EFT for Graphene's Many-Body Problem

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INT Program
Effective Field Theories and
the Many-Body Problem
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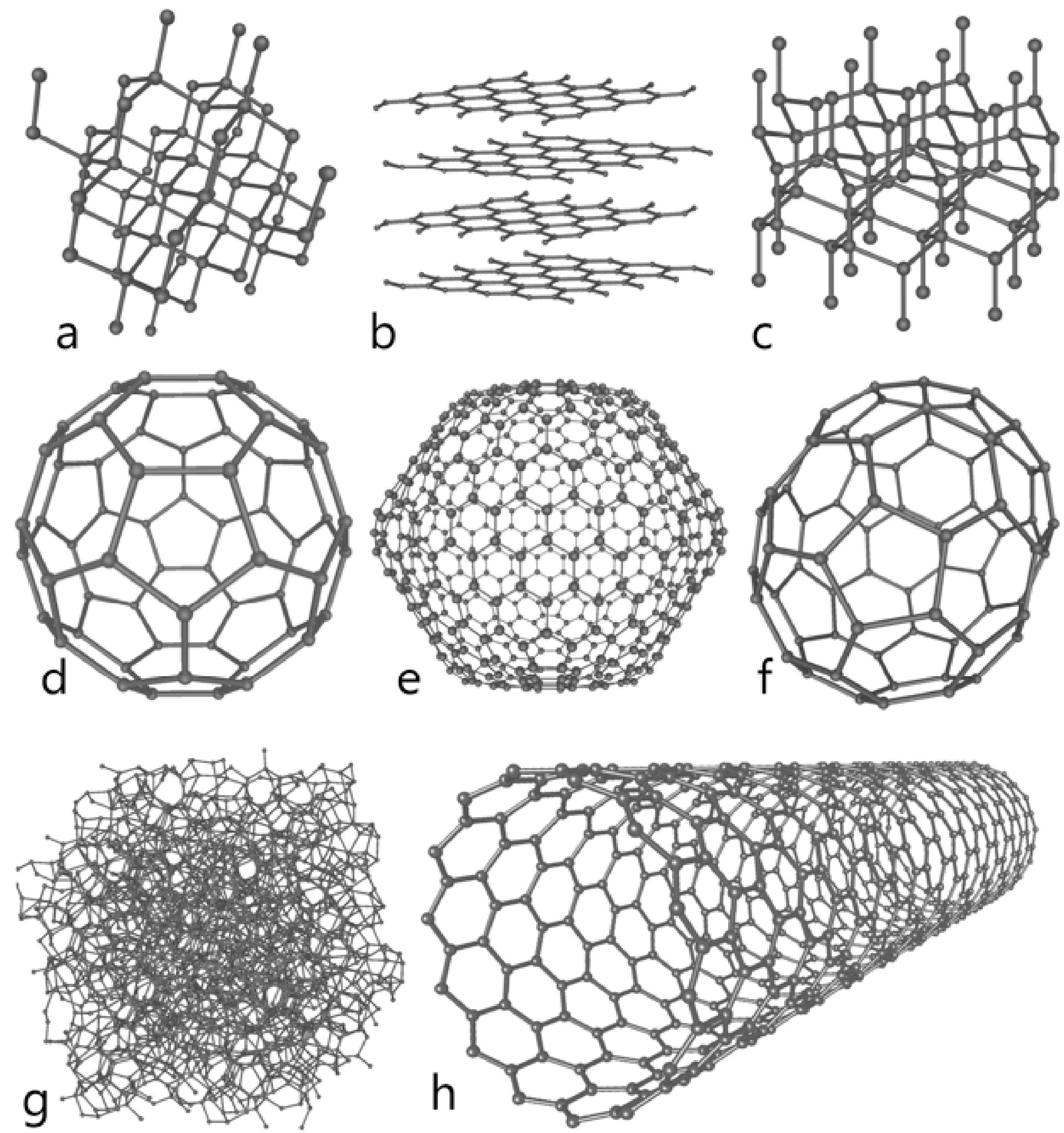
Outline

- What is graphene?
- What makes it interesting?
- Low-energy effective theory
- Graphene on the lattice
- Spontaneous chiral symmetry breaking
- Work in progress

What is graphene?

- An allotrope of C



source: Wikipedia

What is graphene?

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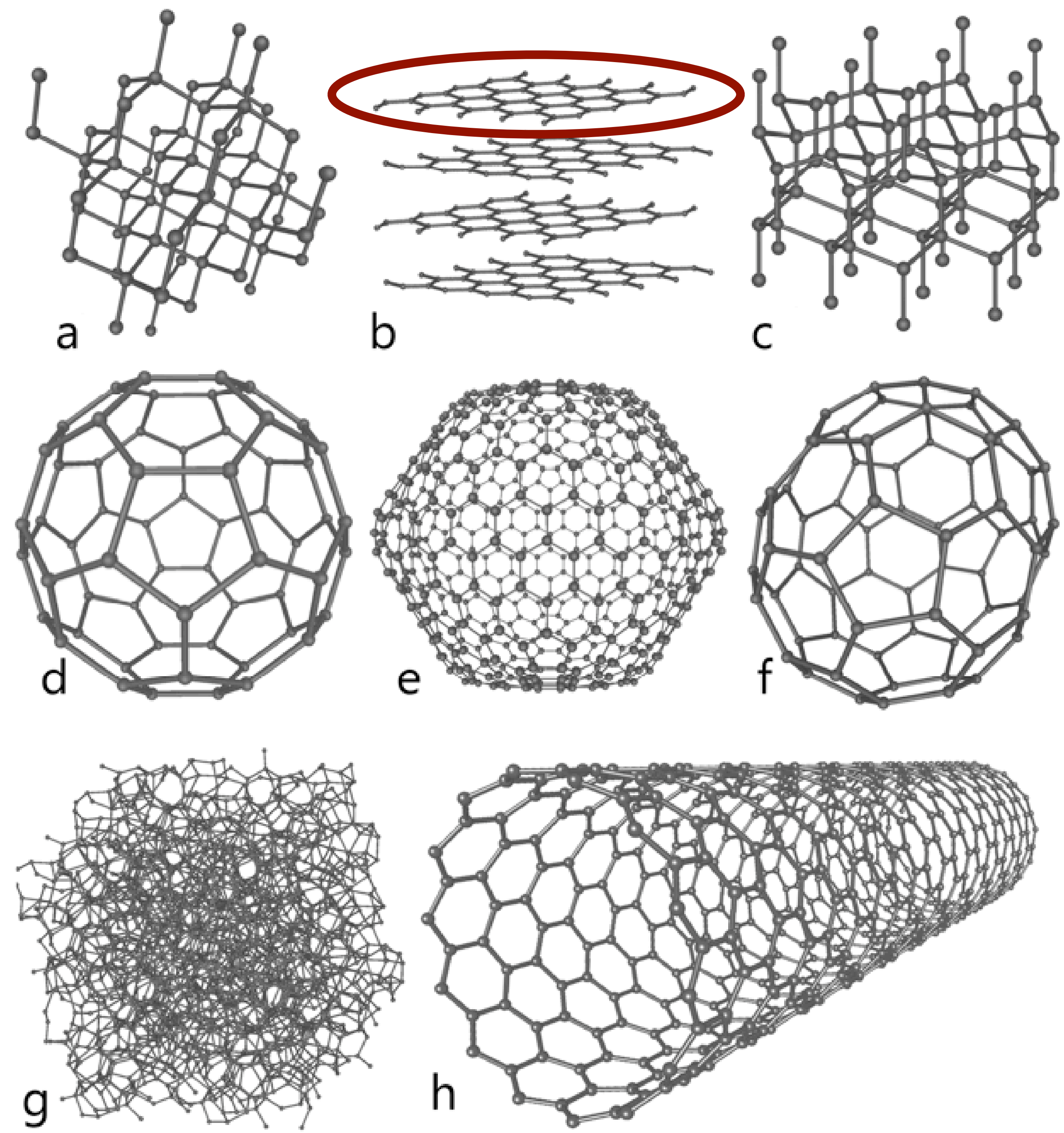


