From the honeycomb lattice to the square lattice: a new look at graphene

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Simulations and Symmetries:
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in collaboration with:
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Lauri Suoranta (Aalto U.)

- **Graphene phenomenology**

  Origin of the semimetallic band structure ...

- **Graphene at low energies**

  Does a gap form due to Coulomb interactions?

- **Lattice Monte Carlo simulation**

  From the honeycomb to the square lattice ...

- **Results**

  Is suspended graphene an insulator?

- **Lattice artifacts**

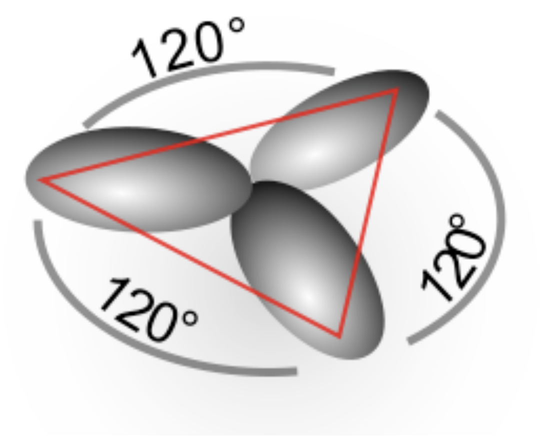
  Are the simulation results realistic?

- **Future projects**

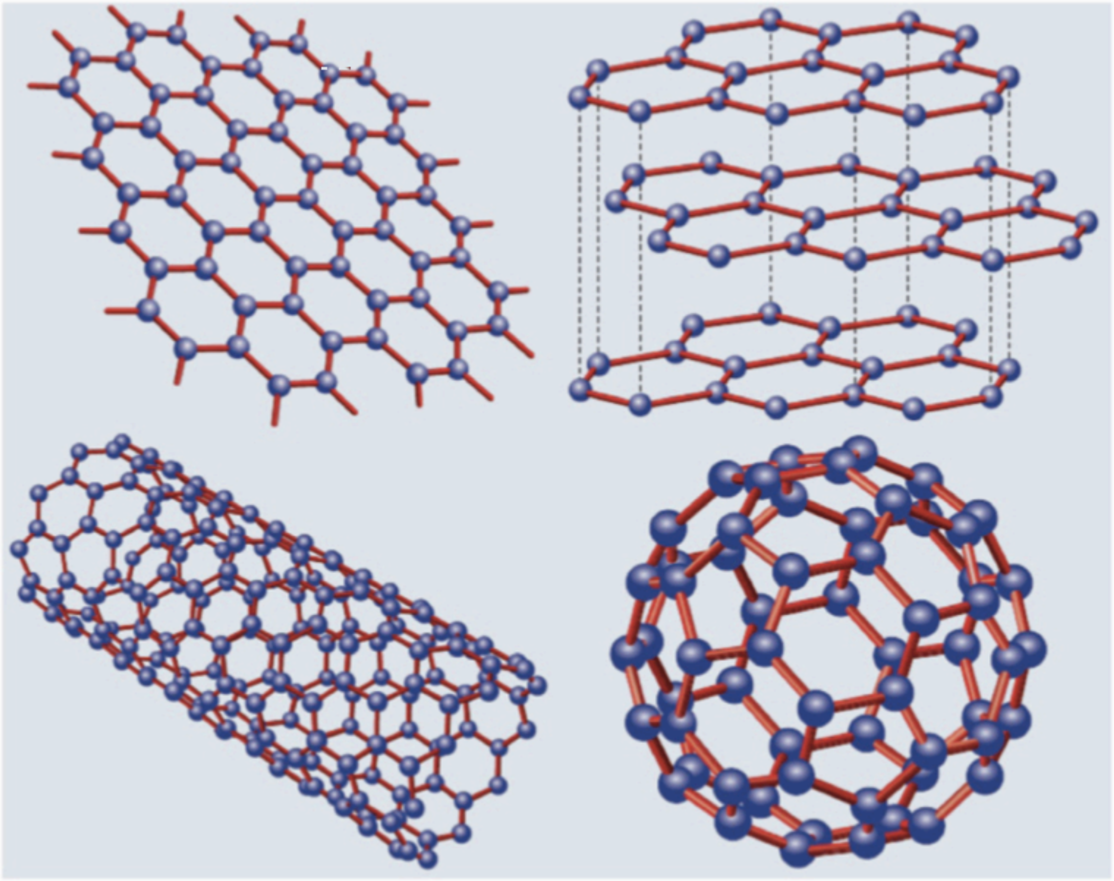
  Where to go from here?

Graphene phenomenology I:
what is graphene?

- Carbon atoms form strong covalent bonds ...



