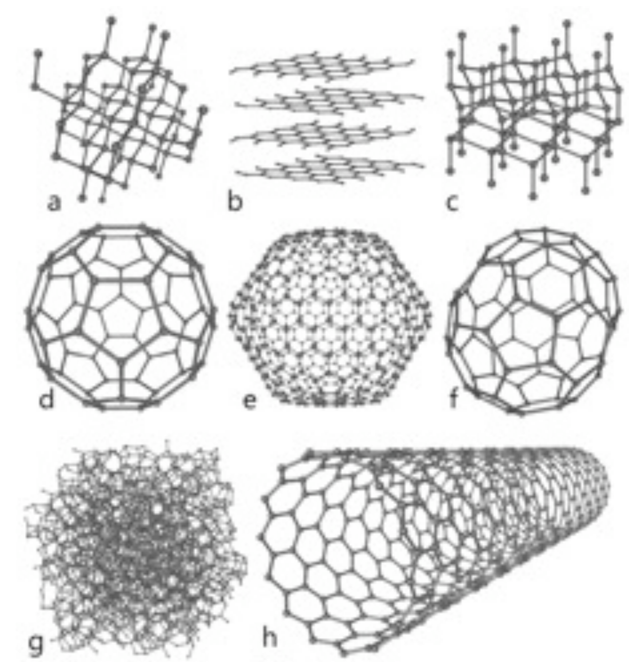


Colleagues

Timo A. Lähde, Lauri Suoranta,
Eero Tölö
Aalto University, Finland

Kyle Wendt
The Ohio State University

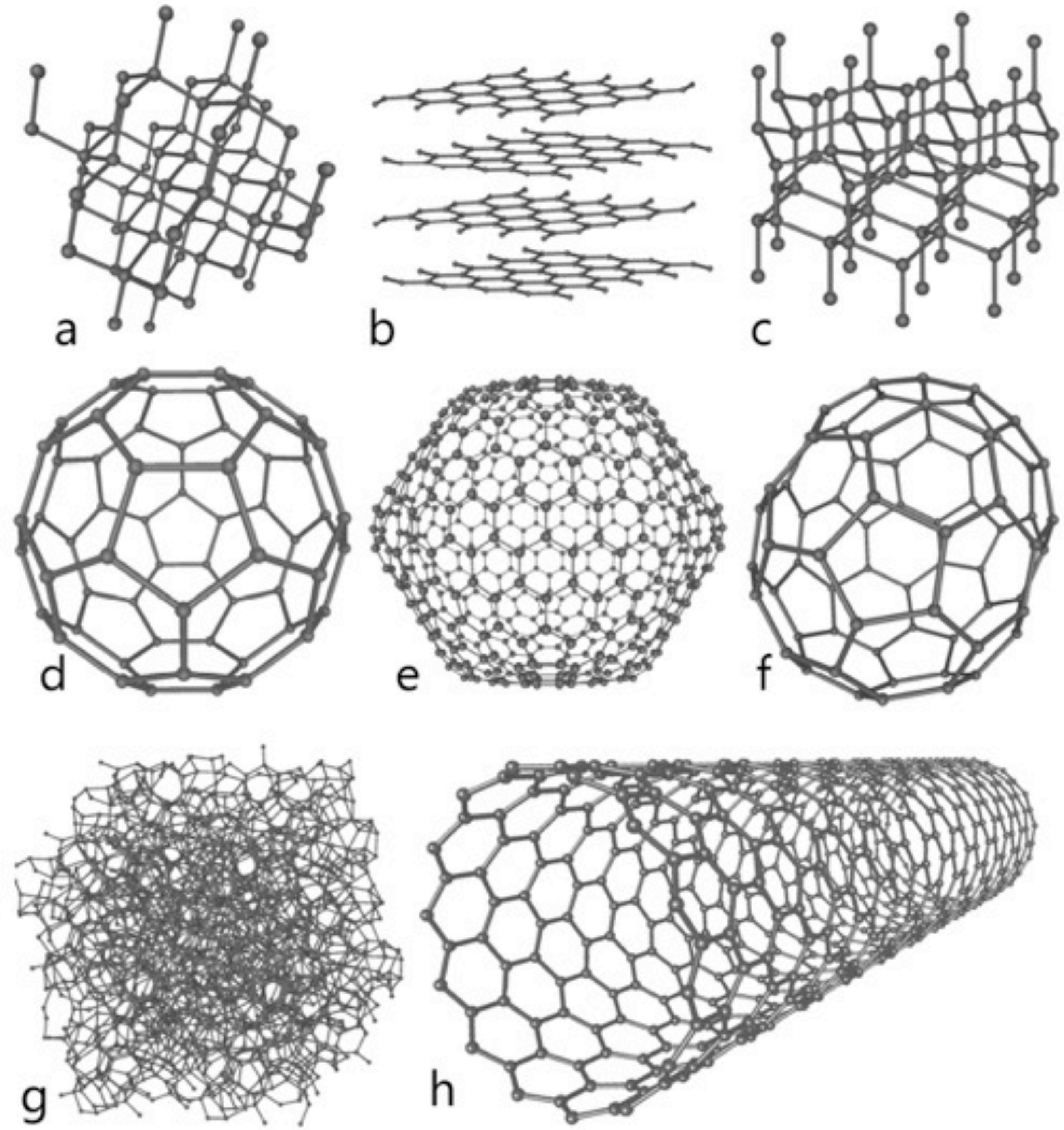
Timour Ten
University of Illinois

Plan

- Graphene
  - What is it? Why is it interesting?
  - What do experiments say?
  - What can we say about it with lattice methods?
- Summary & future work
- From QCD to condensed matter... and back!

What is graphene?

- An allotrope of C



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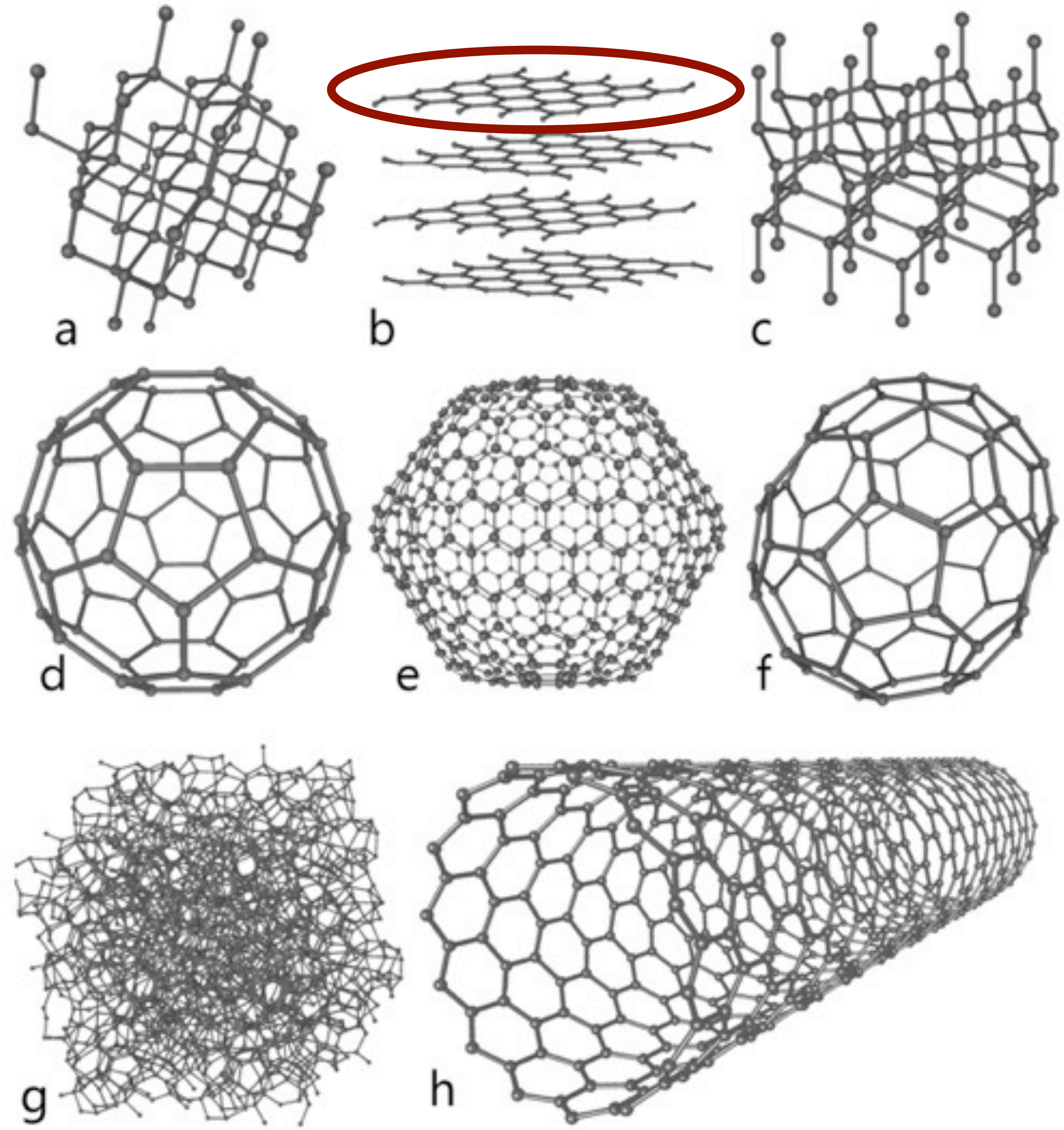
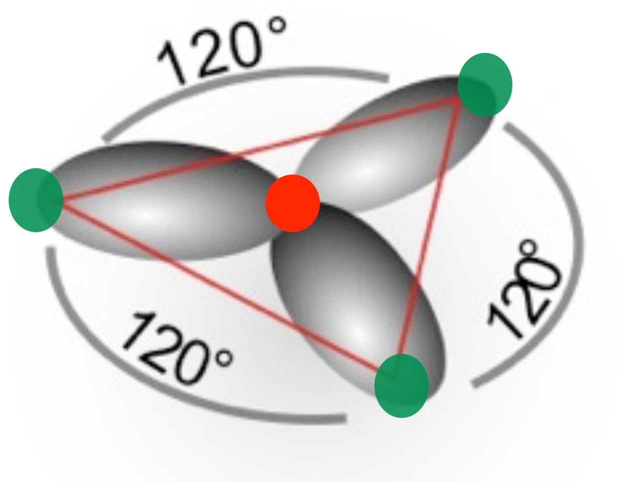


What is graphene?