source: Wikipedia

What is graphene?

- An allotrope of C
- 2D honeycomb lattice
  - Orbital hybridization

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

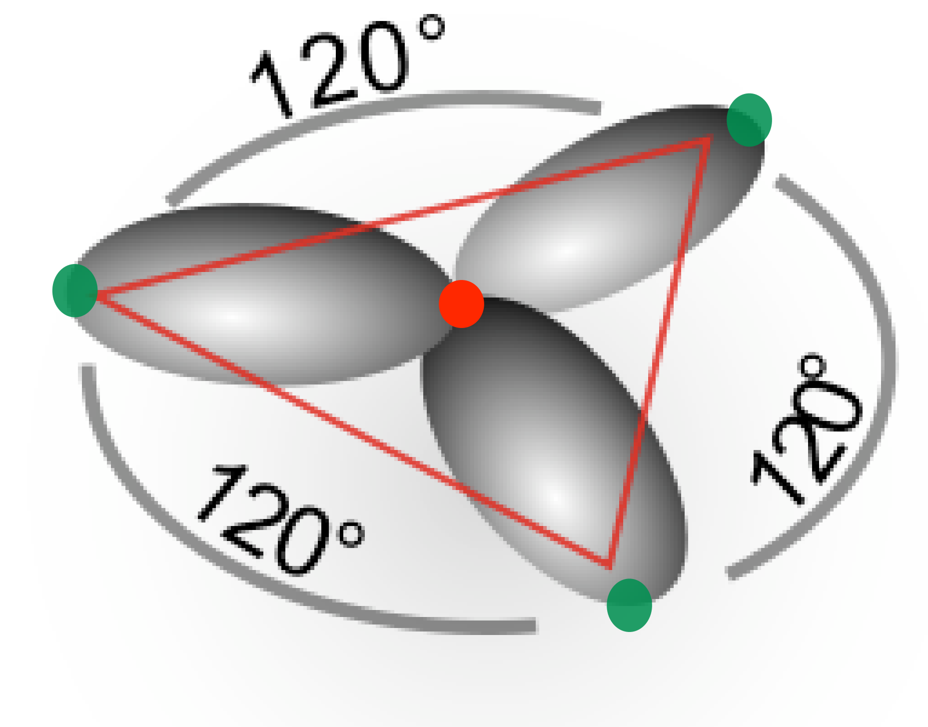
↓

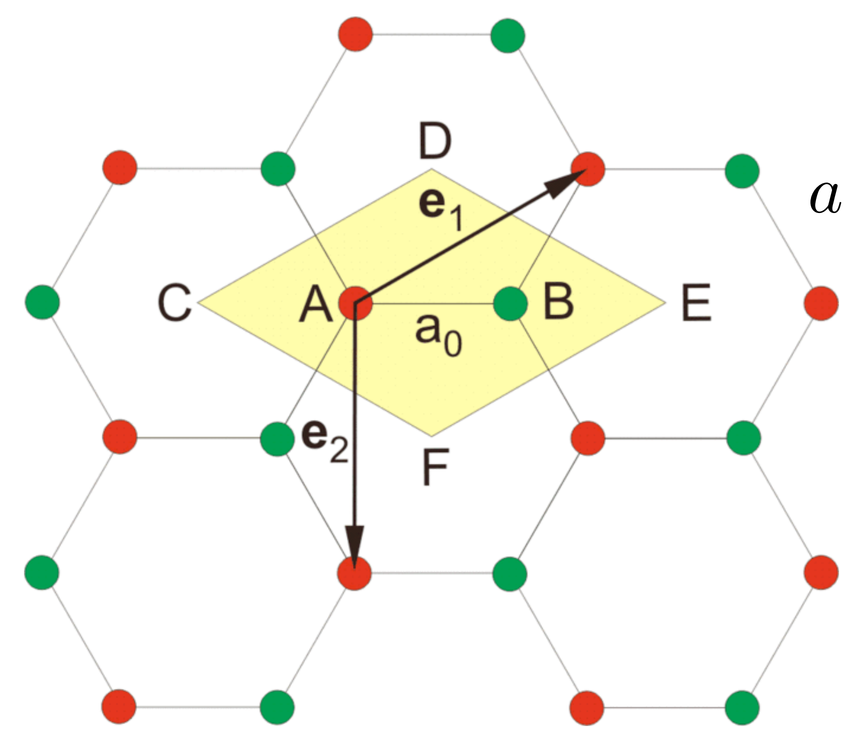
$3\ sp^2 + p$

↓ lattice (σ band)

↓ electron on lattice (π band)

  - Two triangular sublattices A, B





$a = 1.42\text{Å}$

How do we study graphene?