graphene
single graphite layer



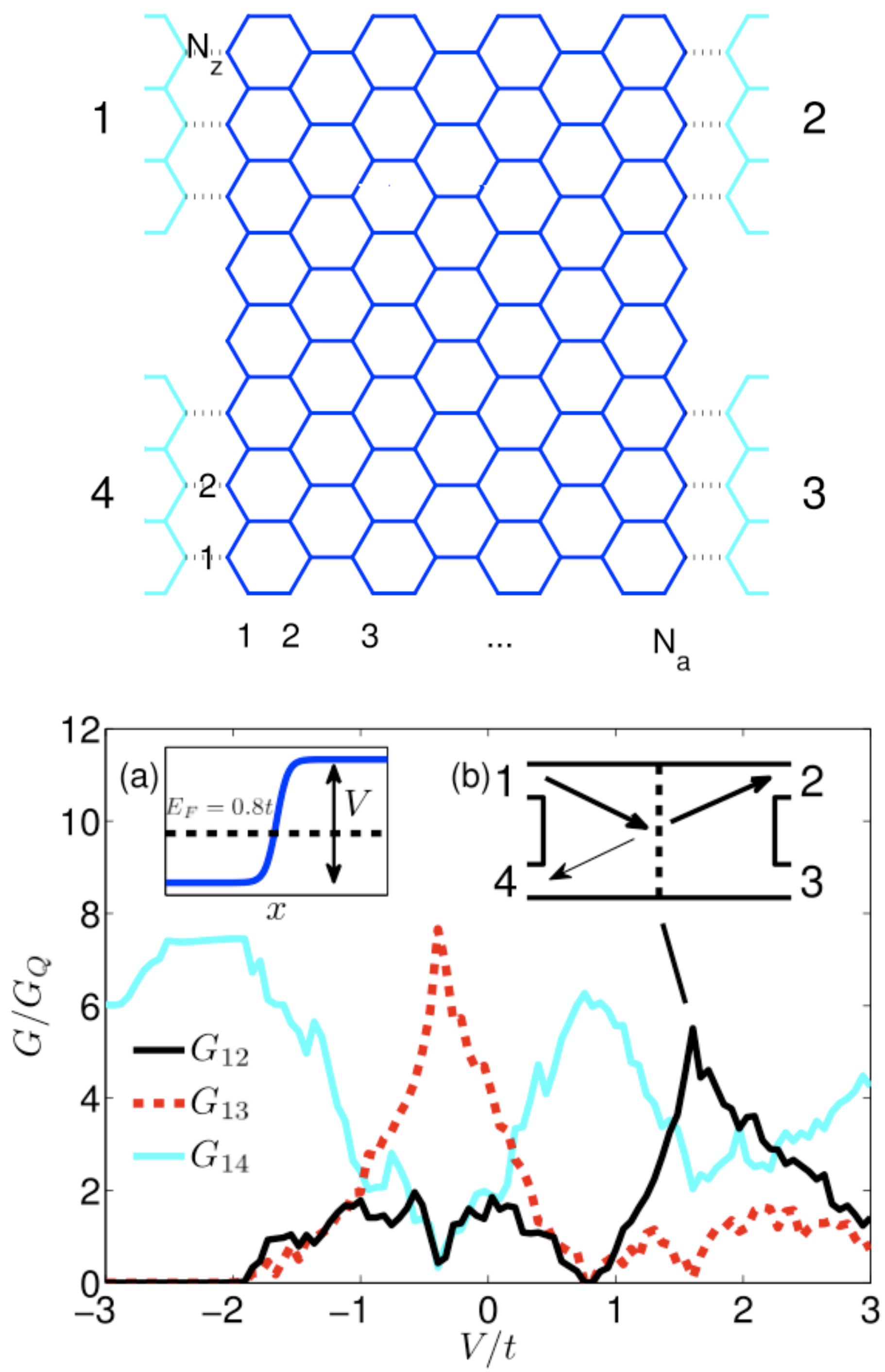
graphite
stacked graphene

nanotube
rolled graphene

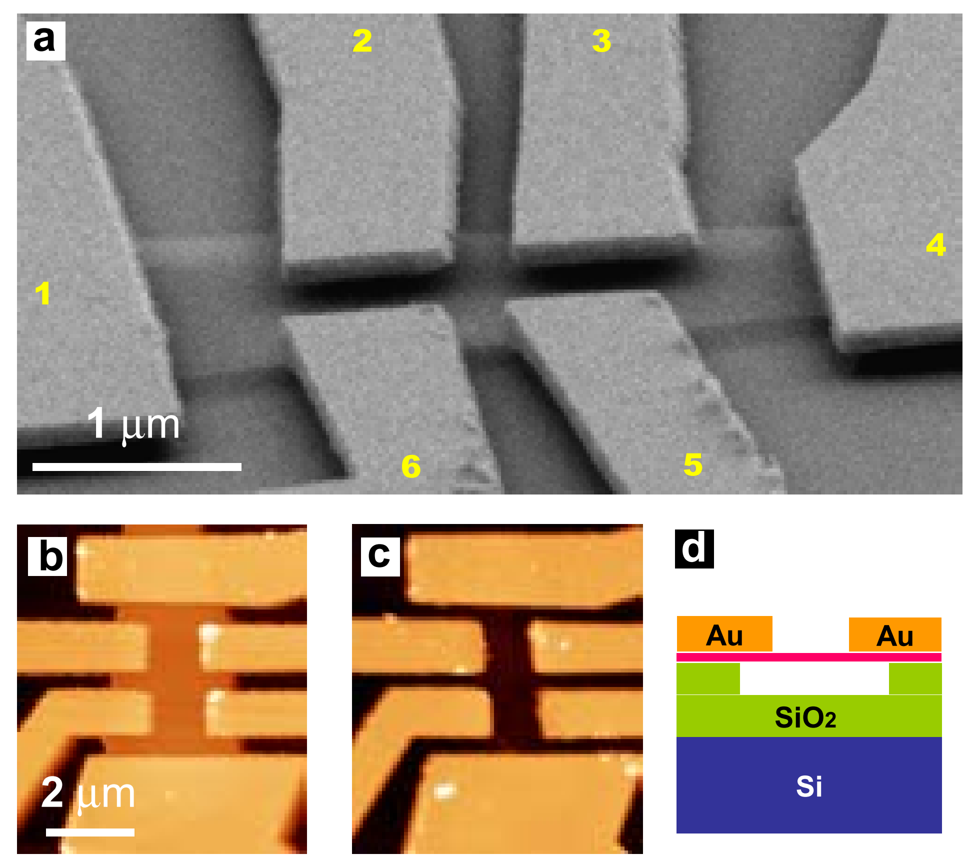
fullerene
wrapped graphene

Graphene phenomenology II:
a promising material for applied physics …

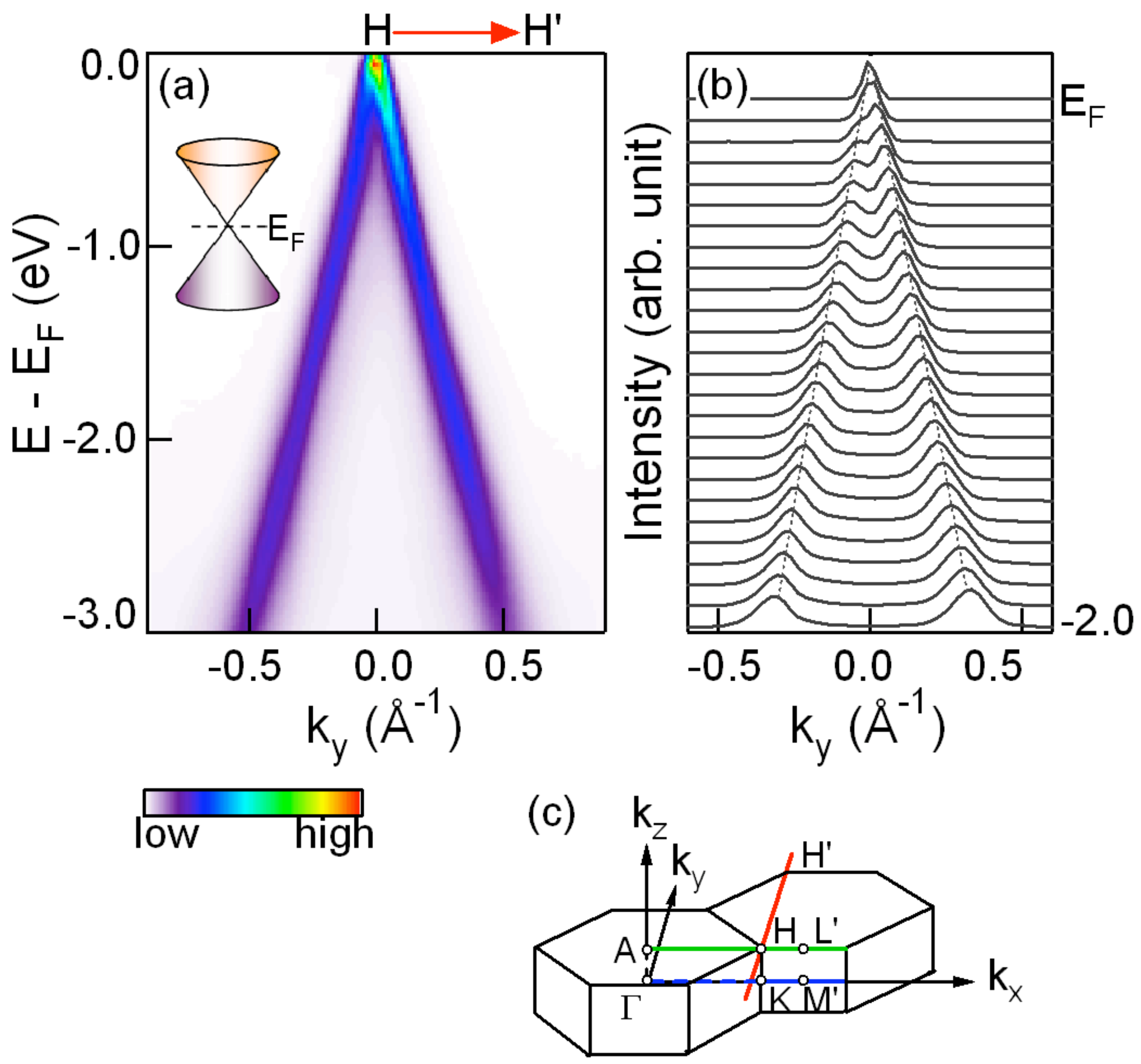
- Graphene-based gate-controlled current switch …
  K. Sääskilahti, A. Harju, P. Pasanen, Appl. Phys. Lett. 95, 092104 (2009).



- Suspended graphene devices …
  K.I. Bolotin et al., Phys. Rev. Lett. 101, 096802 (2008),
  V. Crespi, Physics 1, 15 (2008).

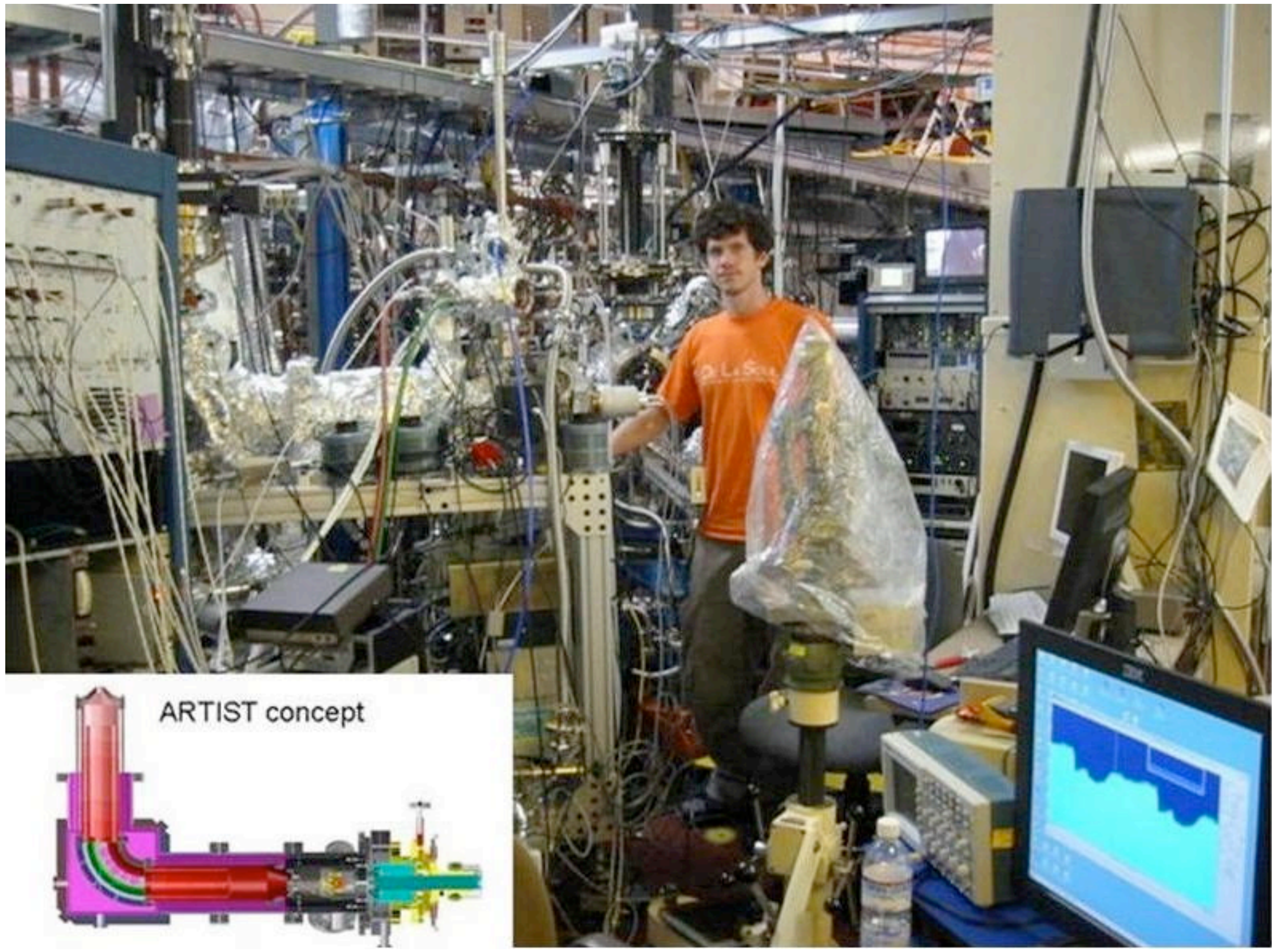


Graphene phenomenology III:
... and for fundamental physics as well!