- An allotrope of C
- 2D hexagonal structure



$a = 1.42\text{Å}$

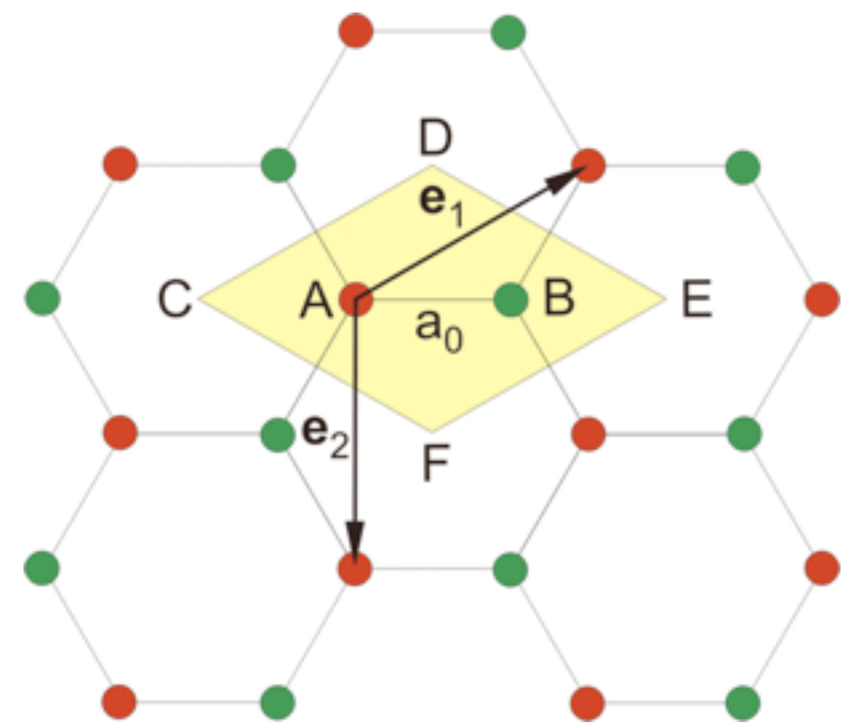
- Orbital hybridization

$1s^2 \quad \underline{2s^2\ 2p^2}$

↓

$3\ sp^2 + p$

↓ lattice ↓ electron on lattice



- Two triangular sublattices A, B

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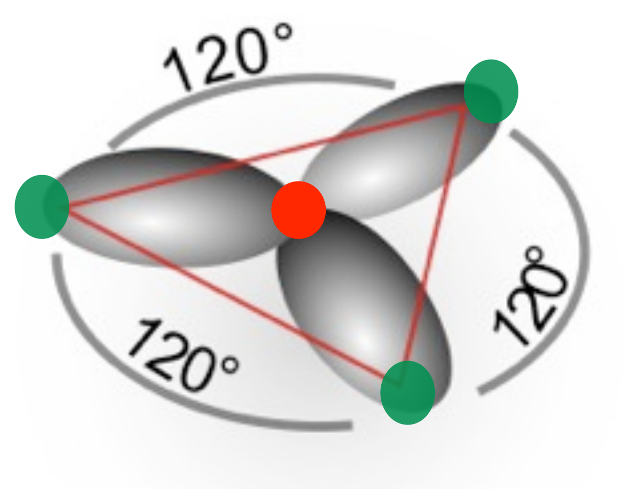

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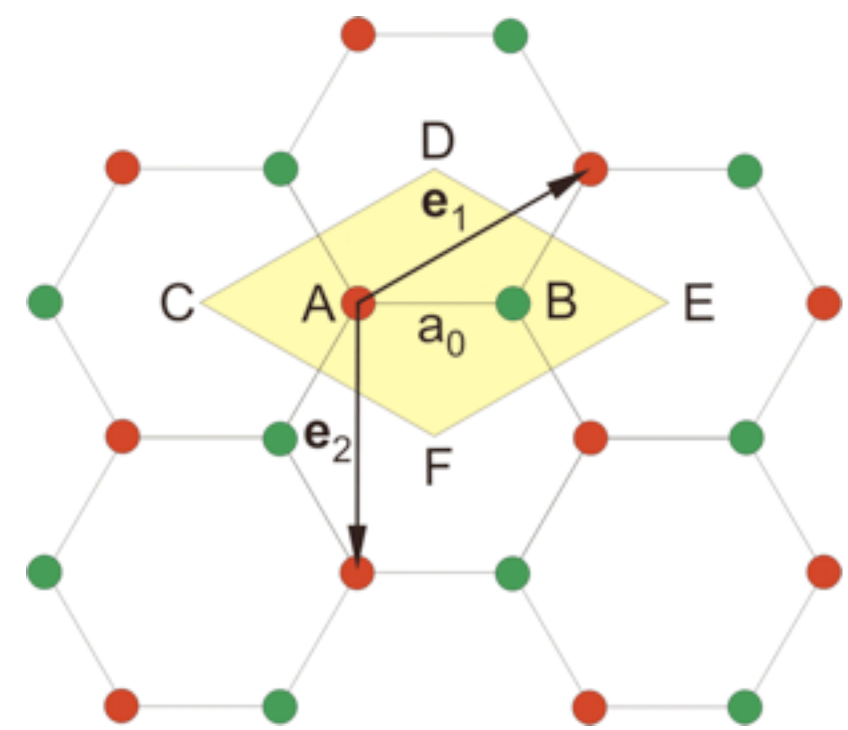


- Tight-binding hamiltonian

$$H = -t \sum_{\langle i,j \rangle, \sigma=\uparrow,\downarrow} \left(a^\dagger_{\sigma,i} b_{\sigma,j} + \text{H.c.} \right)$$
$$-t' \sum_{\langle\langle i,j \rangle\rangle, \sigma=\uparrow,\downarrow} \left(a^\dagger_{\sigma,i} a_{\sigma,j} + b^\dagger_{\sigma,i} b_{\sigma,j} + \text{H.c.} \right)$$

$t \simeq 2.8\ \text{eV} \qquad t' \simeq 0.2t$

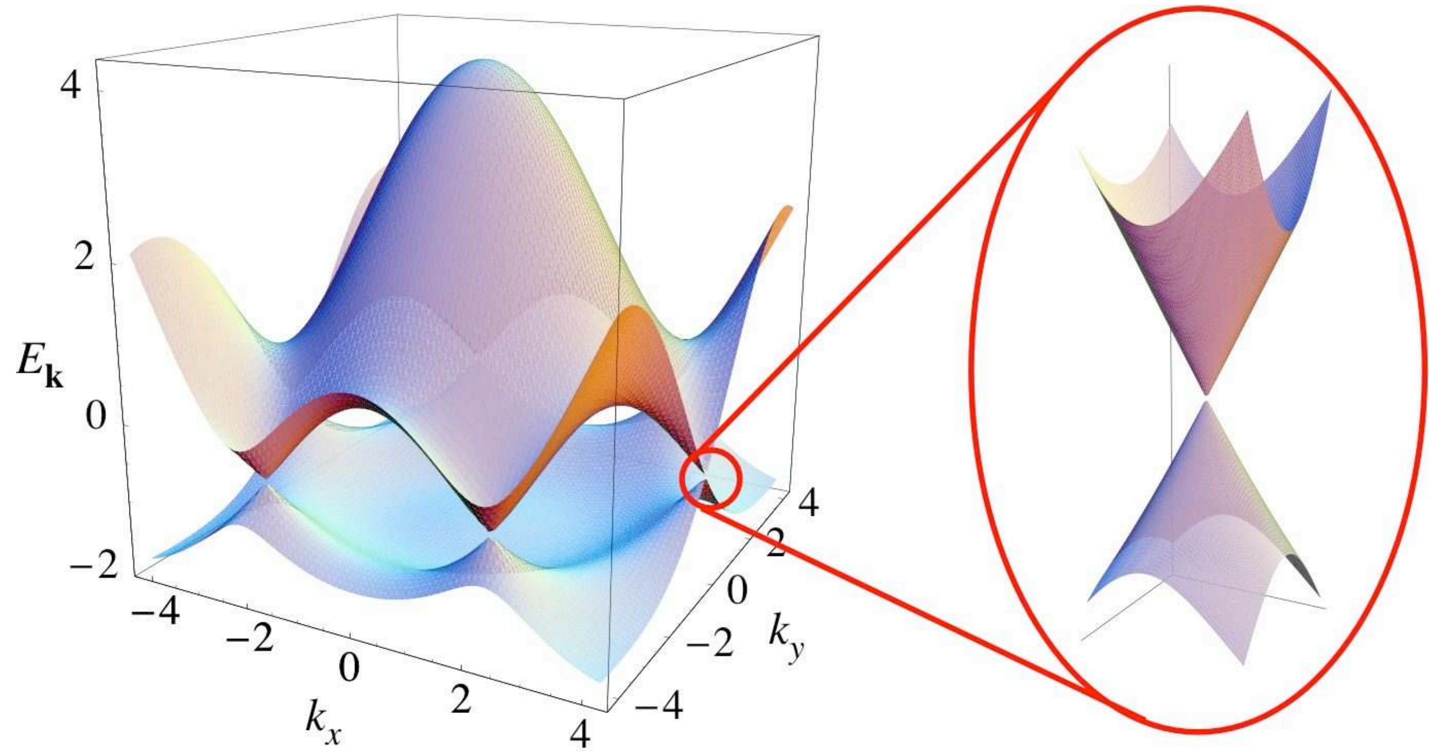
- Two triangular sublattices A, B

What is graphene?