- We could start from...

$$\sum_i \frac{p_i^2}{2m} + \sum_{i<j} V_{ee}(\mathbf{r}_i - \mathbf{r}_j) + \sum_I \frac{p_I^2}{2M} + \sum_{I<J} V_{ii}(\mathbf{R}_I - \mathbf{R}_J) + \sum_{iI} V_{ei}(\mathbf{R}_I - \mathbf{r}_i)$$

...but this is:
- Very hard !
- Unnecessarily general !

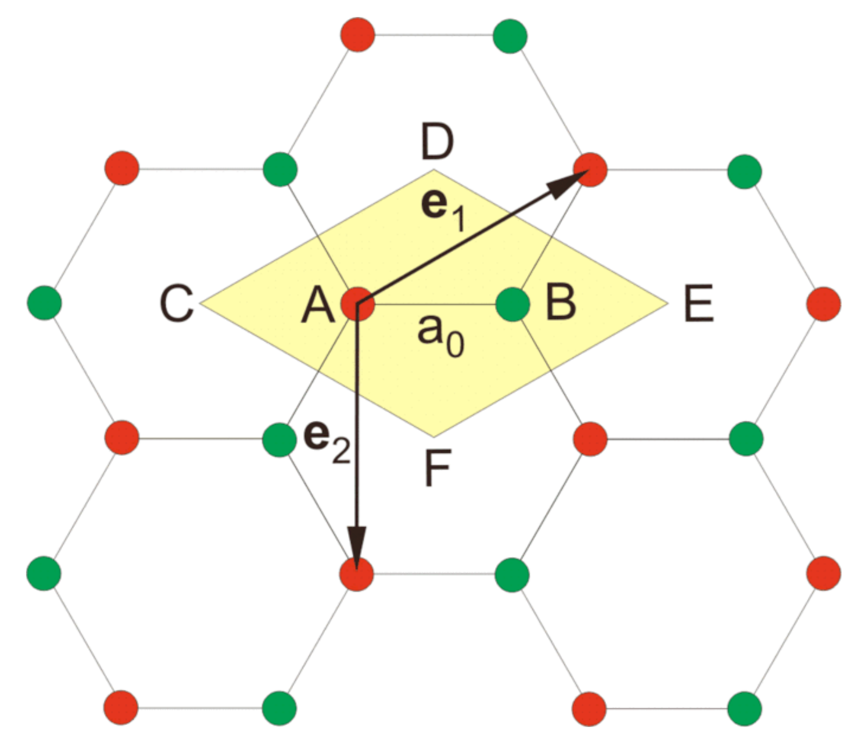
- The EFT approach:
  - Identify the energy scales relevant for the questions you want to answer
  - Identify the relevant degrees of freedom and the associated symmetries

Band structure

- Tight-binding hamiltonian for the honeycomb lattice

$$H = -t \sum_{\langle i,j\rangle,\sigma} (a^{\dagger}_{\sigma,i} b_{\sigma,j} + \text{H.c.}) - t' \sum_{\langle\langle i,j\rangle\rangle,\sigma} (a^{\dagger}_{\sigma,i} a_{\sigma,j} + b^{\dagger}_{\sigma,i} b_{\sigma,j} + \text{H.c.})$$

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



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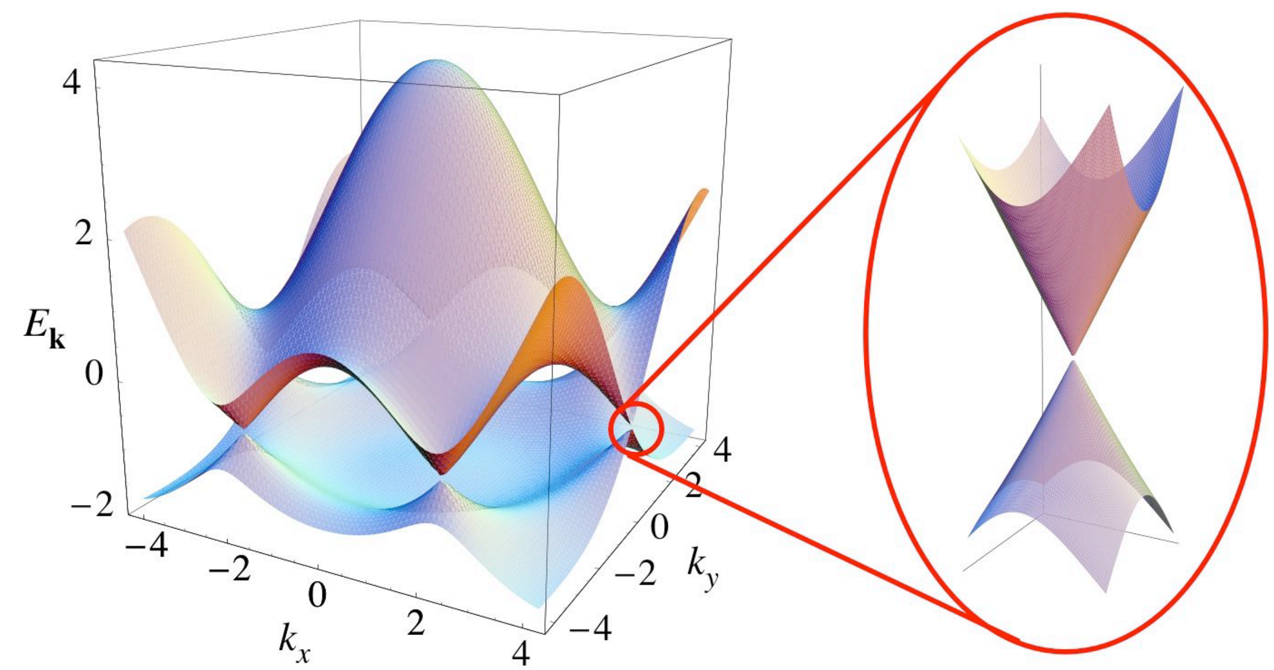

source: talk by A. H. Castro Neto

- At low energies...
  - Two Dirac points K, K'

$$E(\mathbf{q}) \simeq v|\mathbf{q}| \qquad v = \frac{3ta}{2} \simeq c/300$$

  - Electronic spin ↑↓

Low-energy effective degrees of freedom → N=2 flavors of 4-component Dirac fermions in (2+1)d

Low-energy effective theory

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

Fermion sector (a.k.a. electrons)

- 2 Dirac flavors (i.e. two 4-component spinors)

Gauge sector (a.k.a. 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!!!