- Ultrarelativistic (Dirac) dispersion relation in a non-relativistic system ...

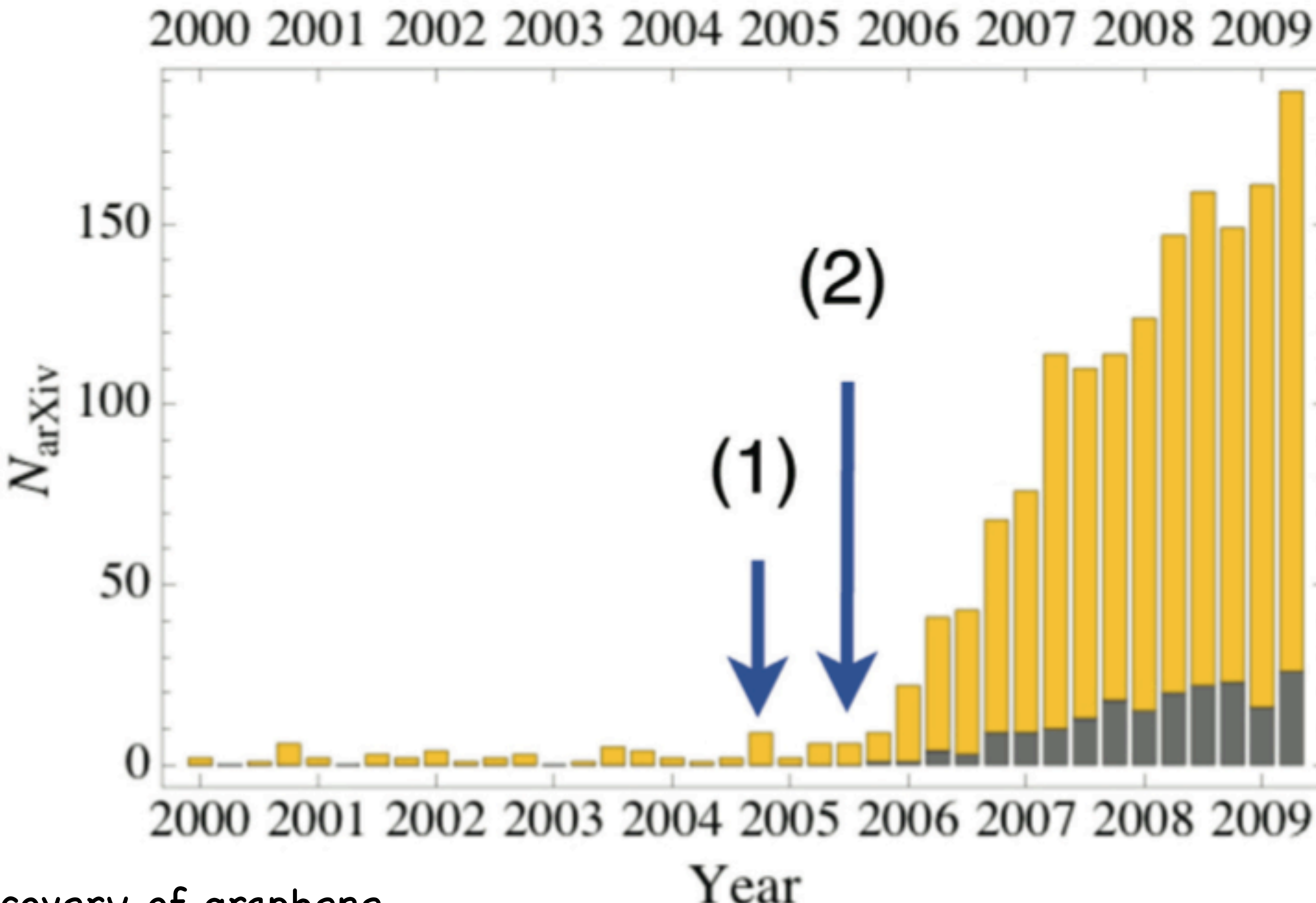
Pictures: Lanzara research group, UC Berkeley



- Direct study of the electronic dispersion relation in graphene and related materials via ARPES ...

Graphene phenomenology IV:
not surprisingly, a very active field of study ...

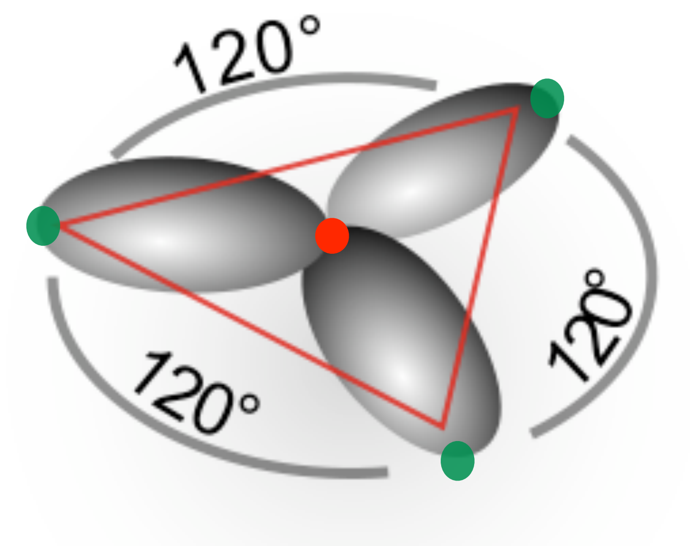
- Quarterly # of publications on graphene (yellow) and bilayer graphene (grey) on arXiv ...



(1) - discovery of graphene
(2) - discovery of the QHE in graphene

Graphene phenomenology V:
a closer look at the physics ...

- Hybridized electron orbitals form a hexagonal "honeycomb" lattice ...



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

⇩

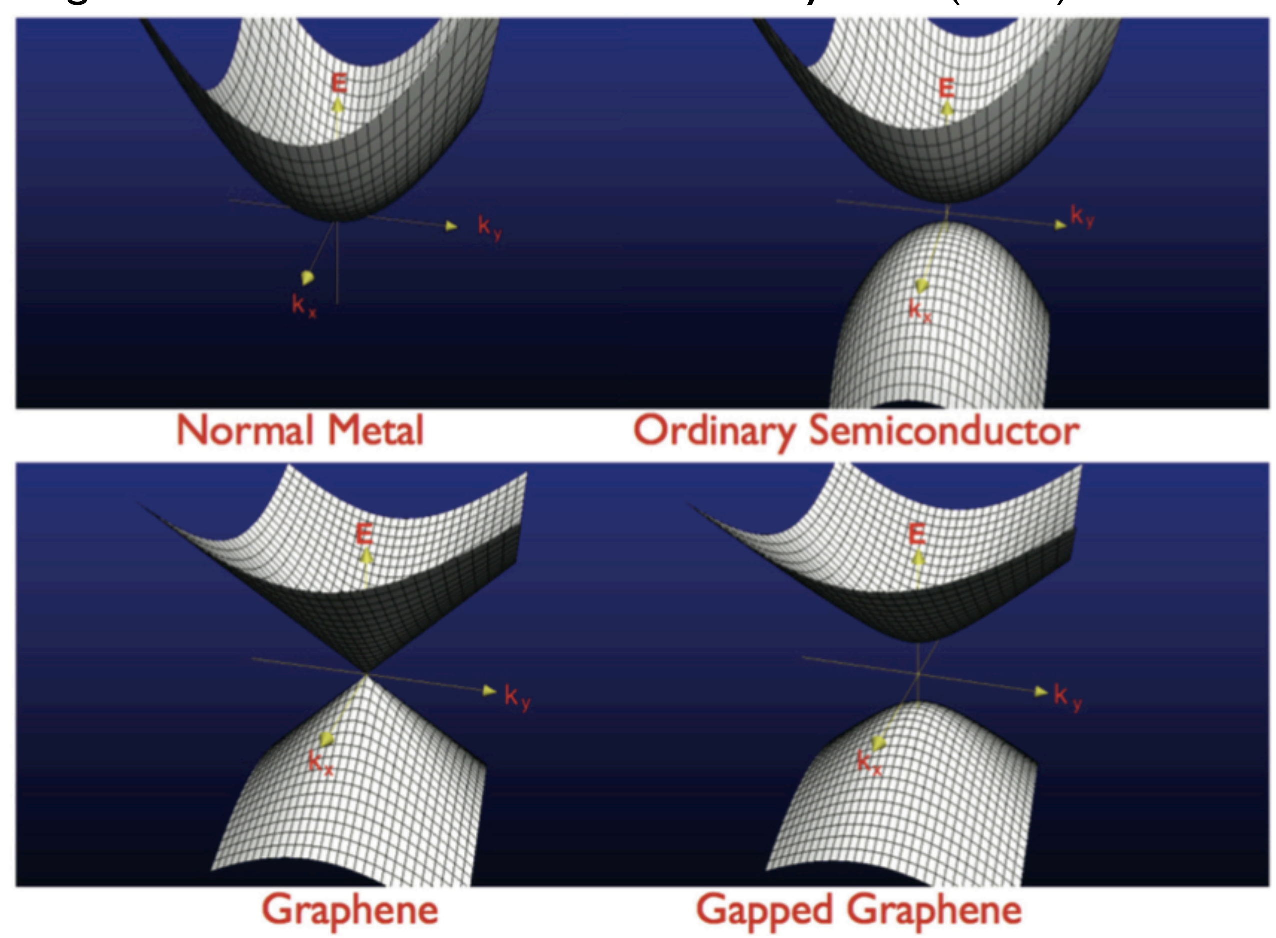
$3\ sp^2 + p$

⇩ lattice ⇩ free electron

- The hexagonal symmetry leads to linear dispersion at low energies ...