- An allotrope of C
- 2D hexagonal structure
- It has 2 Dirac points

  i.e. quasiparticles are relativistic-like...

  $$E_{\pm}(\mathbf{k}) = \pm v|\mathbf{k}|$$



Castro Neto et al, RMP, **81**, 109 (2009)

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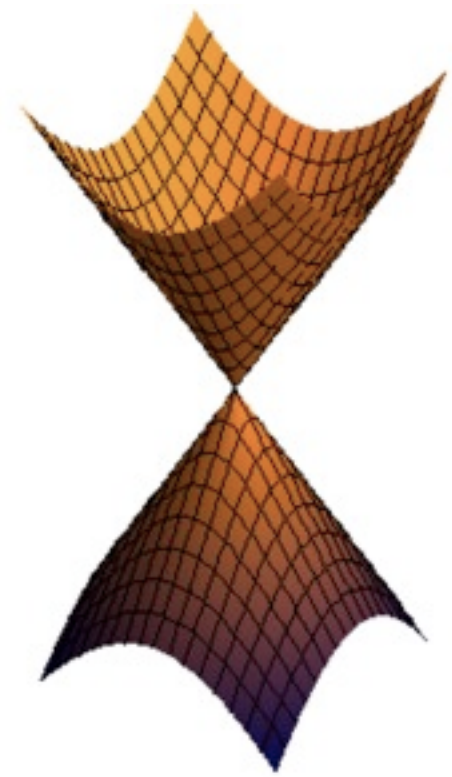

- 2 x 2 x 2 = 8 Fermion d.o.f. → Two 4-component Dirac spinors

Dirac points
Sublattices a.k.a. pseudo-spin
Electron spin

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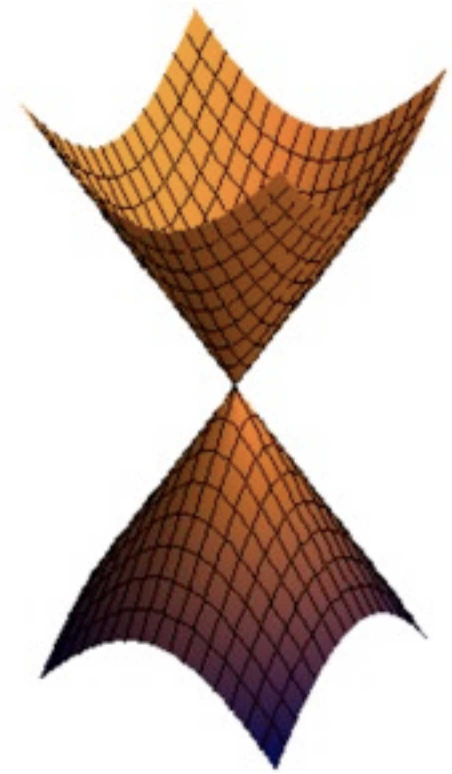

- Two 4-component Dirac spinors, U(4) symmetry

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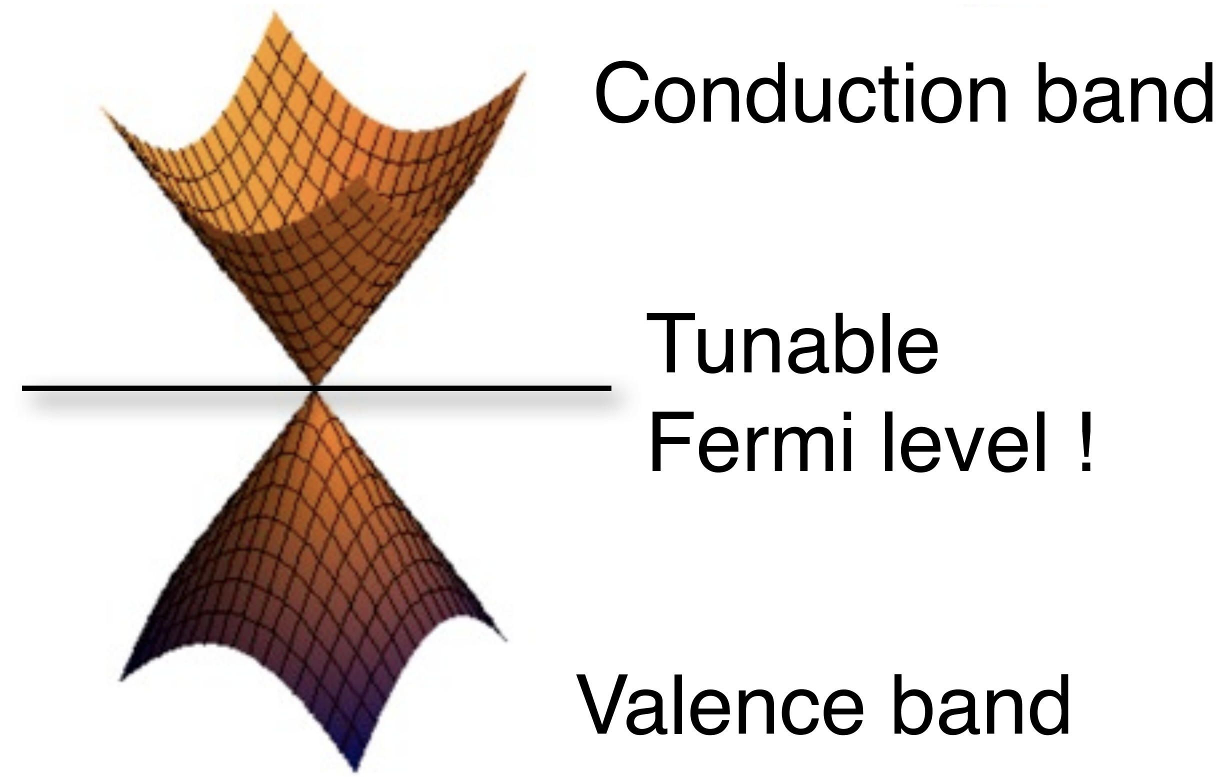

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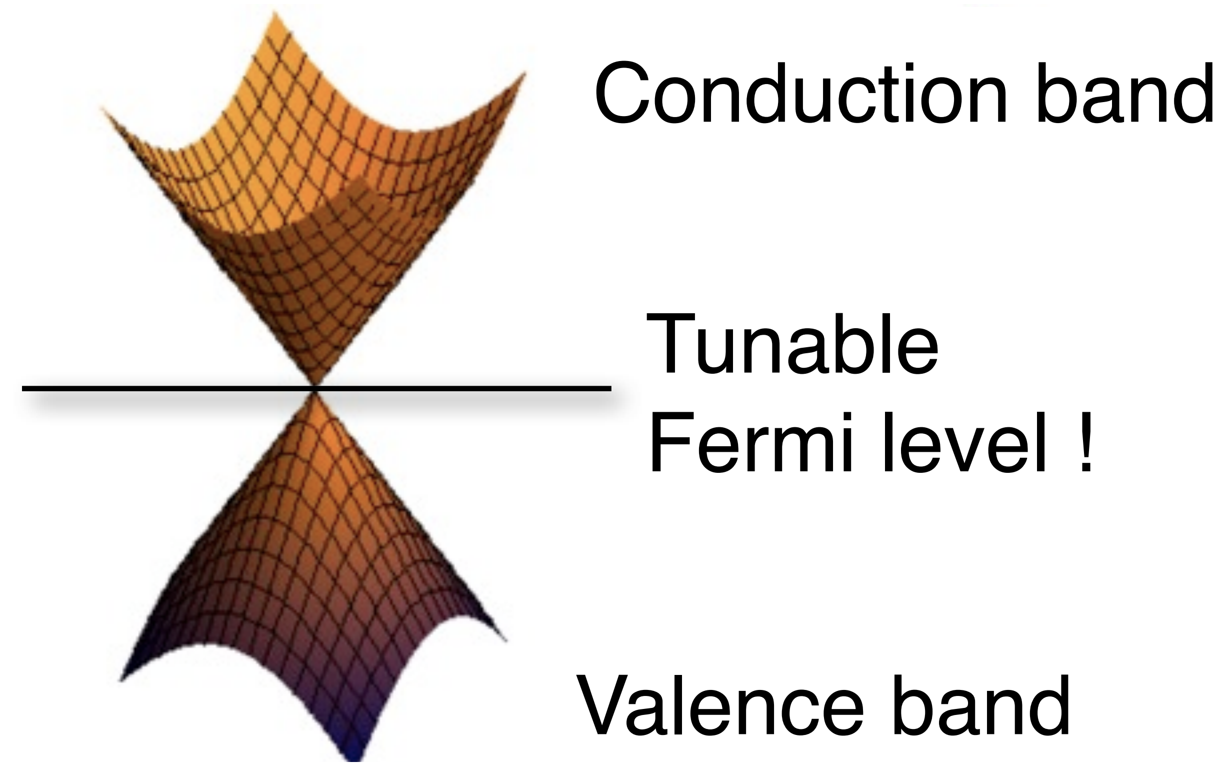
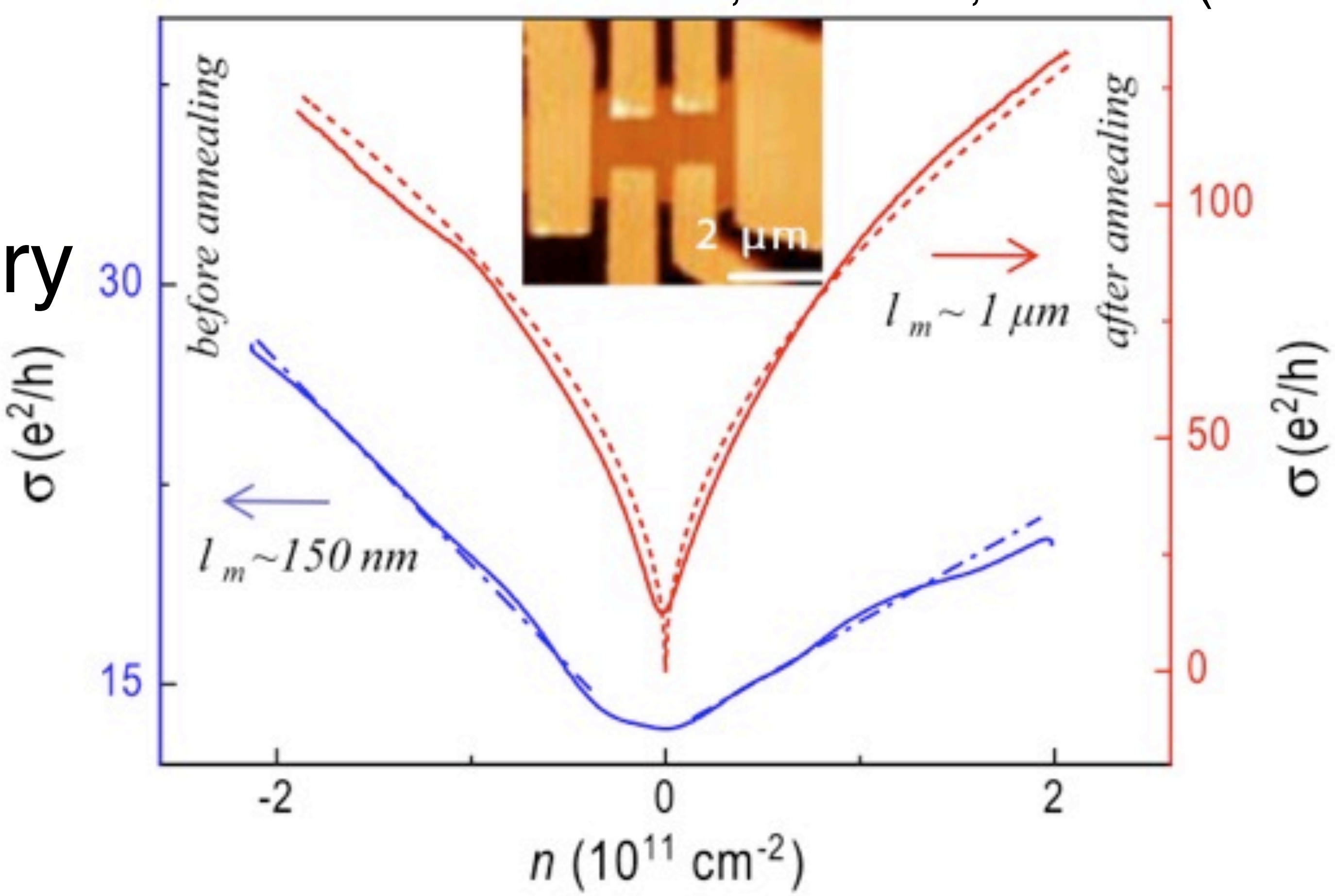