Symmetries and scales (or lack thereof)

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

- Lorentz symmetry (2 + 1) d → Explicitly broken by the Coulomb field
  ↓
  Velocity renormalization

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- Lorentz symmetry (2 + 1) d → Explicitly broken by the Coulomb field ↓ Velocity renormalization

- Chiral symmetry

$$\psi_a(x) \rightarrow e^{-i\vec{\Gamma}\cdot\vec{\Theta}} \psi_a(x)$$

$$\Gamma_i = \{\mathbb{1}, \sigma_1, \sigma_2, \sigma_3\} \times \gamma_\mu$$

U(4)

Symmetries and scales (or lack thereof)

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

- Lorentz symmetry (2 + 1) d → Explicitly broken by the Coulomb field ↓ Velocity renormalization
- Chiral symmetry → Can be spontaneously broken ↓ Chiral condensate

$$\psi_a(x) \to e^{-i\vec{\Gamma}\cdot\vec{\Theta}} \psi_a(x)$$

$$\Gamma_i = \{\mathbb{1}, \sigma_1, \sigma_2, \sigma_3\} \times \gamma_\mu$$

$$\langle \bar{\psi}_a(x) \psi_a(x) \rangle$$

U(4) → U(2) x U(2)

Symmetries and scales (or lack thereof)

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

- Lorentz symmetry (2 + 1) d → Explicitly broken by the Coulomb field ↓ Velocity renormalization
- Chiral symmetry → Can be spontaneously broken ↓ Chiral condensate
- Scales? Cutoff Λ → $\langle \bar{\psi}_a(x) \psi_a(x) \rangle$

What about higher order terms?

- Short-range interactions
  - ➡ Irrelevant according to large-N
- Relativistic corrections (e.g. B field interaction)
  - ➡ Supressed by powers of $v/c \simeq 1/300$
- Tight-binding...

$$E(\mathbf{q}) \simeq \pm v_F|\mathbf{q}| \left[1 \mp \frac{a|\mathbf{q}|}{4} \sin(3\theta_q)\right]$$

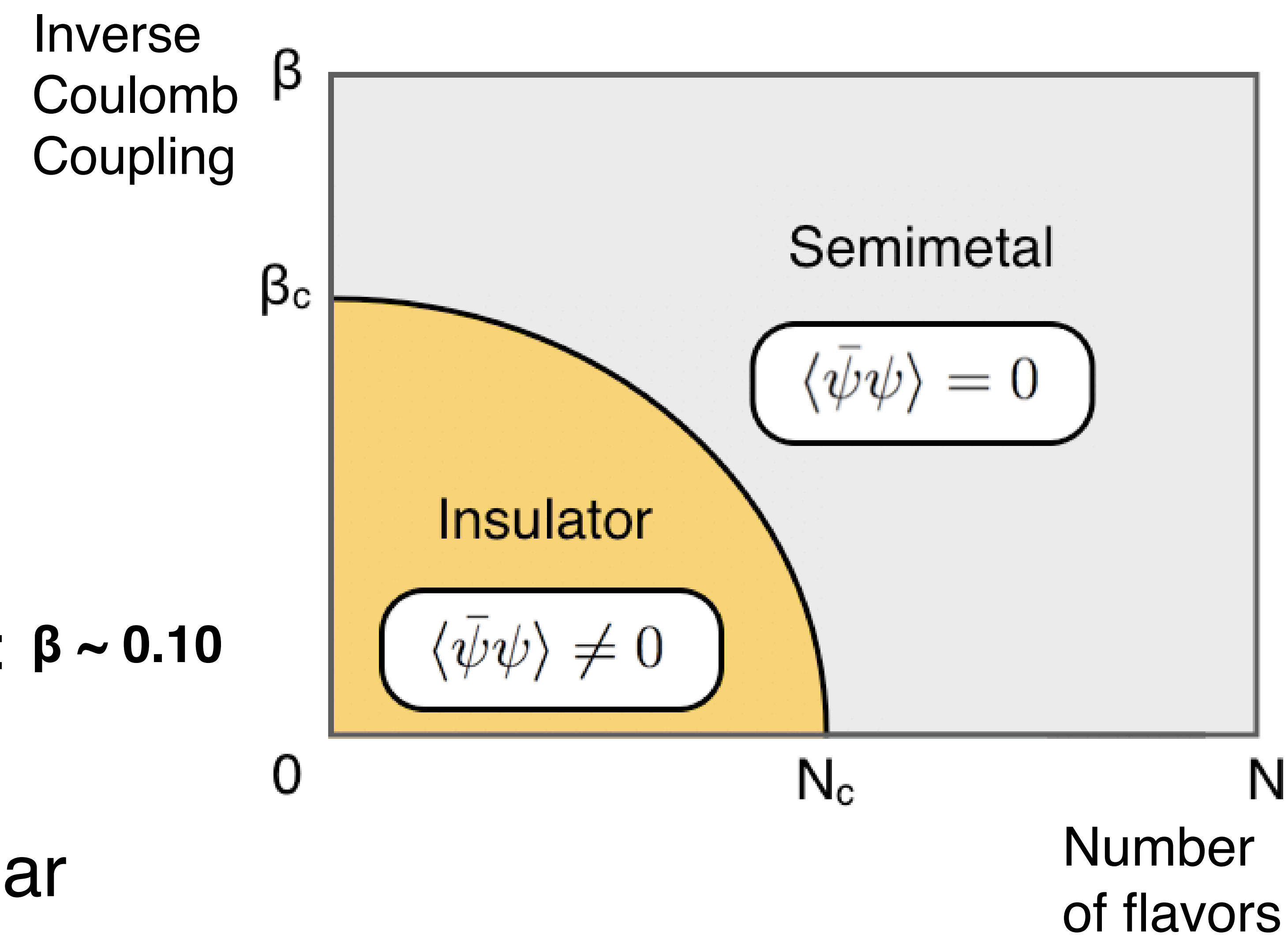
$$\theta_q = \arctan\left(\frac{q_x}{q_y}\right)$$

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 substrate: **β ~ 0.10** is in the semimetallic phase!

  - ... and it should disappear at large enough N (screening ~ N)



- 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).

  $\beta_c \sim 0.06$

Graphene on SiO_2 substrate: **$\beta \sim 0.10$** → Semimetal

suspended: **$\beta \sim 0.037$** → Gapped ?

- How to answer these questions?

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

- Staggered fermions
- Link variables
- Hybrid Monte Carlo

Lattice theory

- Lattice fermions & chiral symmetry
  - Nielsen-Ninomiya theorem

    H.B. Nielsen and M. Ninomiya, Nucl. Phys. B185, 20 (1981); Nucl. Phys. B193, 173 (1981).