  P. R. Wallace, Phys. Rev. 71, 622 (1947).

Figure: A.H. Castro Neto, Materials Today 13, 1 (2010).



Graphene phenomenology VI:
theory of the electronic band structure ...

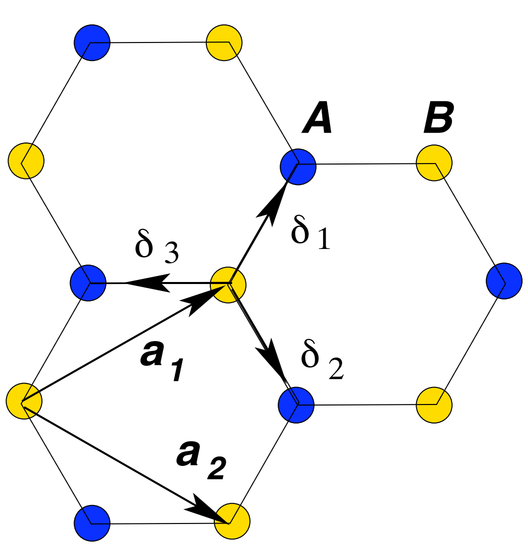
S. Reich *et al*, Phys. Rev. B66, 035412 (2002).

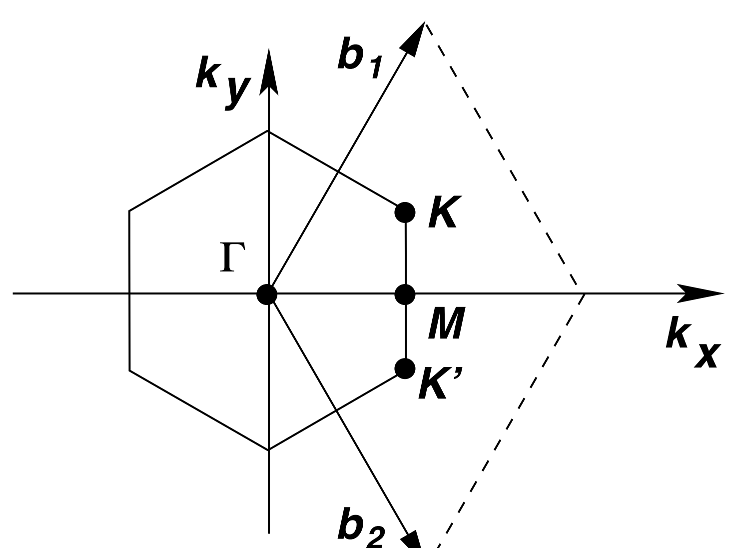
- Tight-binding description of the electron-ion interactions in graphene ...

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

Creation and annihilation operators for electrons on sublattices (A,B)

- Conical dispersion around two "valleys", centered around the "Dirac points" (K,K') ...

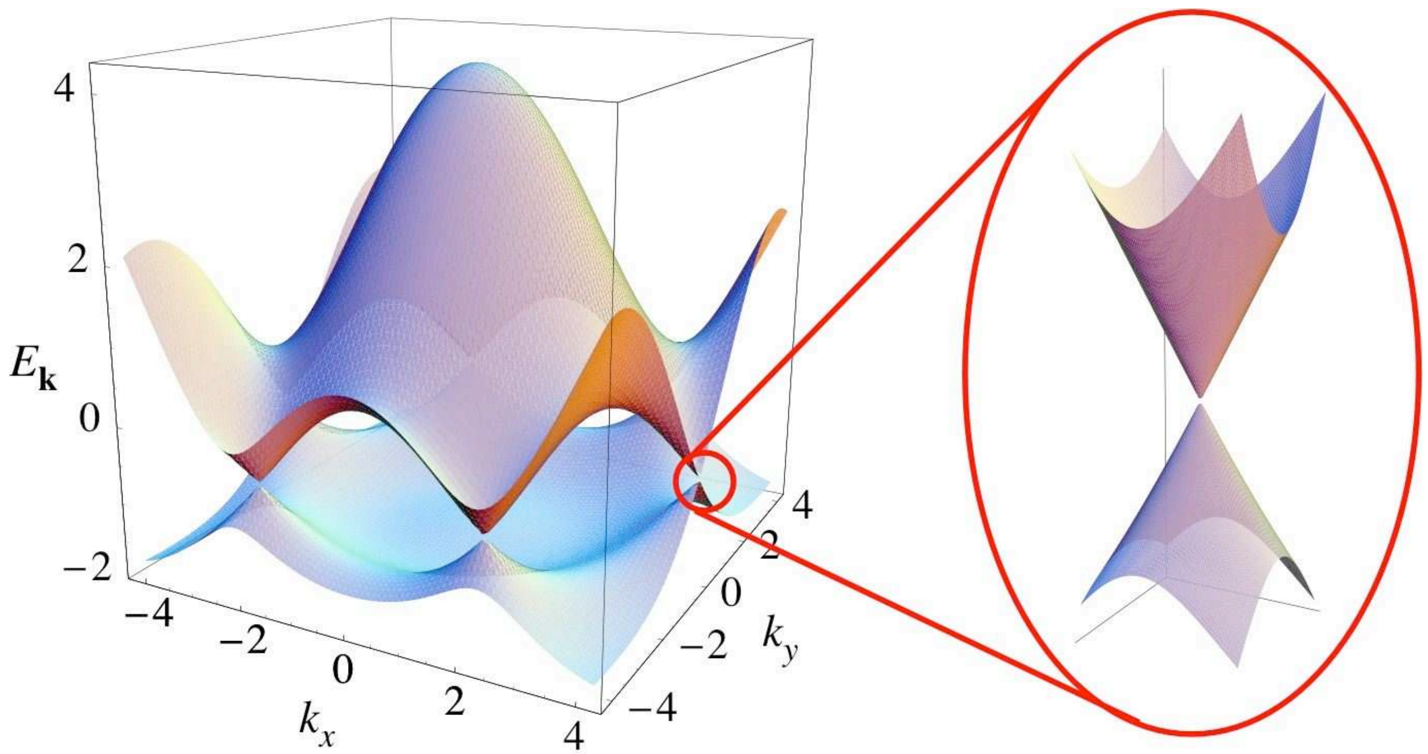




Theory of non-interacting electrons

Graphene at low energies I:
massless Dirac quasiparticles ...

- The non-interacting theory describes a gapless **semimetal** ...
  However: the quasiparticle velocity is a fraction of the speed of light in vacuum!



In the vicinity of a "Dirac point":

$$E_k \simeq vk$$

$$v \simeq c/300$$

Velocity of quasiparticles

Fermions (in 2+1 dimensions)

Dirac flavors, $N_f = 2$ describes a graphene monolayer ...

$$S_E = -\sum_{a=1}^{N_f} \int d^2x \, dt \, \bar{\psi}_a \, D \, \psi_a$$

$$D = \gamma_0 \partial_0 + v \gamma_i \partial_i, \quad i = 1, 2$$

$$\gamma^\mu, \, \mu = 0, 1, 2 \quad \{\gamma^\mu, \gamma^\nu\} = 2\delta^{\mu\nu}$$

Graphene at low energies II:

quasiparticles with instantaneous Coulomb interactions ...

$$S_E = -\sum_{a=1}^{N_f} \int d^2x\, dt\, \bar{\psi}_a\, D[A_0]\, \psi_a + \frac{1}{2g^2} \int d^3x\, dt\, (\partial_i A_0)^2$$

$$D[A_0] = \gamma_0(\partial_0 + iA_0) + v\gamma_i\partial_i, \quad i = 1, 2$$

Gauge field (in 3+1 dimensions)

Electrostatic Coulomb interaction ...

$$A_0 \to A_0 + \alpha(t) \qquad \psi \to \exp\left\{ i \int dt \alpha(t) \right\} \psi$$

Gauge invariance

- Whether the Coulomb interaction is significant depends on the dielectric constant of the environment ...