K. I. Bolotin et al., PRL **101**, 096802 (2008)



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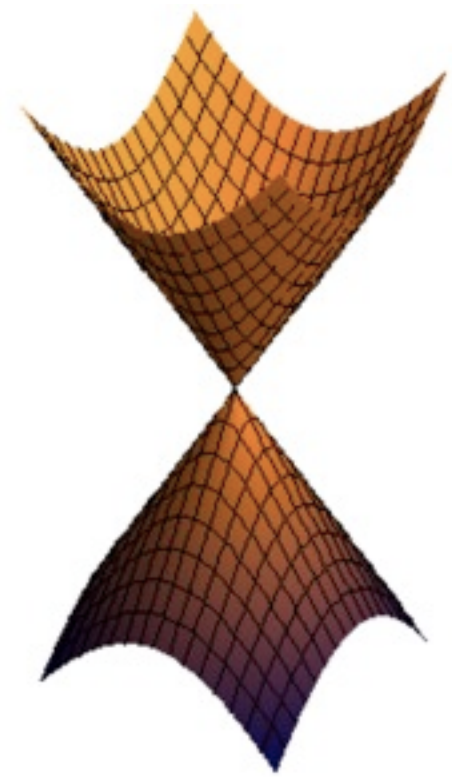

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...but they move very slowly!

$$v = \frac{3ta}{2} \simeq c/300$$

- Strong Coulomb coupling!

$$\alpha_{gr} = \frac{e^2}{4\pi\epsilon_0 v} \simeq 300\alpha \sim 1$$

Maximal for suspended graphene!

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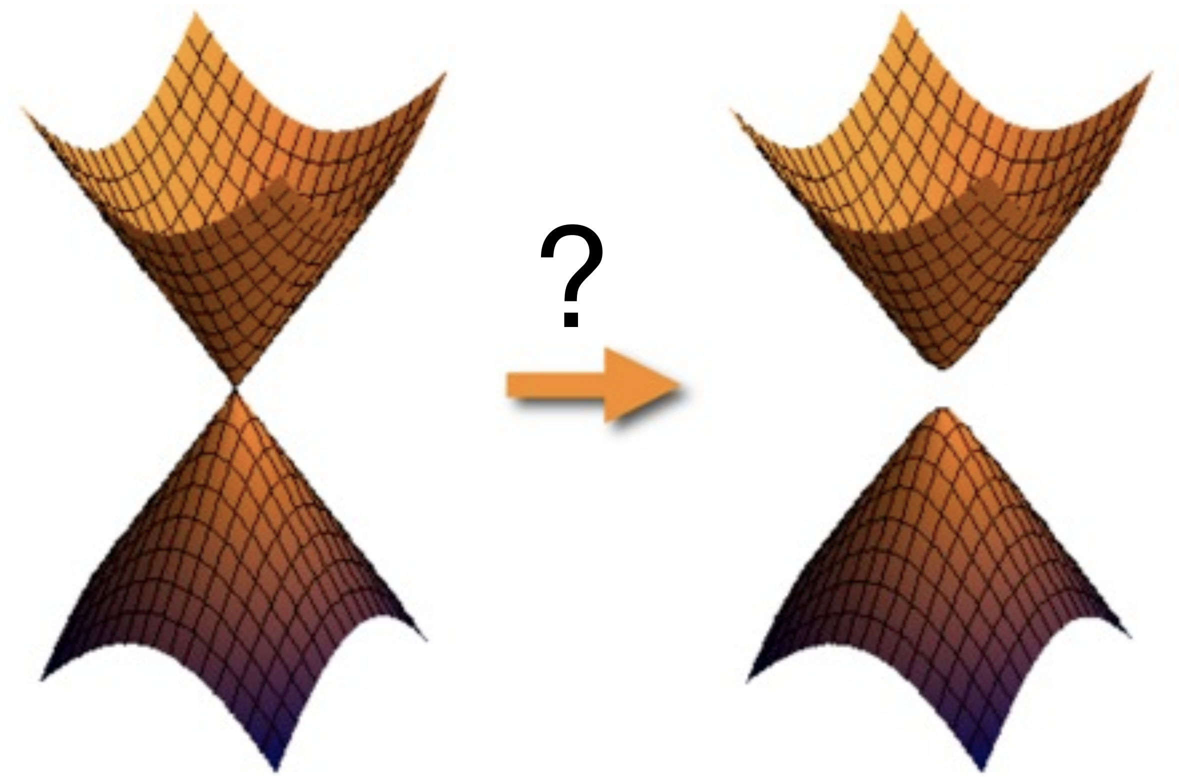


(weak coupling) $\langle\bar{\psi}\psi\rangle = 0$

(strong coupling) $\langle\bar{\psi}\psi\rangle \neq 0$

- Strong Coulomb coupling!

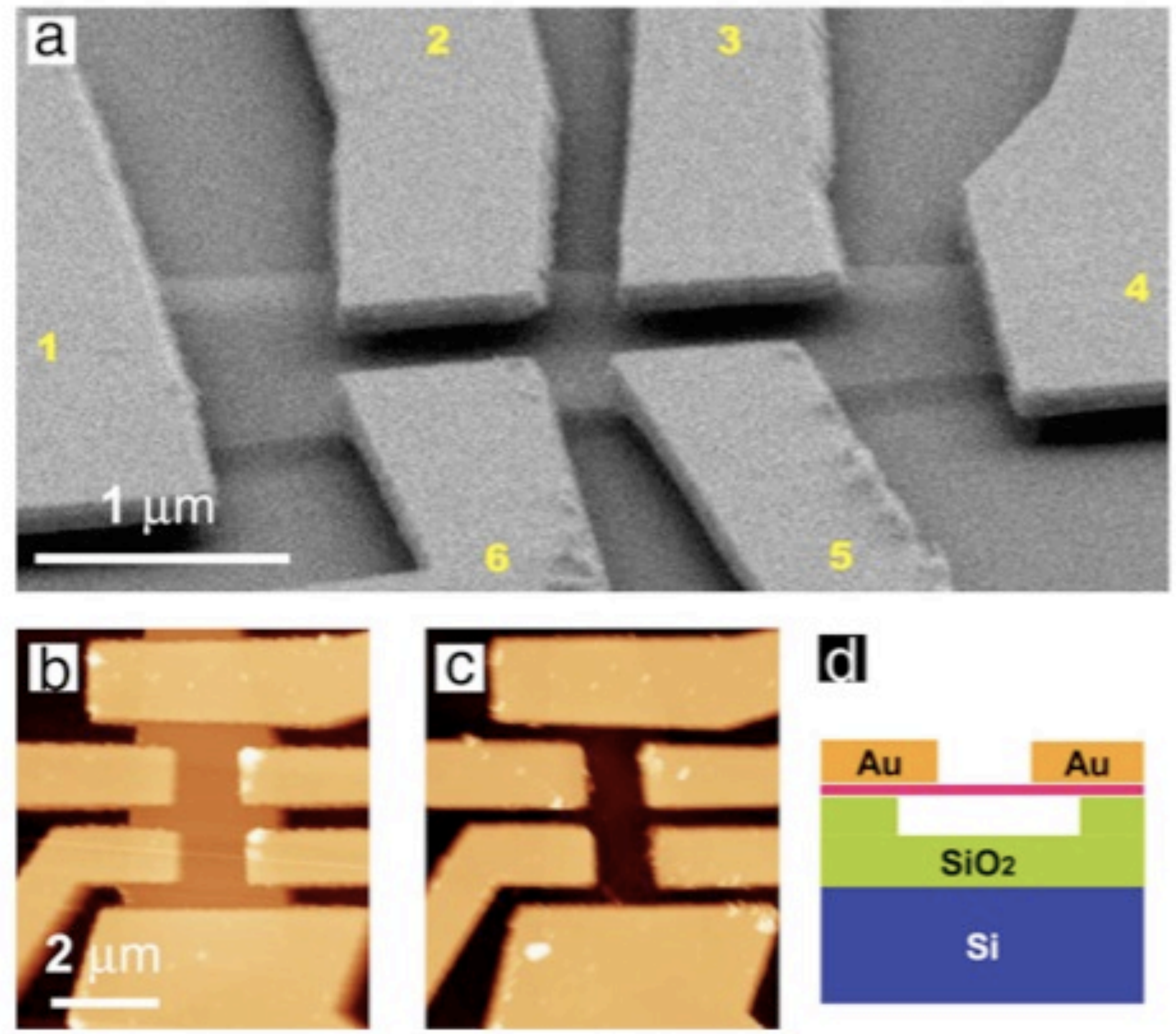
  $$\alpha_{gr} = \frac{e^2}{4\pi\epsilon_0 v} \simeq 300\alpha \sim 1$$

Maximal for suspended graphene!

Is suspended graphene gapped?

What do experiments say?