    - Doubling problem ⟺ Chiral symmetry
  - One partial solution: staggered fermions

    L. Susskind, Phys.Rev. D16, 3031 (1977);
    H. Kluberg-Stern, Nucl. Phys. B220, 447 (1983).

    - Surviving symmetry: U(1) x U(1)

      C. Burden and A.N. Burkitt, Eur. Phys. Lett. 3, 545 (1987).

    - Breaks to U(1) via $\langle\bar{\psi}\psi\rangle$

Lattice theory

- Discrete action

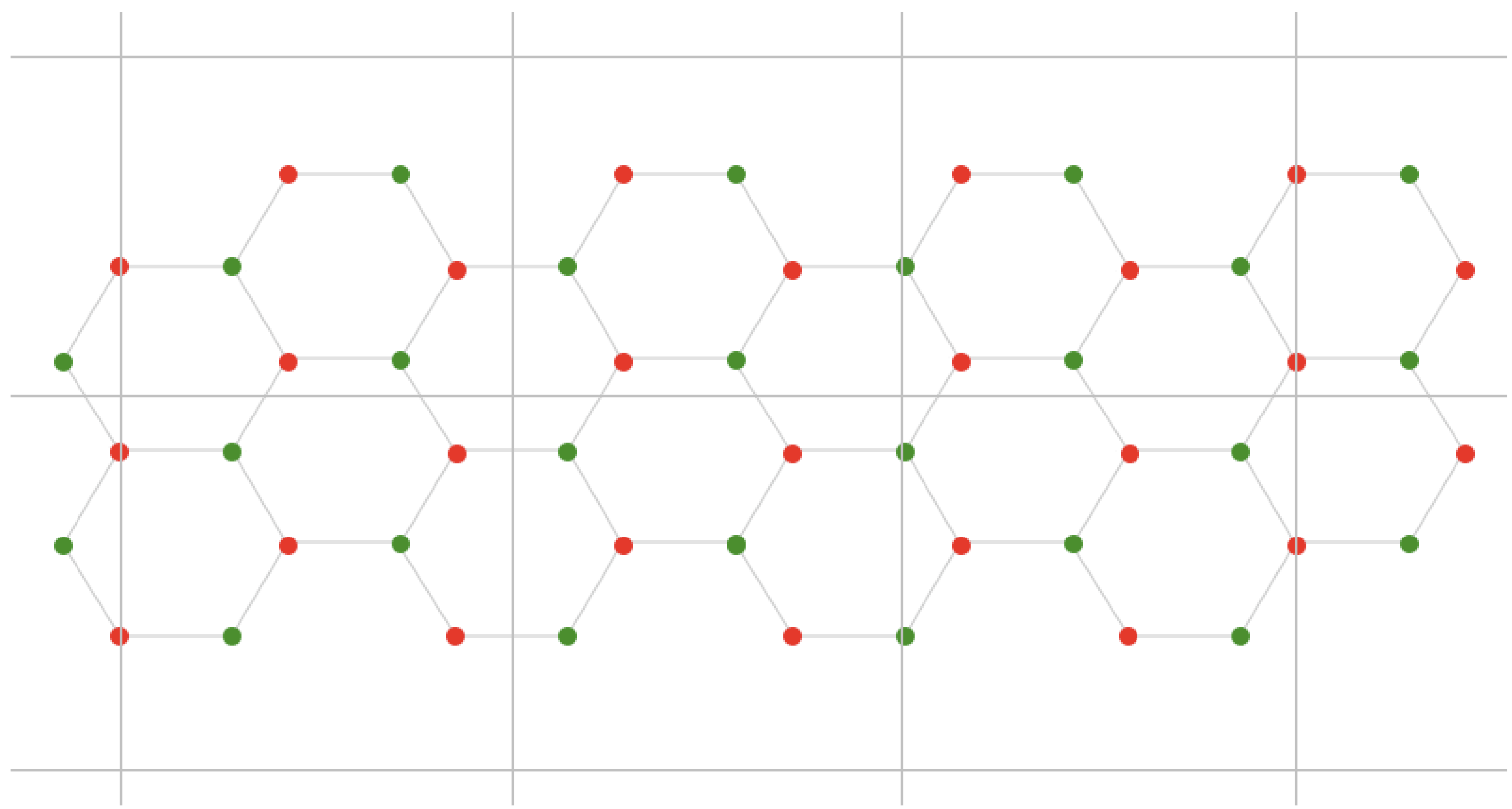
$$S_E^f[\bar{\chi},\chi,U] = -\sum_{\mathbf{n},\mathbf{m}} \bar{\chi}(\mathbf{n}) D_s[U,\mathbf{n},\mathbf{m}]\chi(\mathbf{m})$$

Chiral symmetry breaking parameter (mass)

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

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

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



Lattice theory

- Partition function

$$\mathcal{Z} = \int \mathcal{D}A_0 \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-S_E[\bar{\psi}_a, \psi_a, A_0]} = \int \mathcal{D}A_0 e^{-S_E^g[A_0]} (\det[D[A_0]])^{N_f}$$