$$g^2 = e^2/\epsilon_0$$

$$\alpha_g \equiv \frac{e^2}{4\pi\epsilon_0 \hbar v} \simeq 300\alpha \sim 1$$

Fine-structure constant of graphene

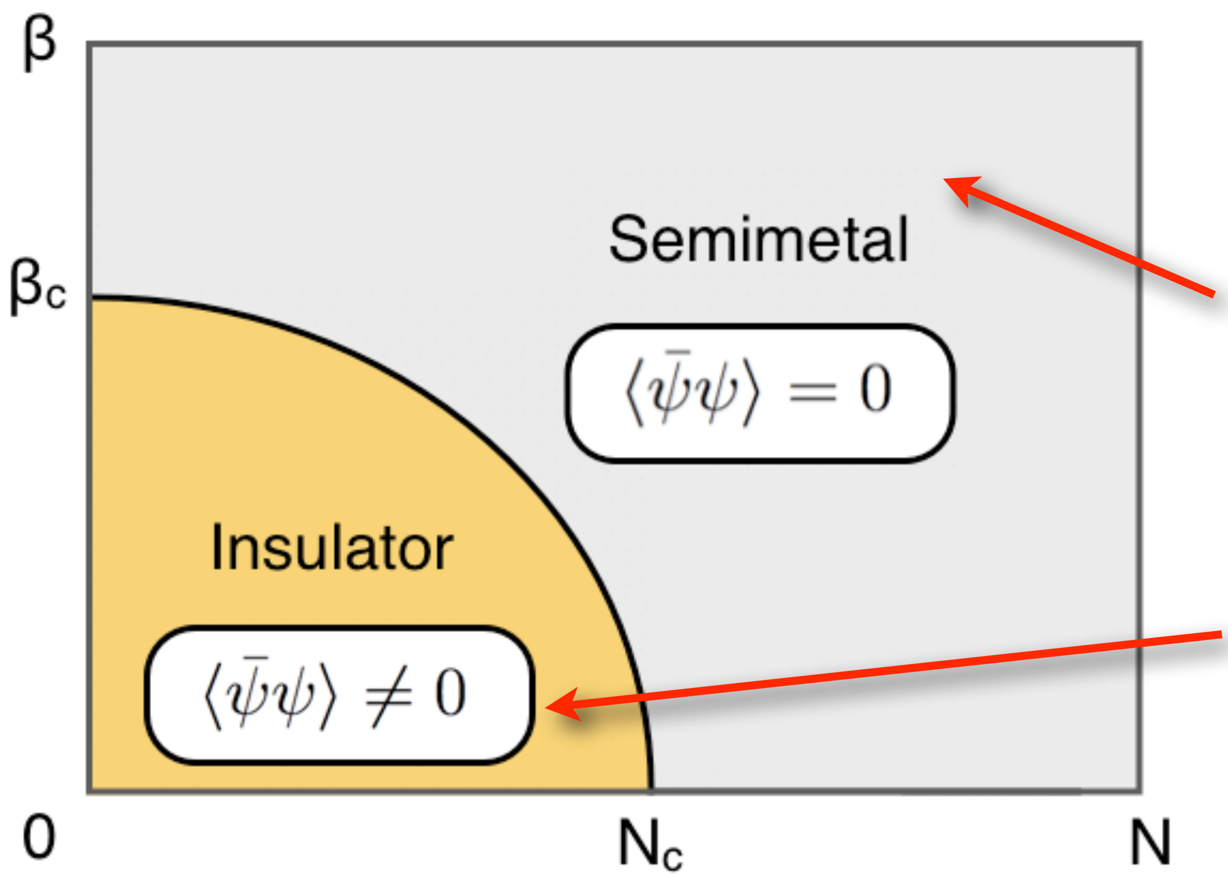
Graphene at low energies III:
spontaneous chiral symmetry breaking ...

G.W. Semenoff, Phys. Rev. Lett. 54, 2449 (1984),
C. Burden, A.N. Burkitt, Eur. Phys. Lett. 3, 545 (1987).

- The massless quasiparticles possess **chiral symmetry**, which can be spontaneously broken ...

$U(2N_f) \rightarrow U(N_f) \times U(N_f)$ $\langle \bar{\psi}_a(x) \psi_a(x) \rangle$ Order parameter, chiral condensate

- A conjectured electronic phase diagram, as a function of inverse coupling and fermion flavors ...



chiral symmetry **unbroken,** quasiparticles remain **massless.**

chiral symmetry **spontaneously broken,** quasiparticles **massive.**

Lattice Monte Carlo simulation I:
evaluating the condensate ...

J.E. Drut, T.A. Lähde, Phys. Rev. B79, 165425 (2009).

- Integrate out the fermion fields ...

$$\mathcal{Z} = \int \mathcal{D}A_0 \; \underline{\exp(-S_{\text{eff}}[A_0])} \qquad S_{\text{eff}}[A_0] = -N_f \ln\det(D[A_0]) + S_E^g[A_0]$$

Positive definite probability measure
for MC calculation

- Evaluate observables stochastically by generating snapshots of the gauge field ...

$$\sigma = \frac{1}{V\mathcal{Z}} \int \mathcal{D}A_0 \, \text{Tr}(D^{-1}[A_0]) \exp(-S_{\text{eff}}[A_0])$$

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

- Compute the condensate at different (inverse) interaction strengths ...

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

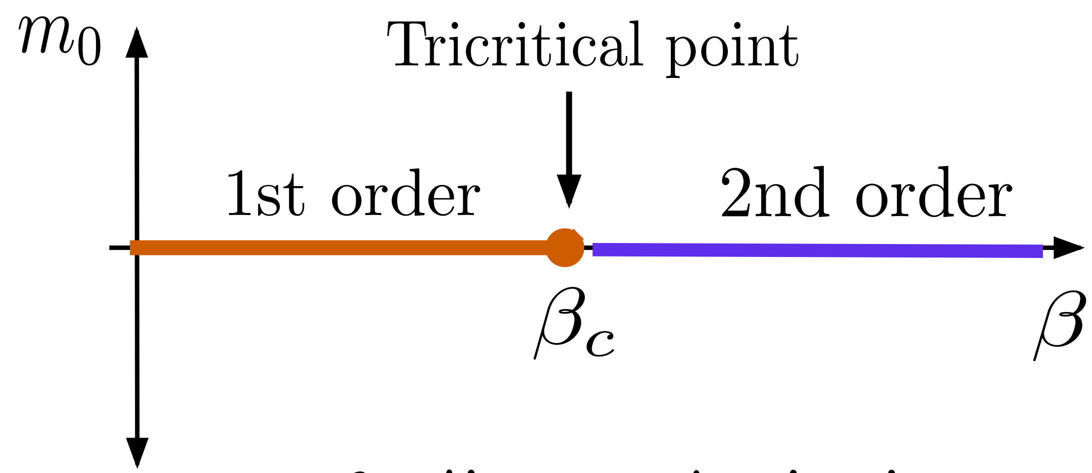
Lattice Monte Carlo simulation II:
finding the transition ...

M. Göckeler *et al*, Nucl. Phys. B487, 313 (1997).

- Discretize on a square lattice with finite lattice spacing (acts as an UV cutoff) ...

- Perform calculations at finite fermion mass (acts as an IR cutoff) ...

$$\int d^2x\, dt\, m_0 \bar{\psi}_a \psi_a$$



Continuum physics is recovered in the vicinity of the second-order transition

- We want to study the critical region of the theory, however:

  1) Dirac operator develops small eigenvalues

  2) Large finite-volume effects (correlation length diverges)

- In practice, extrapolate using results obtained at different masses and couplings ...

Lattice Monte Carlo simulation III: discretized theory ...

H. Rothe, "Lattice gauge theories", World Scientific (2005).

- Non-compact gauge action ...

$$S_E^g[\theta_0] \;=\; \frac{\beta}{2}\sum_n \left[\sum_{i=1}^{3}\left(\theta_{0,n} - \theta_{0,n+\hat{e}_i}\right)^2\right]$$

- Doubling problem for chiral lattice fermions: 1 staggered fermion flavor gives 2 continuum flavors!

  H.B. Nielsen, M. Ninomiya, Nucl. Phys. B185, 20 (1981); Nucl. Phys. B193, 173 (1981).
  C. Burden, A.N. Burkitt, Eur. Phys. Lett. 3, 545 (1987).

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

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

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

- Gauge invariance on the lattice: "gauge links" in the fermion action ...

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

Lattice Monte Carlo simulation IV:

generation of gauge configurations, Hybrid Monte Carlo ...

S. Duane *et al.*, Phys. Lett. B 195, 216 (1987).

- Add to the Euclidean action a random Gaussian noise component ...

$$H = \sum_{\mathbf{n}} \frac{\pi_{\mathbf{n}}^2}{2} + S_E[\theta]$$

Enables global updates of the lattice gauge potential

- Introduce pseudofermions to provide efficient updating of the fermion action ...

$$\det(Q) \propto \int \mathcal{D}\phi^\dagger \mathcal{D}\phi \, \exp(-S_E^p) \qquad S_E^p = \sum_{\mathbf{n},\mathbf{m}} \phi_{\mathbf{n}}^\dagger \, Q_{\mathbf{n},\mathbf{m}}^{-1}[\theta] \, \phi_{\mathbf{m}} = \sum_{\mathbf{n}} \xi_{\mathbf{n}}^\dagger \xi_{\mathbf{n}}$$

- Evolve the gauge field by numerically integrating the EOM (Molecular Dynamics) ...

$$H = \sum_{\mathbf{n}} \frac{\pi_{\mathbf{n}}^2}{2} + S_E^g + S_E^p$$

$$\begin{aligned} \dot{\theta}_{\mathbf{n}} &= \frac{\delta H}{\delta \pi_{\mathbf{n}}} = \pi_{\mathbf{n}}, \\ \dot{\pi}_{\mathbf{n}} &= -\frac{\delta H}{\delta \theta_{\mathbf{n}}} \equiv F_{\mathbf{n}}^g + F_{\mathbf{n}}^p \end{aligned}$$

- Exact method: MD evolution error corrected by Metropolis step ...