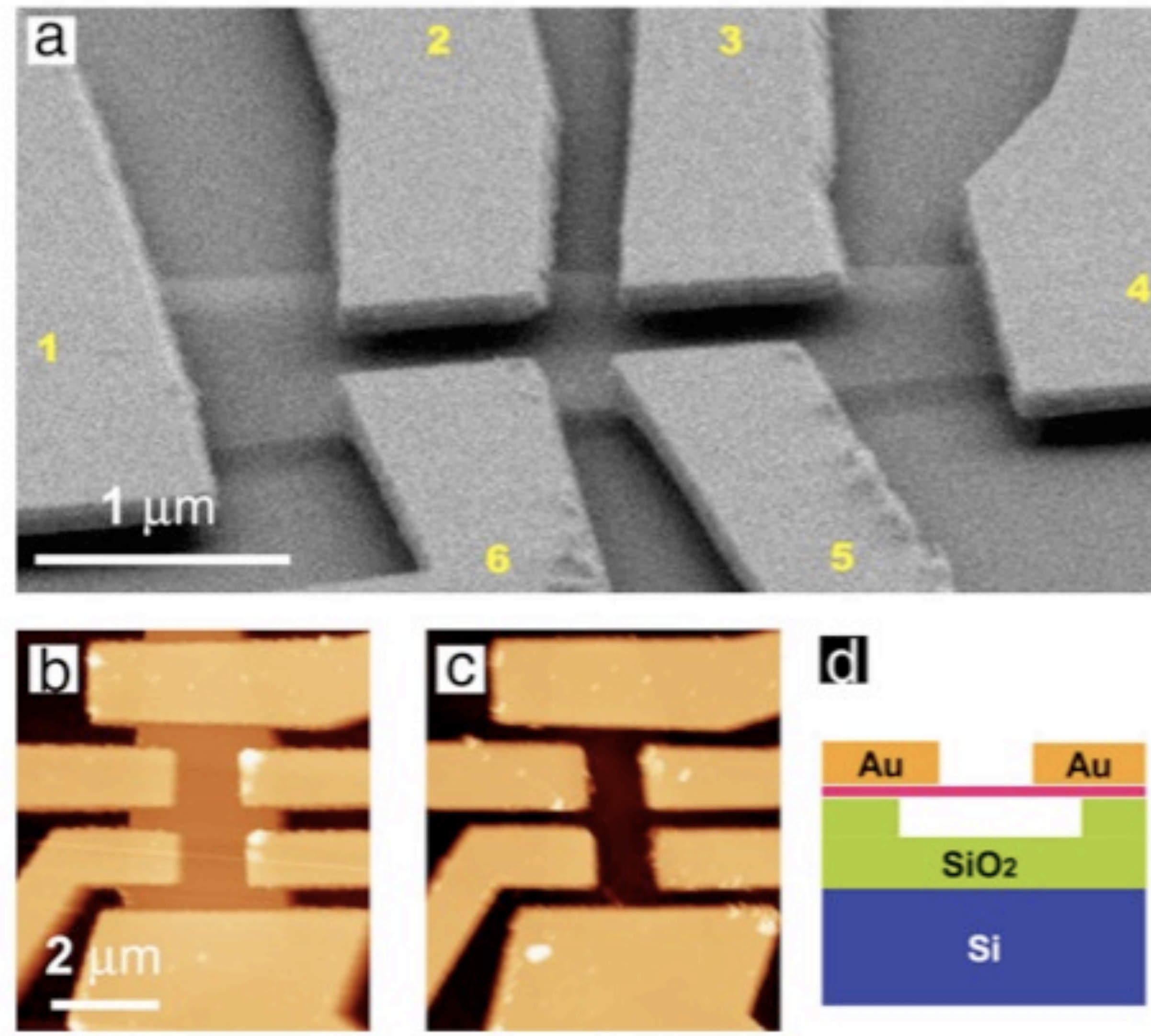
- Very few experiments on suspended graphene



K. I. Bolotin et al., Solid State Comm. **146**, 351, (2008)

What do experiments say?

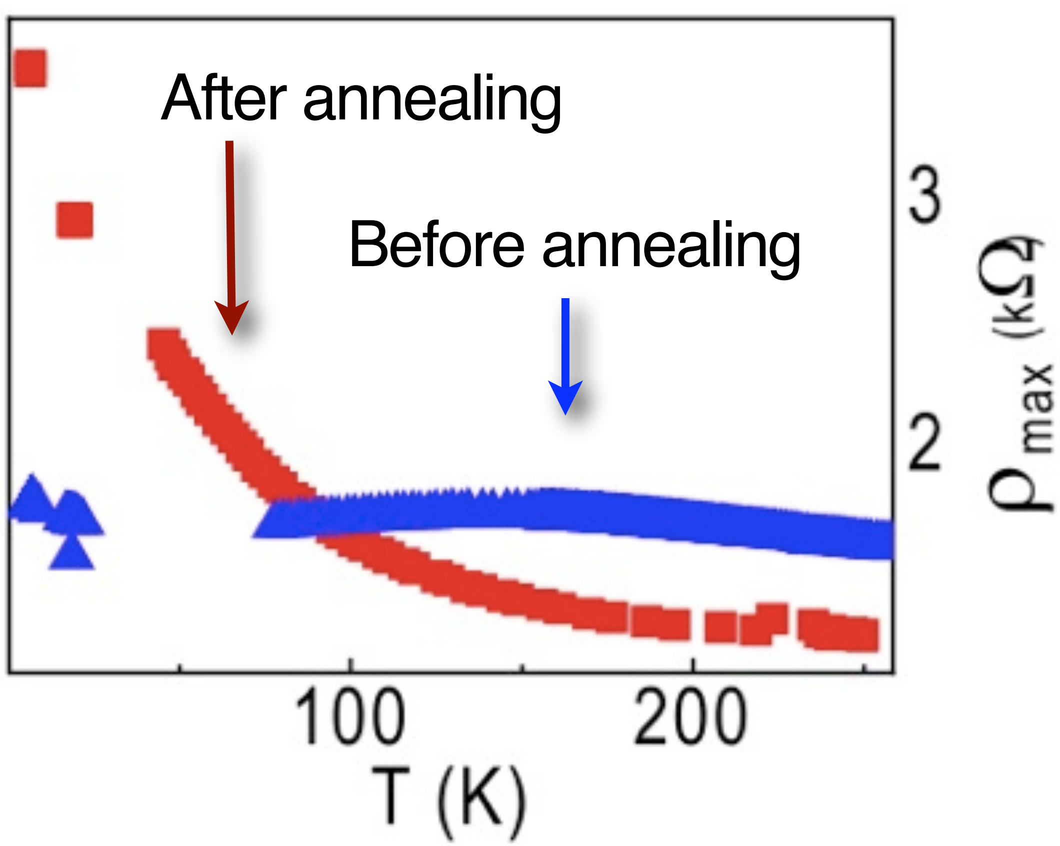
- Very few experiments on suspended graphene
- Annealing techniques are necessary



K. I. Bolotin et al., Solid State Comm. **146**, 351, (2008)

What do experiments say?

- Very few experiments on suspended graphene
- Annealing techniques are necessary
- **Surprising results!**



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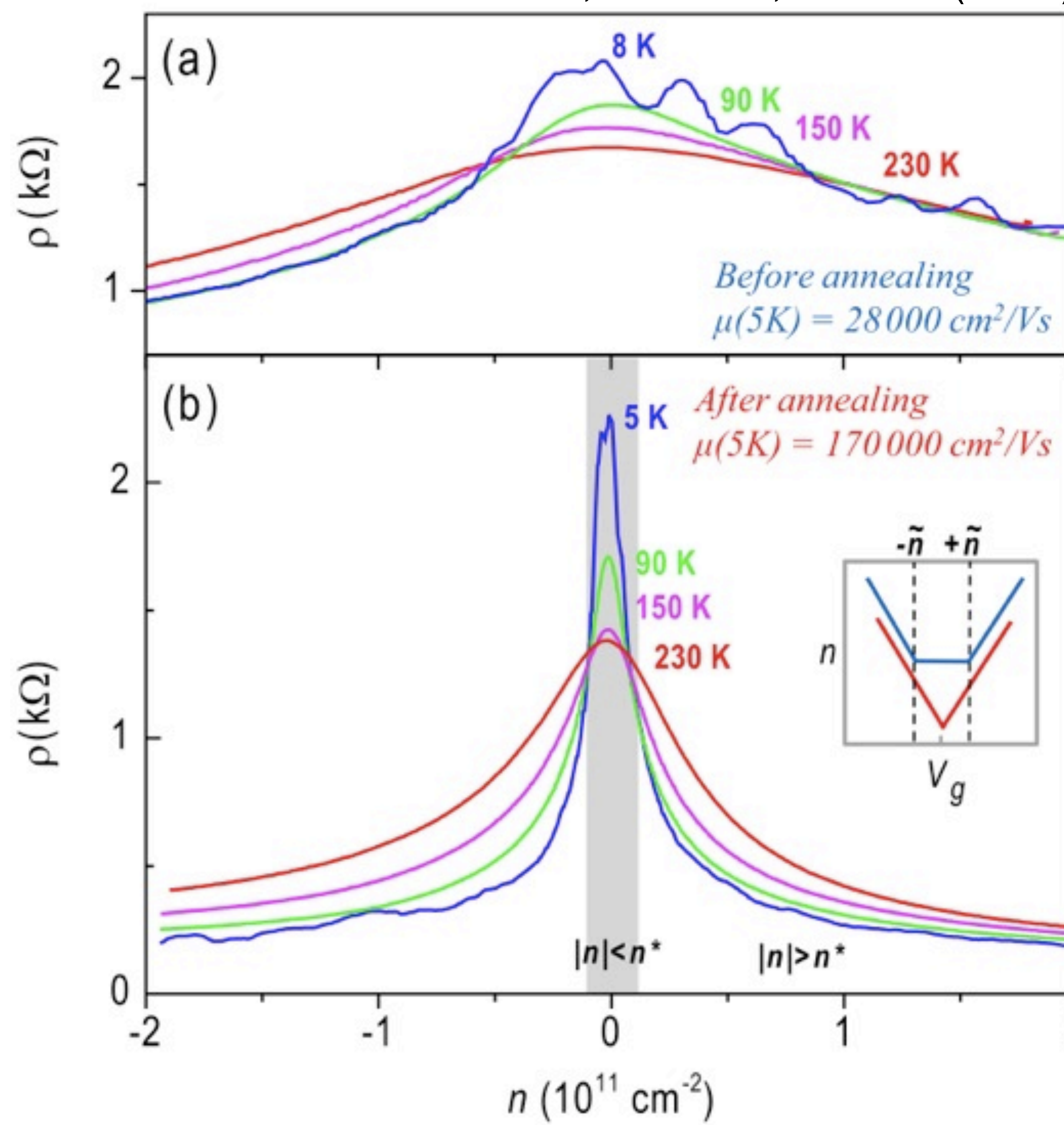
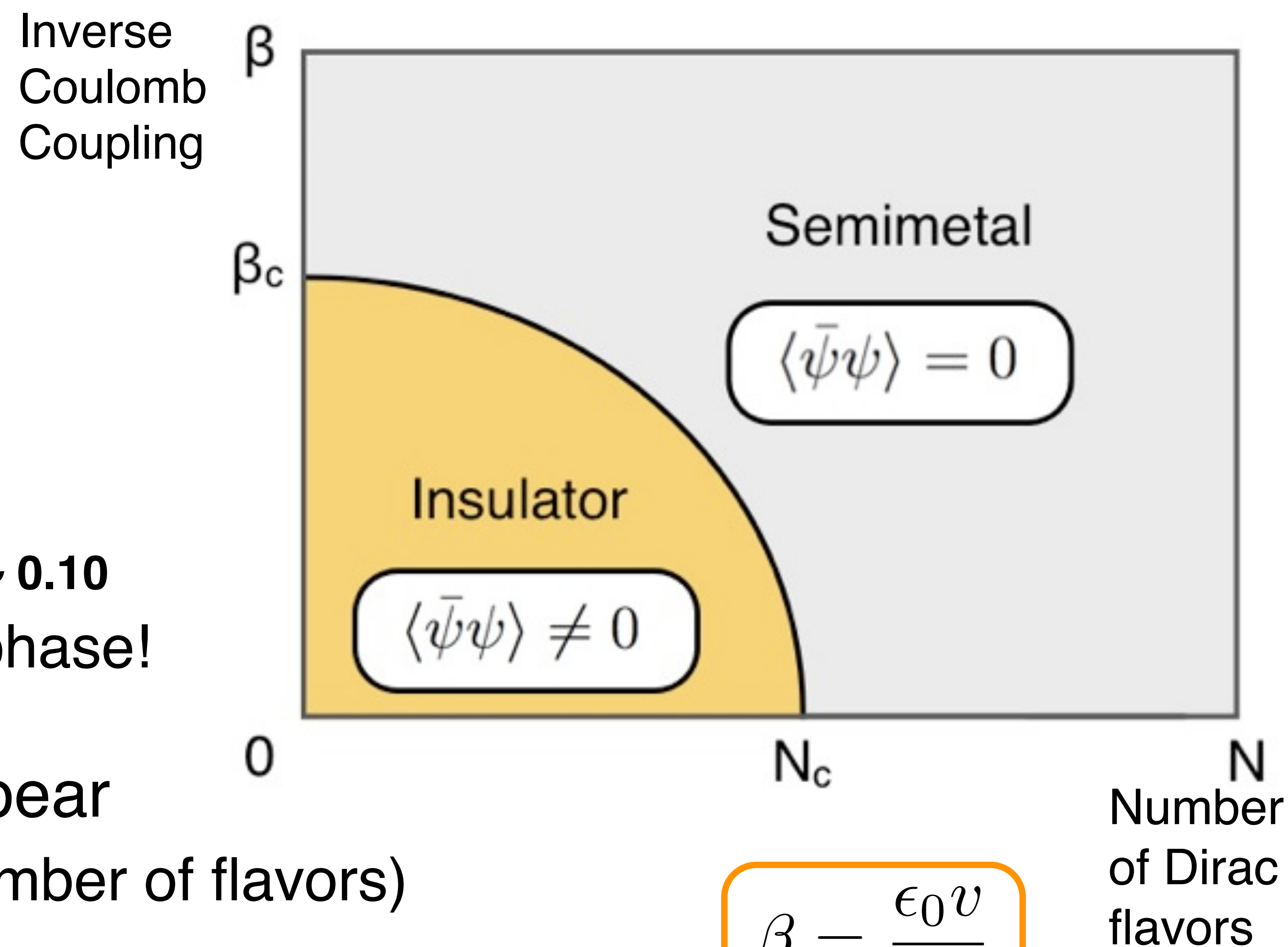