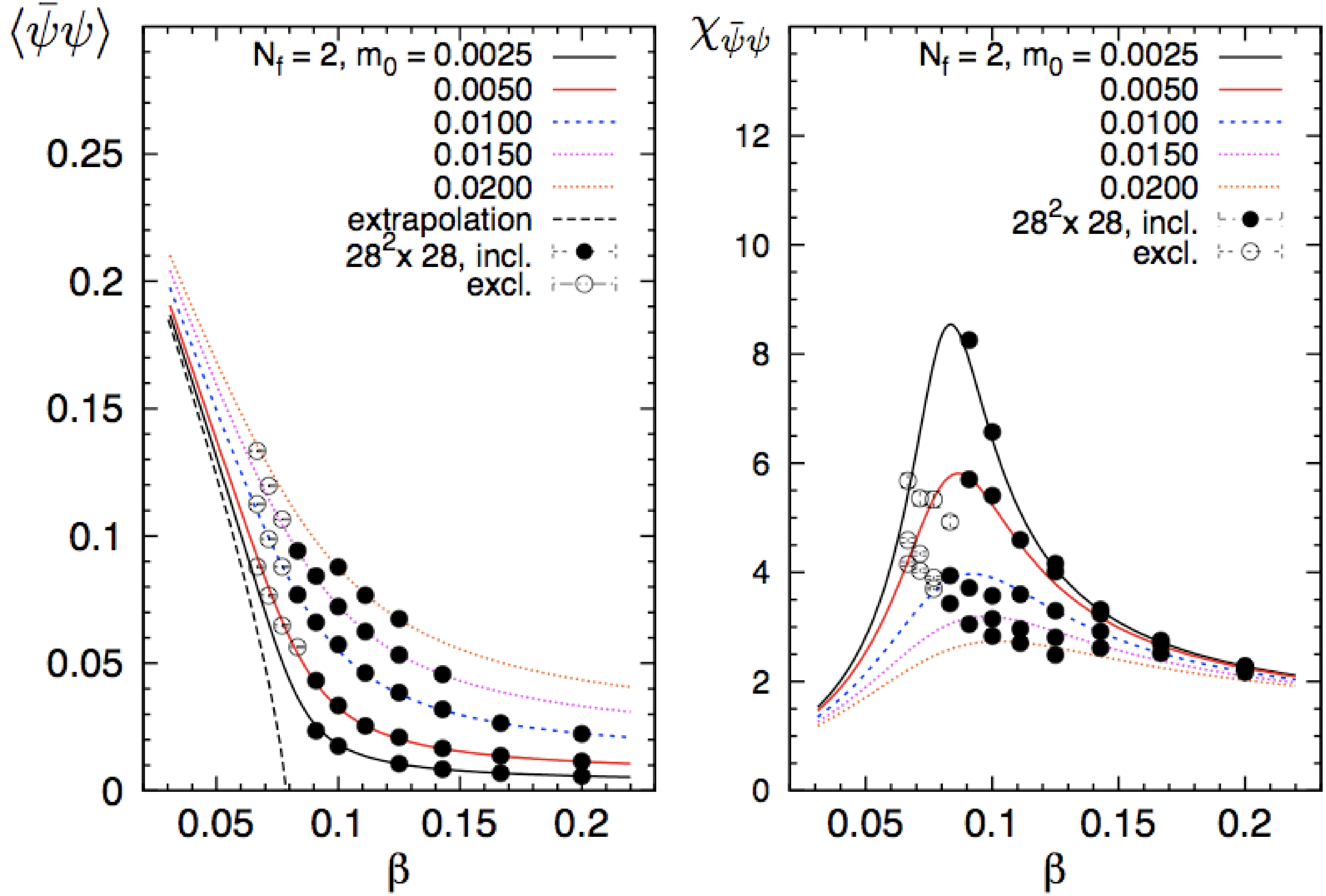
- Condensate & Susceptibility

$$\langle \bar{\psi}_b \psi_b \rangle = \frac{1}{V} \langle \mathrm{Tr}\left[D^{-1}[A_0] \right] \rangle$$

$$\chi_{\bar{\psi}\psi} = \frac{1}{V} \left[\langle \mathrm{Tr}^2 \left[D^{-1} \right] \rangle - \langle \mathrm{Tr}\left[D^{-2} \right] \rangle - \langle \mathrm{Tr}\left[D^{-1} \right] \rangle^2 \right]$$

- Monte-Carlo strategy
    - Metropolis Monte Carlo
    - Hybrid Monte Carlo

Condensate & susceptibility



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

Logarithmic derivative R

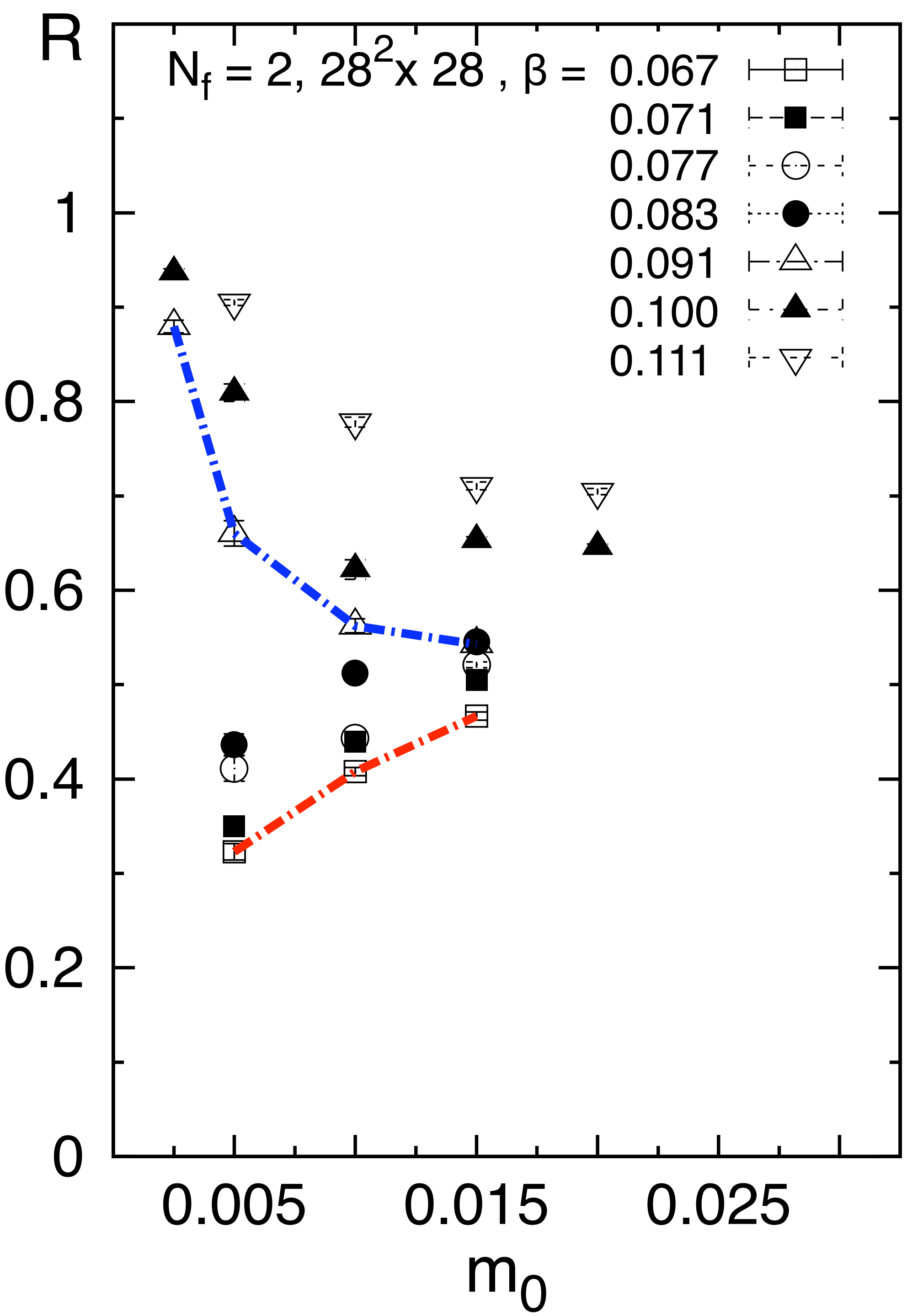
$$R = \frac{m_0}{\langle \bar{\psi}\psi \rangle} \chi_{\bar{\psi}\psi}$$