Lattice Monte Carlo simulation V:
extrapolation to the critical point ...

A. Kocić, J.B. Kogut, K.C. Wang, Nucl. Phys. B398, 405 (1993).
M. Göckeler *et al*, Nucl. Phys. B487, 313 (1997).

- "Equation of state" analysis ...

$$m_0 = f(\sigma, \beta)$$

$$\sigma \equiv \langle \bar{\chi}\chi \rangle$$

$$\chi_l \equiv \frac{\partial \sigma}{\partial m_0}$$

Simultaneous fit to condensate and susceptibility

- Trial function (also for QED4) ...

$$m_0 X(\beta) = Y(\beta) f_1(\sigma) + f_3(\sigma)$$

Dependence on σ:
Information on critical exponents δ, β_m !

$$f_1(\sigma) = \sigma^{\delta - 1/\beta_m}$$
$$f_3(\sigma) = \sigma^{\delta}$$

Dependence on β:
Information on critical coupling β_c!

$$X(\beta) = X_0 + X_1(1 - \beta/\beta_c)$$
$$Y(\beta) = Y_1(1 - \beta/\beta_c)$$

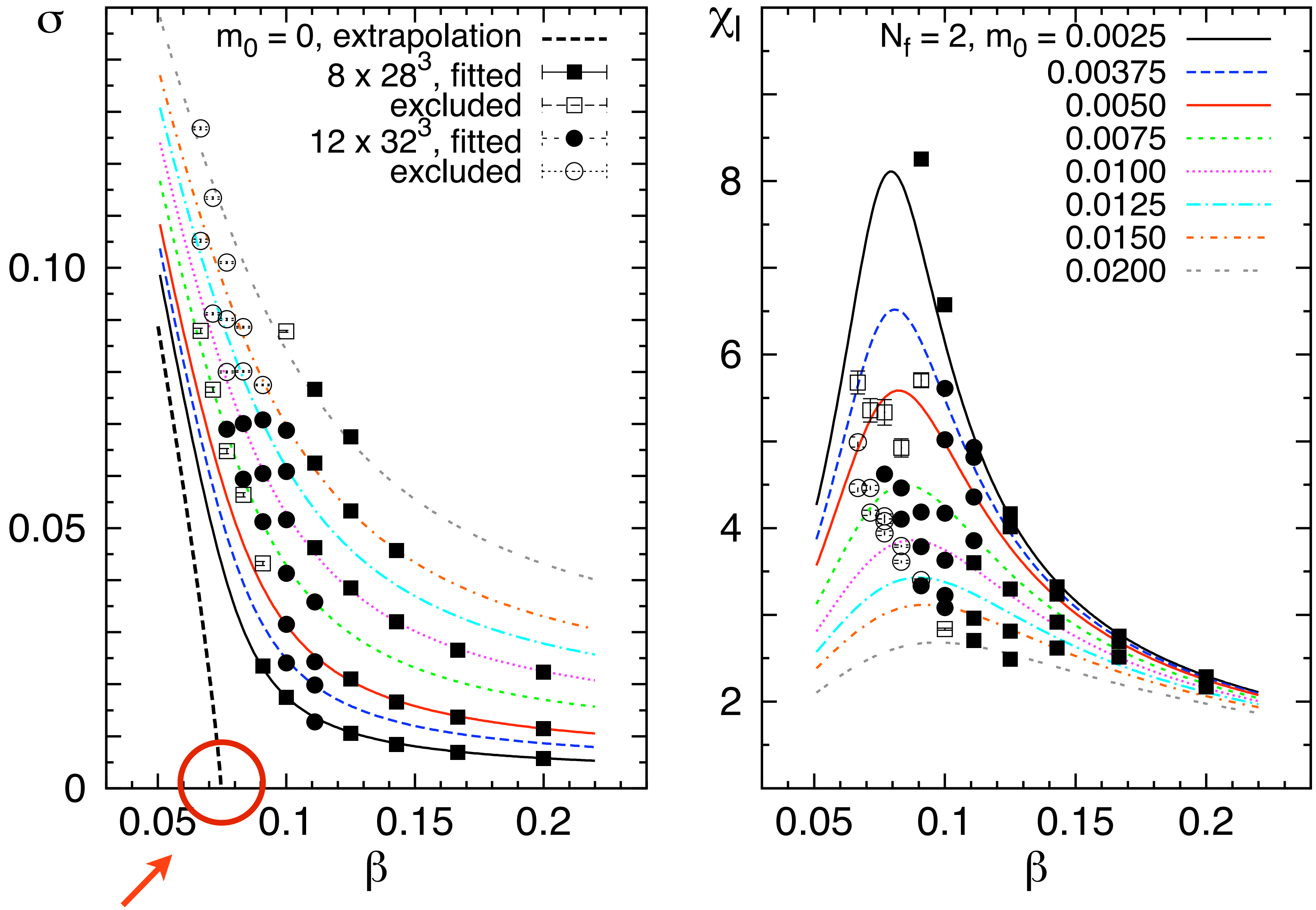
Results I:

quantum phase transition into a gapped phase ...

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

J.E. Drut, T.A. Lähde, Phys. Rev. B79 (2009) 165425

$\beta_c \sim 0.073 \pm 0.002$



Critical coupling from EOS analysis!

Results II:
is the semimetal-insulator transition observable?

Graphene on a SiO_2 substrate
$\beta \sim 0.10$

Our critical coupling
$\beta_c \sim 0.073$

Suspended graphene
$\beta \sim 0.037$

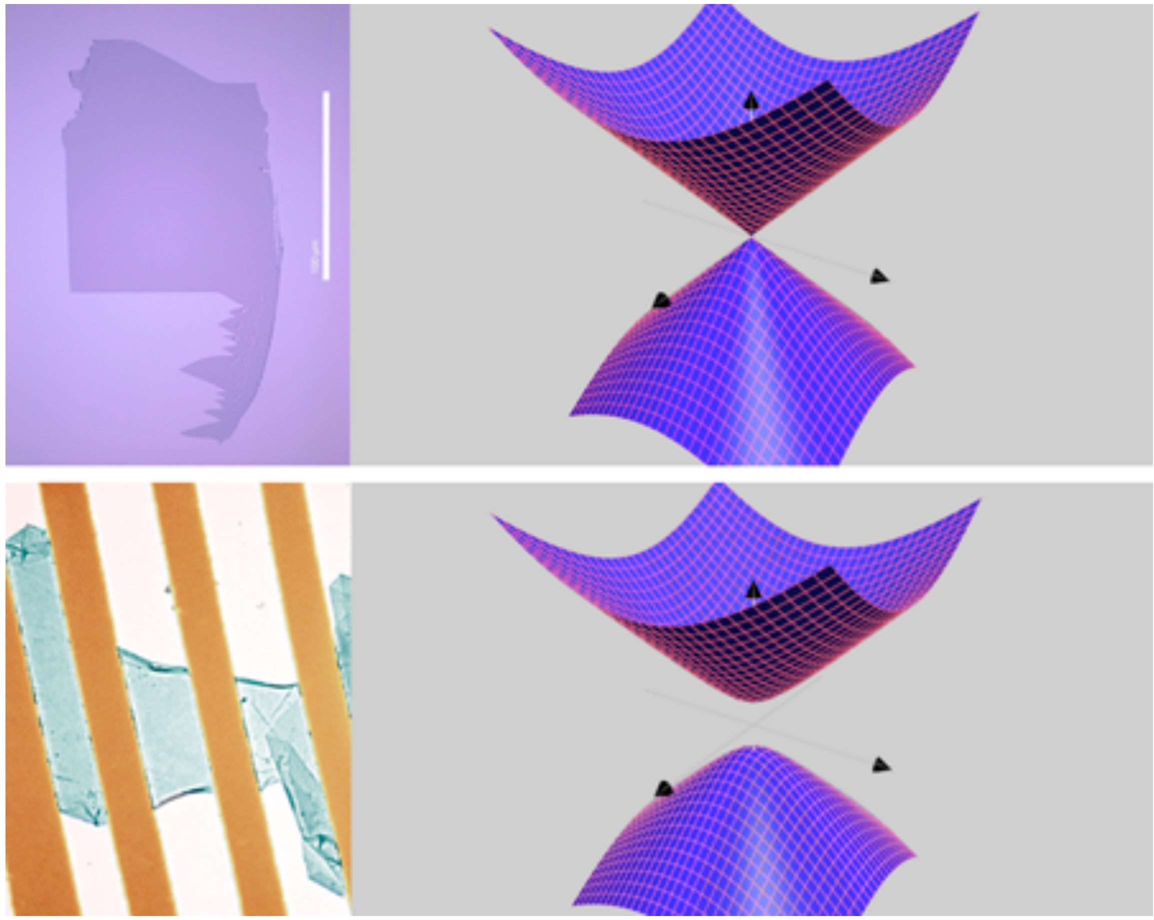


Figure: A.H. Castro Neto, Physics 2, 30 (2009)

Under ideal circumstances: should be observable for **suspended** graphene samples!!

Results III:
critical exponents, critical # of flavors ...