Can we say anything about this?

Is there an excitonic gap?

- If there is a gapped phase...
  - ... it should disappear at large enough β (weak coupling limit)

    Graphene on SiO_2: **β ~ 0.10** is in the semimetallic phase!
  - ... and it should disappear at large enough N (number of flavors)



$$\beta = \frac{\epsilon_0 v}{e^2}$$

Is there a gapped phase at small enough N or β ?

If so, what are the values of N_c and β_c?

Is there an excitonic gap?

- What is the value of N_c ?

  D.V Khveschenko, H. Leal,
  Nucl. Phys. 687, 323 (2004);
  E.V. Gorbar *et al.*,
  Phys. Rev. B 66, 045108 (2002).

  $N_c \sim 2.6$

  S. Hands, C. Strouthos,
  Phys. Rev. B 78, 165423 (2008).

  $N_c = 4.8(2)$

- What is the value of β_c ?

  E.V. Gorbar *et al.*,
  Phys. Rev. B 66 045108 (2002).

  $\beta_c \sim 0.03$

  D.V. Khveschenko,
  Phys. Rev. Lett. 87, 246802 (2001).

  $\beta_c \sim 0.06$

- How to answer these questions?

→ Lattice Monte Carlo simulations
of the low-energy theory of graphene!

Low-energy action (in detail)

$$S_E = -\int dt\, d^2x\, \left(\bar{\psi}_a \gamma^0 \partial_0 \psi_a + v \bar{\psi}_a \gamma^i \partial_i \psi_a + i A_0 \bar{\psi}_a \gamma^0 \psi_a\right)$$

- Fermion sector (Low-energy electrons)
  - 2 Dirac flavors (i.e. two 4-component spinors)

Fermi velocity

$$v \simeq c/300$$

Low-energy action (in detail)

$$S_E = -\int dt\, d^2x\, \left(\bar{\psi}_a \gamma^0 \partial_0 \psi_a + v \bar{\psi}_a \gamma^i \partial_i \psi_a + i A_0 \bar{\psi}_a \gamma^0 \psi_a\right) + \frac{1}{2g^2} \int dt\, d^3x (\partial_i A_0)^2$$

- Fermion sector (Low-energy electrons)
  - 2 Dirac flavors (i.e. two 4-component spinors)
- Gauge sector (Coulomb interaction)
  - Only one component: A_0 living in 3+1 d
  - Fine structure constant

$$\alpha_{gr} = \frac{e^2}{4\pi\epsilon_0 v} \simeq 300\alpha \sim 1$$

Fermi velocity

$$v \simeq c/300$$

Inverse Coulomb coupling

$$\beta = \frac{\epsilon_0 v}{e^2}$$

Strongly coupled!

Lattice theory

- Discrete action $S_E = S_E^f + S_E^g$

$$S_E^f[\bar{\chi}, \chi, U] = -\sum_{\mathbf{n},\mathbf{m}} \bar{\chi}(\mathbf{n}) D_s[U, \mathbf{n}, \mathbf{m}] \chi(\mathbf{m})$$

Chiral symmetry breaking parameter (mass)

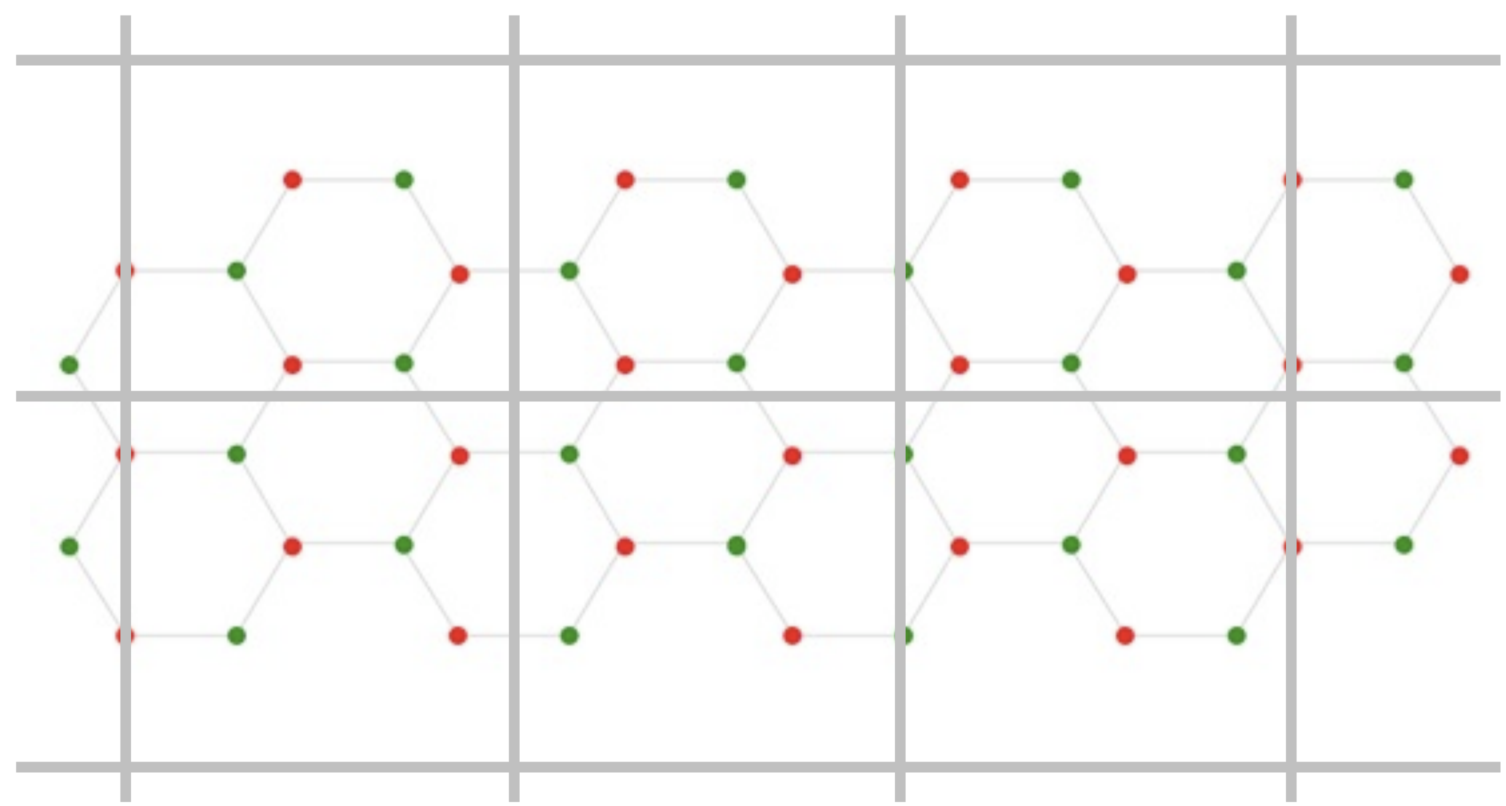
$$D_s[U, \mathbf{n}, \mathbf{m}] = \frac{1}{2}(\delta_{\mathbf{n}+\mathbf{e}_0,\mathbf{m}} U(\mathbf{n}) - \delta_{\mathbf{n}-\mathbf{e}_0,\mathbf{m}} U^\dagger(\mathbf{m})) + \frac{v}{2}\sum_i \eta^i(\mathbf{n})(\delta_{\mathbf{n}+\mathbf{e}_i,\mathbf{m}} - \delta_{\mathbf{n}-\mathbf{e}_i,\mathbf{m}}) + m_0 \delta_{\mathbf{n},\mathbf{m}}$$

$$S_E^g[\theta] = \frac{\beta}{2}\sum_{\mathbf{n}}\sum_{i=1}^{3}[\theta(\mathbf{n}) - \theta(\mathbf{n}+\mathbf{e}_i)]^2$$