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

→ $0.071 < \beta_c < 0.091$



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Conclusions

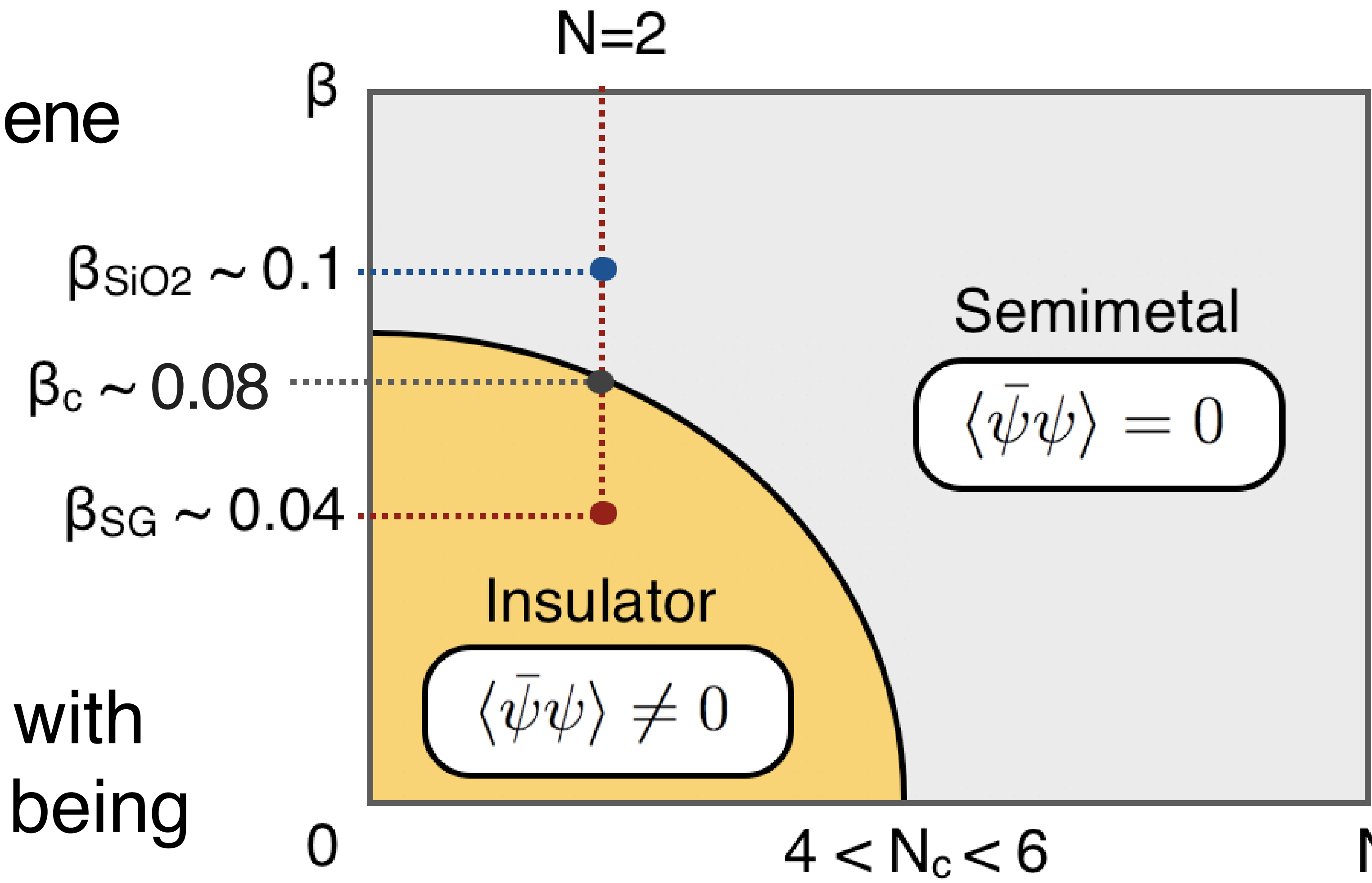
- Critical coupling for chiral symmetry breaking in graphene

$$\beta_c = 0.075 \pm 0.005$$

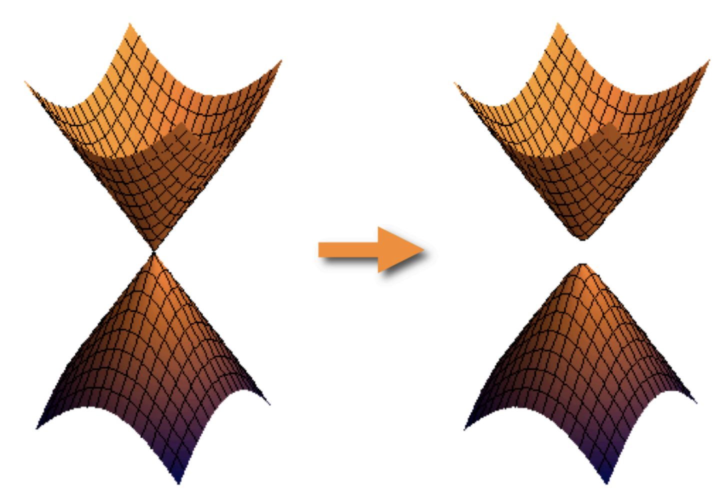
- Critical number of flavors

$$4 < N_c < 6$$

- Our results are consistent with graphene **on a substrate** being a semimetal.