- The EOS extrapolation indicates a second-order transition, critical exponents:

$$\delta = 2.2 \pm 0.1$$
$$\bar{\beta} = 0.83 \pm 0.05$$
$$\gamma = 1.0 \pm 0.04$$

$$\delta \equiv \left[\frac{\partial \ln \sigma}{\partial \ln m_0}\right]^{-1}\Bigg|_{\beta=\beta_c, m_0 \to 0}$$

$$\bar{\beta} \equiv \frac{\partial \ln \sigma}{\partial \ln(\beta_c - \beta)}\Bigg|_{m_0=0, \beta \nearrow \beta_c}$$

$$\gamma \equiv -\frac{\partial \ln \chi}{\partial \ln(\beta_c - \beta)}\Bigg|_{m_0=0, \beta \to \beta_c}$$

Consistent with $\bar{\beta}(\delta - 1) = \gamma$

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

- Simulations for N_f = 4 show a transition at stronger coupling, for N_f = 6 nothing is observed:

$$4 < N_{crit} < 6$$

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

Results IV:
supporting results by other groups (some examples) ...

- Analytical Dyson-Schwinger calculations:
  consistent with our results, however infinite-order transition ...

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

  E.V. Gorbar et al., Phys. Rev. B66, 045108 (2002)

- Lattice Monte Carlo simulations:
  strong-coupling limit, closely related to Thirring model in (2+1) dimensions ...

  S.J. Hands, C. Strouthos, Phys. Rev. B78, 165423 (2008)

  S.J. Hands, C. Strouthos, W. Armour, arXiv:0910.5646

- Large N_f treatment:
  second-order transition verified, critical exponents disagree ...

  I. Herbut, V. Juričić, O. Vafek, Phys. Rev. B80, 075432 (2009)

- Strong-coupling expansion of the lattice theory:
  chiral EFT technique, transition to insulating phase confirmed ...

  Y. Araki, T. Hatsuda, arXiv:1003.1769

Lattice artifacts I:
photon self-interactions on the lattice ...

- We chose arbitrarily to simulate the non-compact theory of graphene ...

$$S_E^{g,nc}[\theta] \;=\; \frac{\beta}{2}\sum_n \left[\sum_{i=1}^{3}\left(\theta_{\mathbf{n}} - \theta_{\mathbf{n}+\mathbf{e}_i}\right)^2\right]$$

- Equally well, we could simulate the compact theory instead, identical continuum limit ...

$$S_E^{g,c}[\theta] = \beta \sum_{\mathbf{n}} \left[3 - \sum_{i=1}^{3} \Re\left(U_{\mathbf{n}} U^{\dagger}_{\mathbf{n}+\mathbf{e}_i}\right)\right]$$

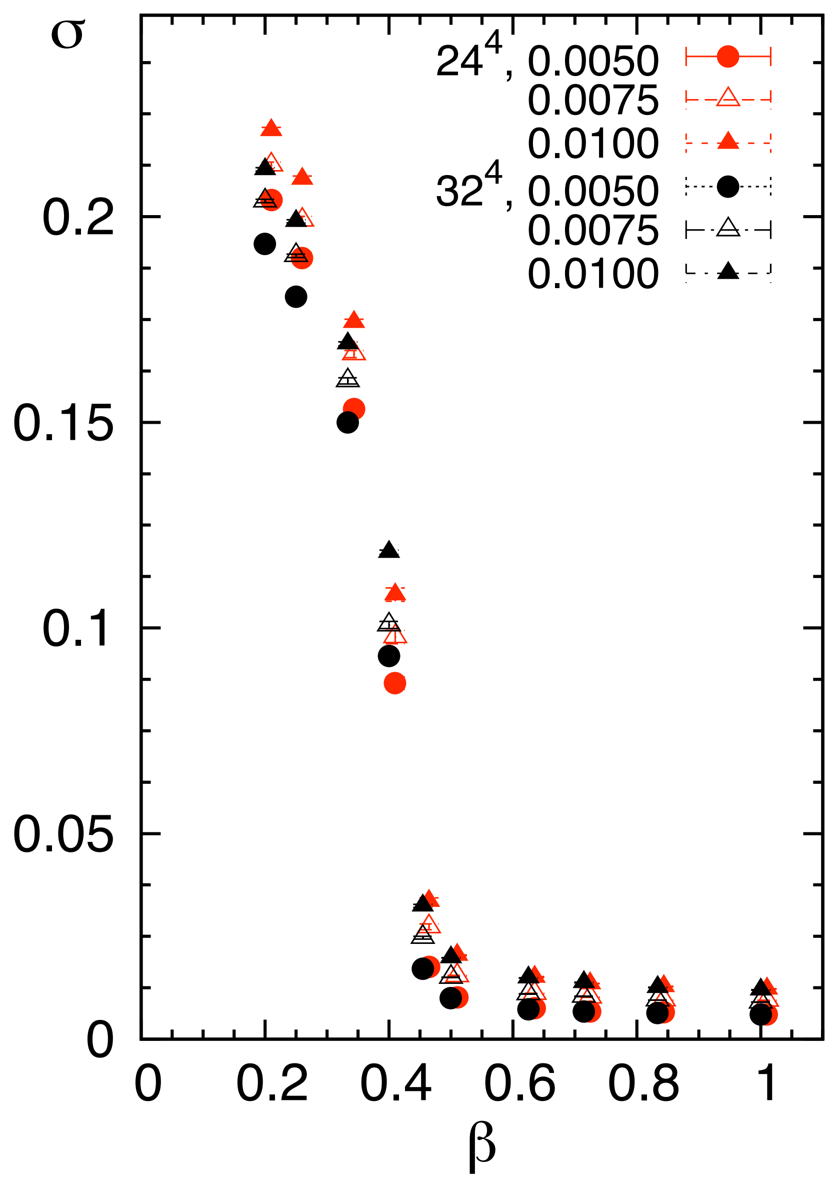
- Gauge links introduce higher-order vertices (self-interactions, tadpoles) .... How do these affect the simulation?

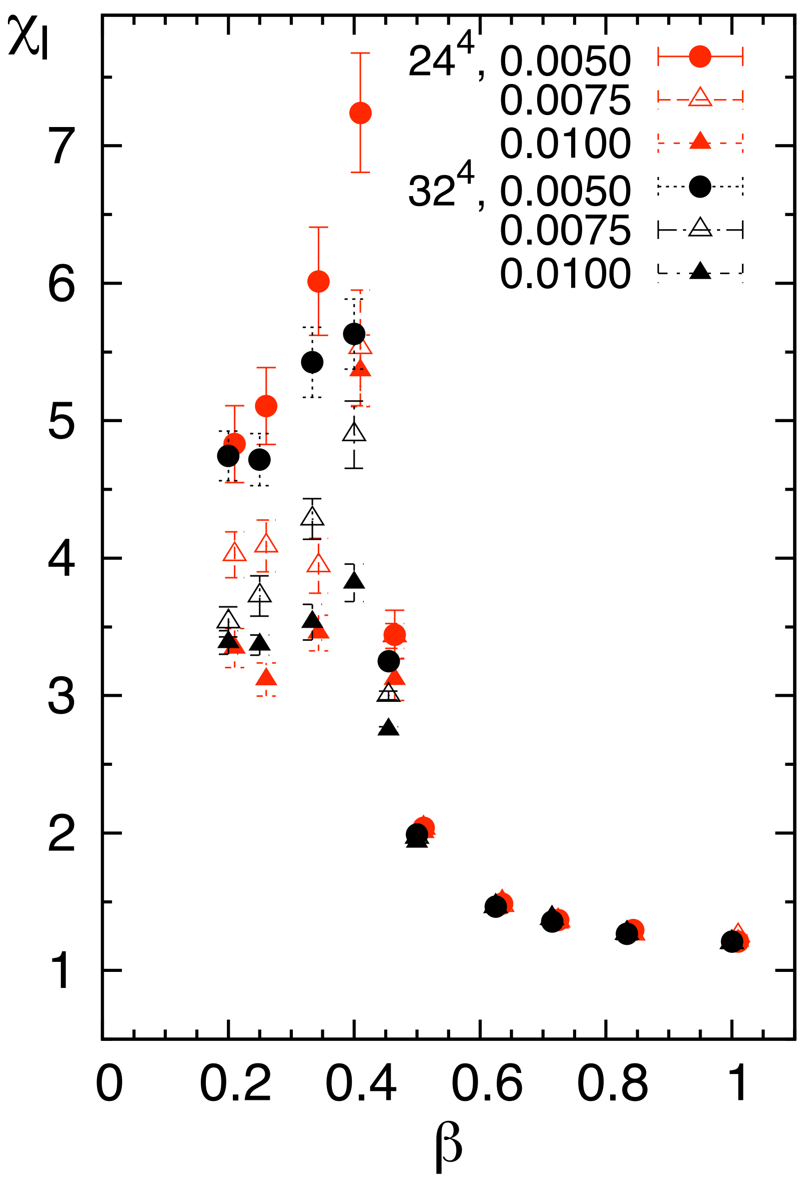
Lattice artifacts II:
effects of photon self-interactions in the compact theory ...

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

- First order transition, no approach to the continuum limit (!)

$\beta_c \sim 0.40$





- As for (3+1) dimensional QED, the compact theory of graphene bears little resemblance to continuum physics ...

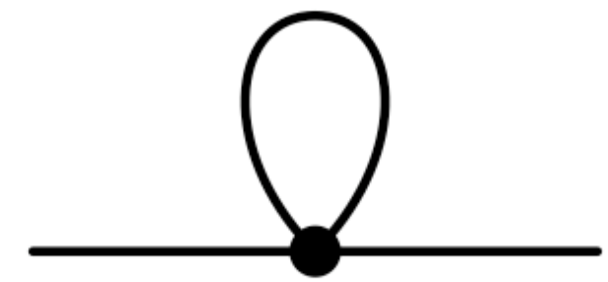
Lattice artifacts III:

tadpole improvement ...