Exactly 8 dof, **no rooting needed!**

$$U(\mathbf{n}) = \exp\{i\theta(\mathbf{n})\}$$

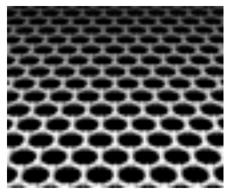
$$\begin{aligned} \eta^0(\mathbf{n}) &= 1 \\ \eta^1(\mathbf{n}) &= (-1)^{n_0} \\ \eta^2(\mathbf{n}) &= (-1)^{n_0+n_1} \end{aligned}$$



First results: Condensate

J. E. Drut and T. A. Lähde,
Phys. Rev. Lett **102**, 026802 (2009)

- $N_f = 2$



  Possible transition below $\beta \sim 0.10$

- $N_f = 4$

  Possible transition below $\beta \sim 0.05$

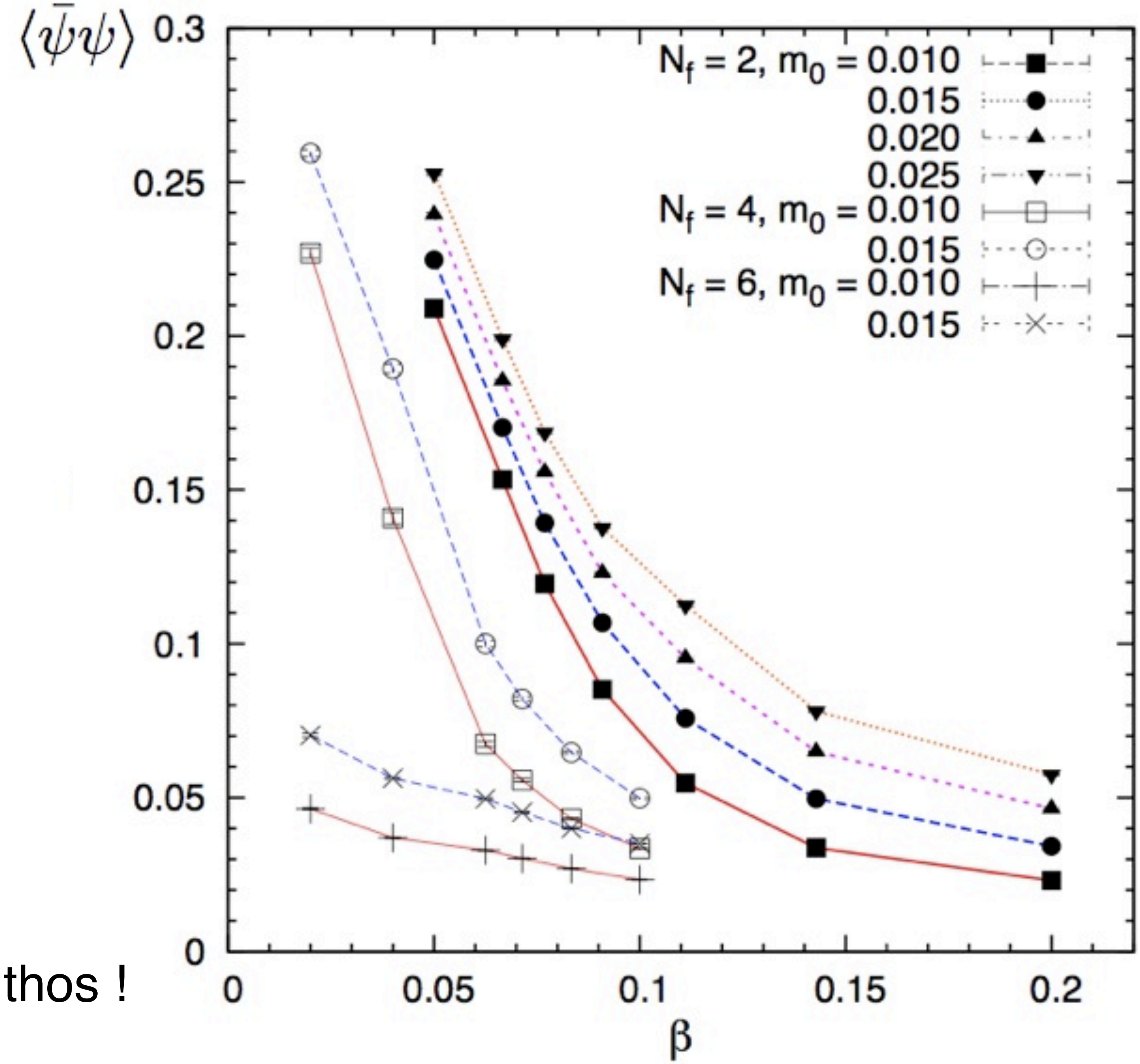
- $N_f = 6$

  No transition ?!

→ $4 < N_c < 6$

Agrees with Hands & Strouthos !

$N_c = 4.8(2)$



Logarithmic derivative R

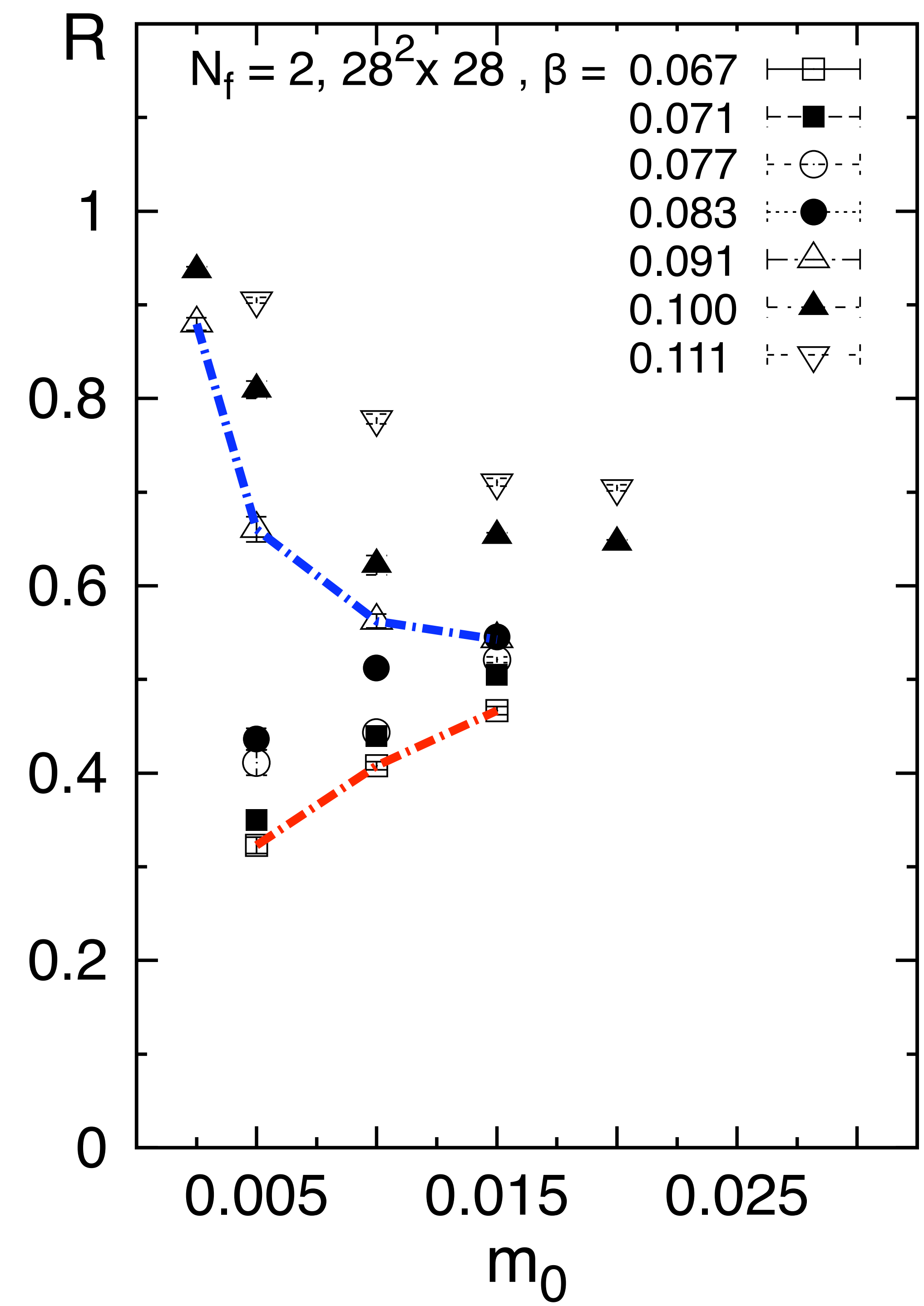
$$R = \frac{m_0}{\langle\bar{\psi}\psi\rangle}\chi_{\bar{\psi}\psi}$$