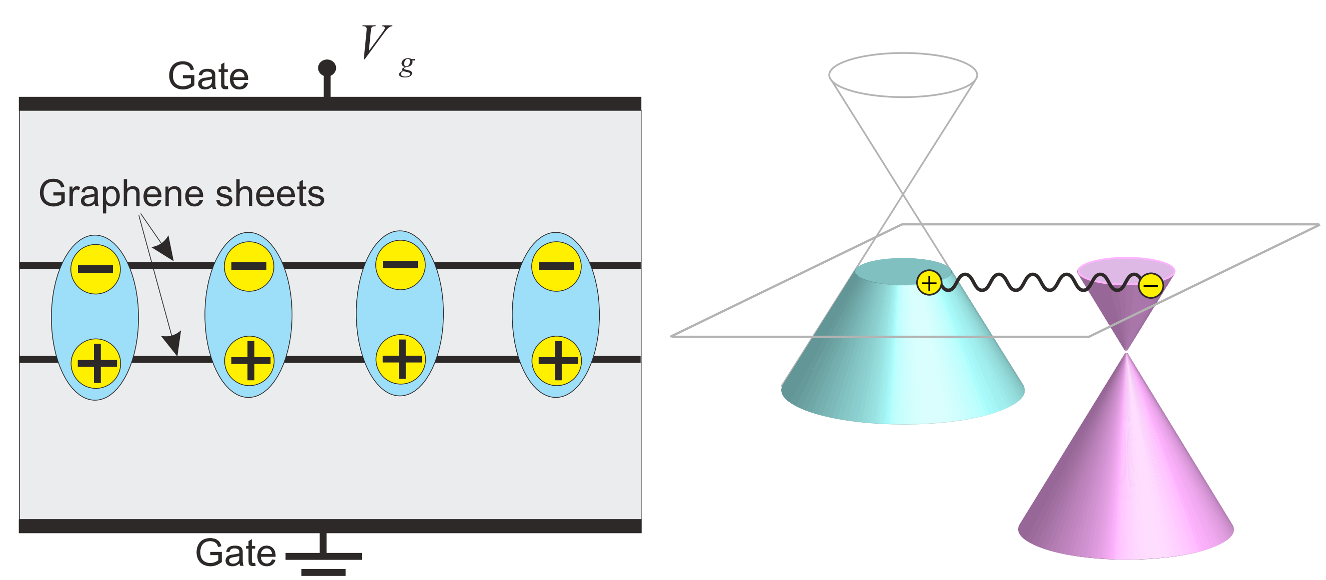
- Is **suspended** graphene an insulator?
  - Velocity renormalization?
  - Magnitude of the gap?



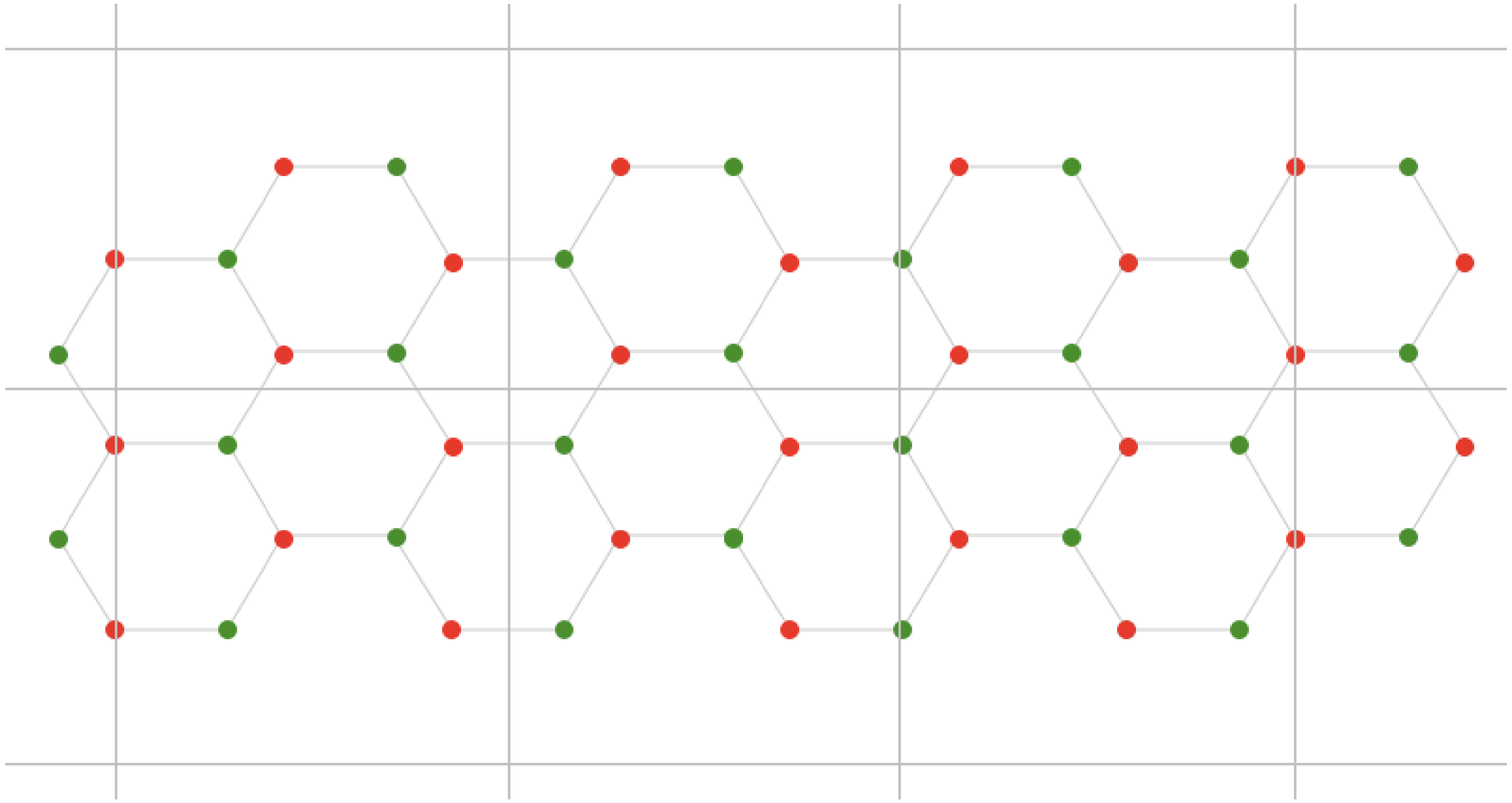
Semimetal (weak coupling) **Insulator (strong coupling)**

Work in progress...

- What is the true nature of the transition?
    - Infinite order (Miransky scaling)? ✘
    - Second order ? ✔
- What is the gap?
- Calculation of the conductivity
- Exciton condensation in bilayers



from Kharitonov & Efetov, arXiv [0808.2164]



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