Gapless: $\langle\bar{\psi}\psi\rangle \sim m_0$ → $R \to 1$

Critical: $\langle\bar{\psi}\psi\rangle \sim m_0^{1/\delta}$ → $R \to 1/\delta$

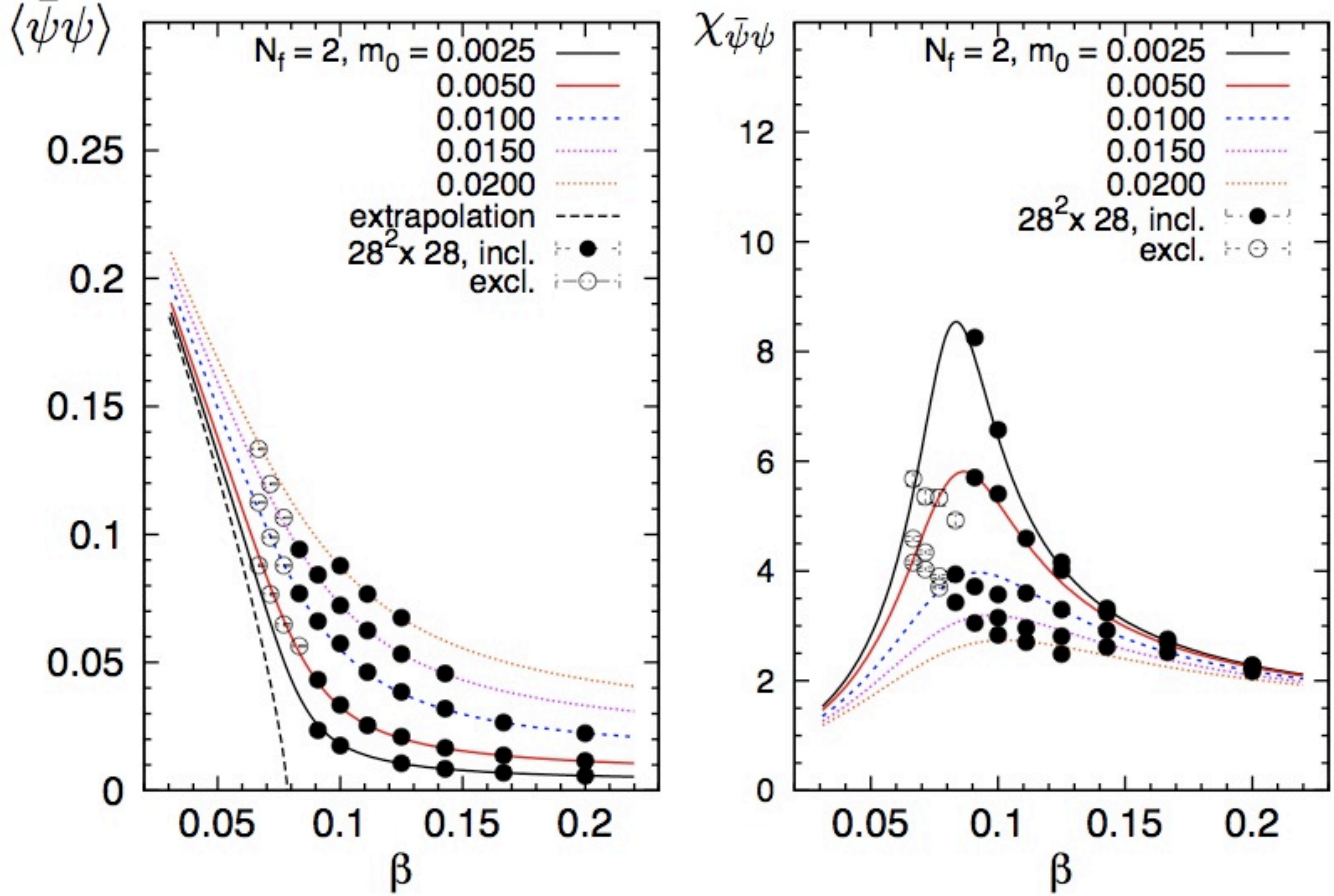
Gapped: $\langle\bar{\psi}\psi\rangle \to const.$ → $R \to 0$

→ $0.071 < \beta_c < 0.091$



J. E. Drut and T. A. Lähde,
Phys. Rev. Lett **102**, 026802 (2009)
Phys. Rev. B **79**, 165425 (2009)

EOS extrapolation



J. E. Drut and T. A. Lähde,
Phys. Rev. Lett **102**, 026802 (2009)
Phys. Rev. B **79**, 165425 (2009)

$$m_0 A(\beta) = B_0(\beta - \beta_c)\sigma^b + \sigma^\delta$$

$$A(\beta) = A_0 + A_1(\beta - \beta_c) \qquad \sigma = \langle\bar{\psi}\psi\rangle$$

Summary

- Critical coupling for chiral symmetry breaking in graphene

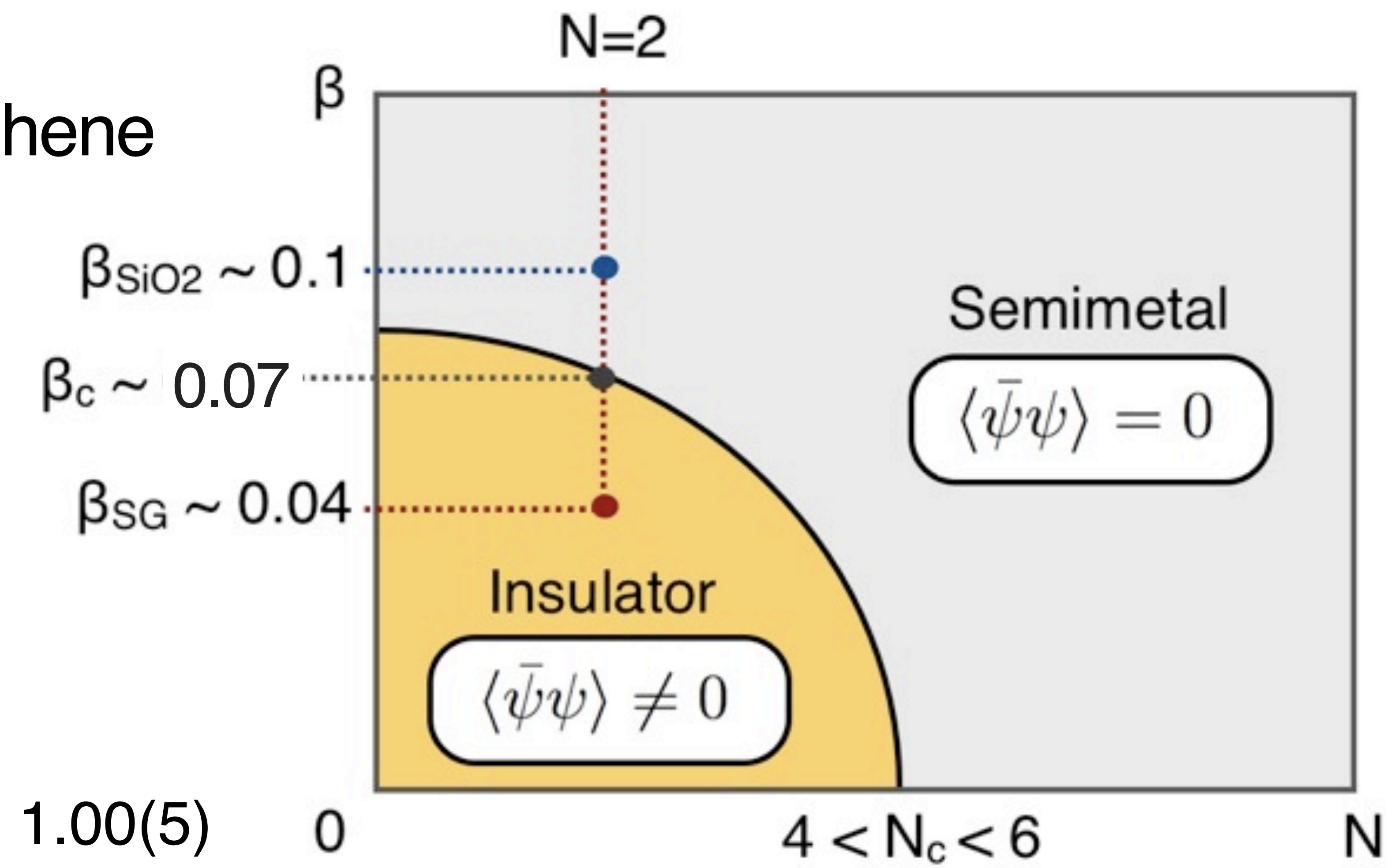
$$\beta_c = 0.073 \pm 0.002$$

- Critical number of flavors

$$4 < N_c < 6$$

- Critical exponents

$\delta \cong 2.26(6)$ $\beta_m \cong 0.78(5)$ $\gamma \cong 1.00(5)$



- Is **suspended** graphene in the gapped phase?
    - Velocity renormalization?
    - Magnitude of the gap?

J. E. Drut and T. A. Lähde,
Phys. Rev. Lett **102**, 026802 (2009)
Phys. Rev. B **79**, 165425 (2009)

J. E. Drut, T. A. Lähde, L. J. Suoranta
arXiv:1002.1273

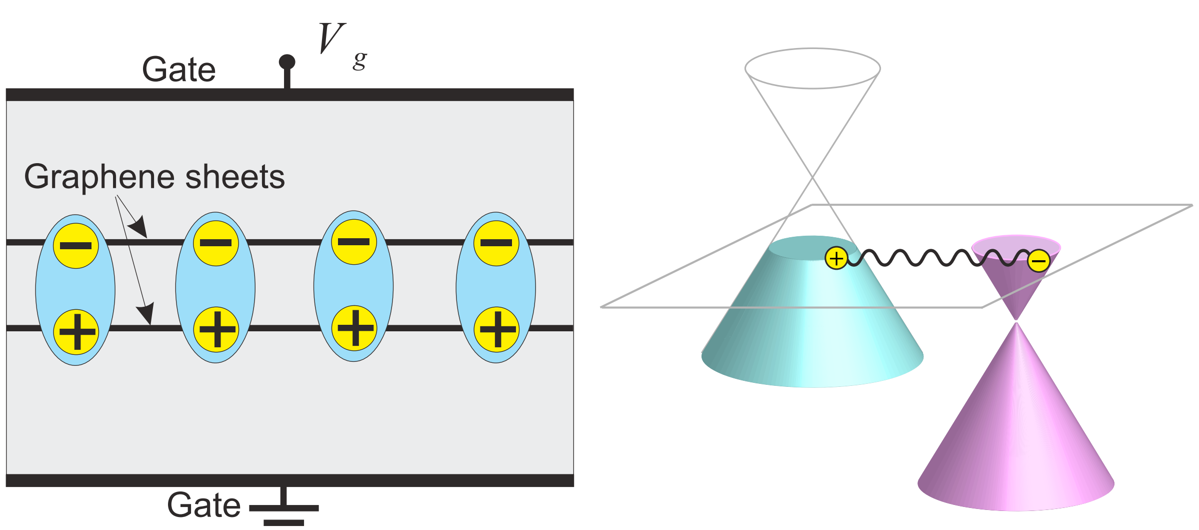
Recent and in-progress work

- What is the nature of the transition?
  - Infinite order (Miransky scaling)? ✘
  - Second order ? ✔
- What happens as a function of N_f ? ✔

Phys. Rev. B **79**, 165425 (2009)

Phys. Rev. B **79** , 241405(R) (2009)

- Velocity renormalization
  (with T. A. Lähde and L. J. Suoranta)
- Magnitude of the gap
  (with T. A. Lähde and E. Tölö)
- Improved actions
  (with T. A. Lähde and L. J. Suoranta)
- Exciton condensation in bilayers
  (with T. A. Lähde and A. H. MacDonald)



from Kharitonov & Efetov,
Phys. Rev. B **78**, 241401R (2008)

To be continued...

Thanks!!!