G.P. Lepage, P.B. Mackenzie, Phys. Rev. D48, 2250 (1993).

$$U_\mu(x) \equiv e^{iagA_\mu(x)} \rightarrow 1 + iagA_\mu(x)$$

- However, UV divergent "tadpole" contributions do not vanish as a power of the lattice spacing ...



- Integrate out the tadpole contributions by "renormalizing" the gauge links ...

$$U_\mu \rightarrow u_0\, e^{iagA_\mu^{\mathrm{IR}}} \approx u_0\,(1 + iagA_\mu^{\mathrm{IR}})$$

- Renormalized gauge links give results closer to the continuum limit, estimate the correction *a posteriori* ...

$$U \rightarrow U/u_0$$

$$u_0 \equiv \langle P \rangle^{1/2}, \quad P = \frac{1}{V}\sum_{\mathbf{n}} U_{\mathbf{n}} U^\dagger_{\mathbf{n}+\mathbf{e}_i}$$

Lattice artifacts IV:

tadpole improvement of the non-compact theory ...

J. Giedt, A. Skinner, S. Nayak, arXiv: 0911.4316

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

$$D^I_{\mathbf{n},\mathbf{n}'}[\theta] = \frac{1}{2}\left[\delta_{\mathbf{n}+\mathbf{e}_0,\mathbf{n}'}\,U_{\mathbf{n}} - \delta_{\mathbf{n}-\mathbf{e}_0,\mathbf{n}'}\,U^\dagger_{\mathbf{n}'}\right] + \frac{v'}{2}\sum_i \eta_{i,\mathbf{n}}\left[\delta_{\mathbf{n}+\mathbf{e}_i,\mathbf{n}'} - \delta_{\mathbf{n}-\mathbf{e}_i,\mathbf{n}'}\right] + m_0'\,\delta_{\mathbf{n},\mathbf{n}'}$$

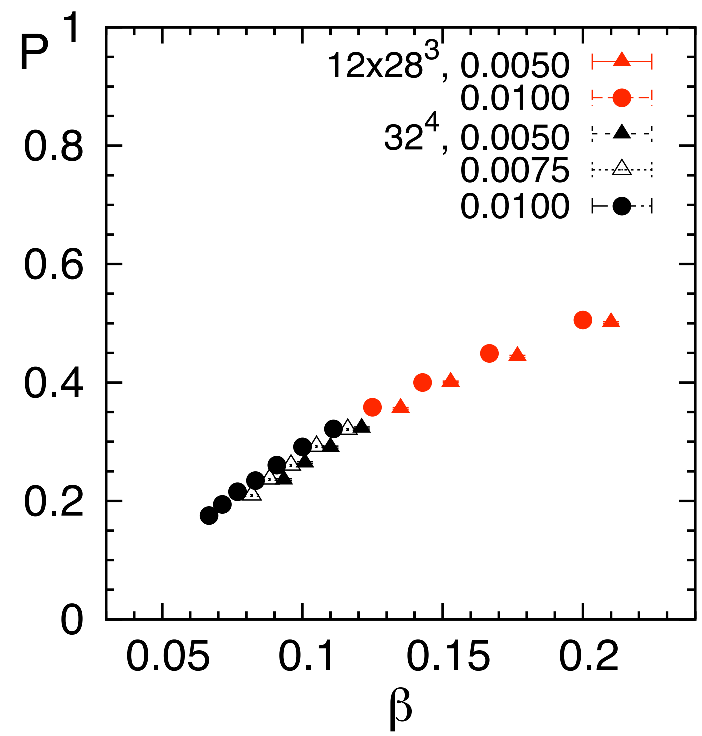
- Overall: effectively a shift in the parameters of the theory!

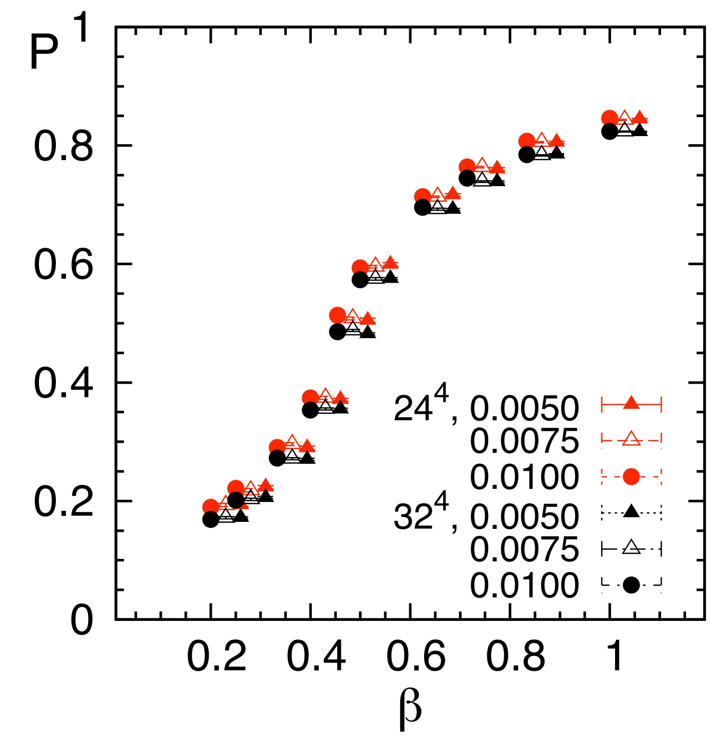
$$\sigma' \equiv \sigma/u_0, \quad v' \equiv u_0 v, \quad m_0' \equiv u_0 m_0 \qquad \chi \equiv \sqrt{u_0}\,\chi'$$

- Additionally, for the compact theory:

$$g' \equiv u_0 g$$

Average plaquettes in the non-compact and compact theories ...



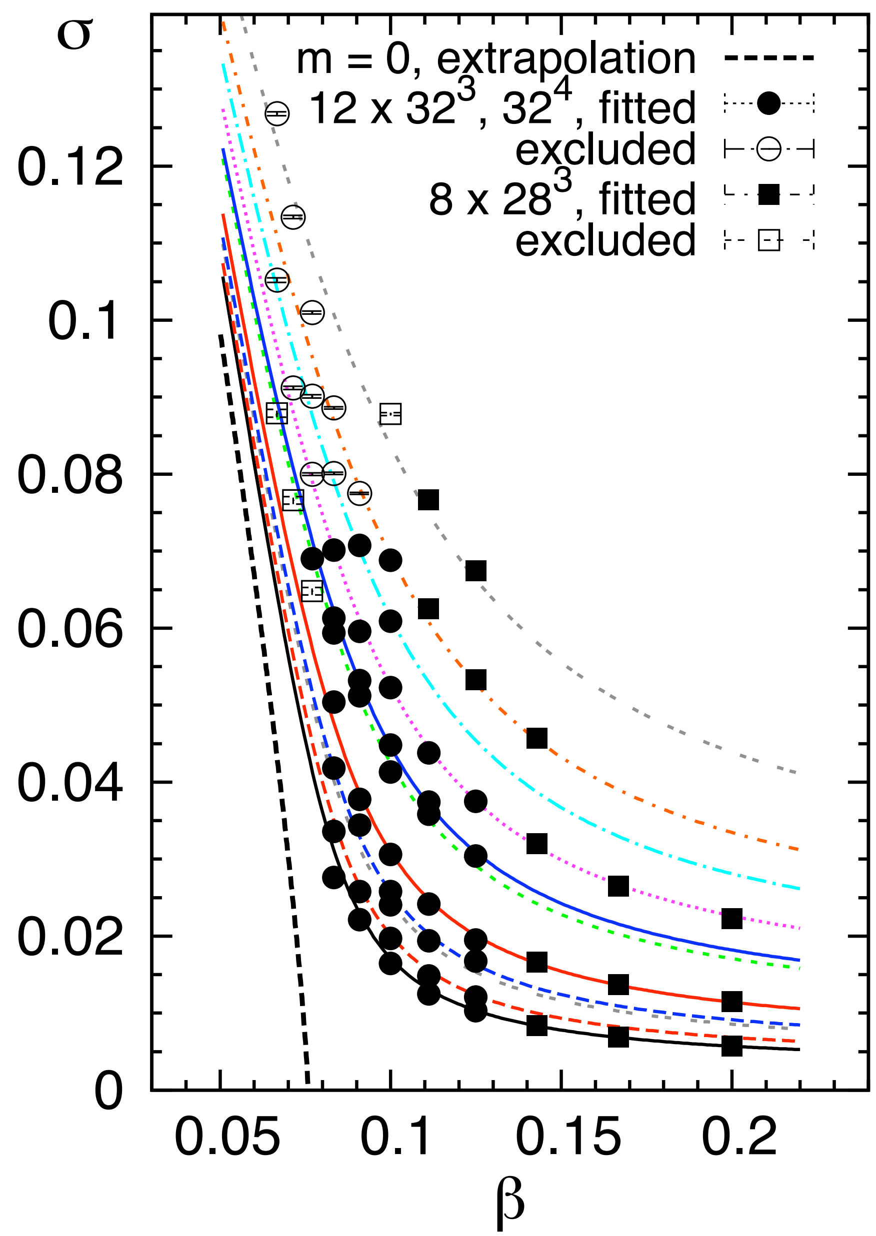


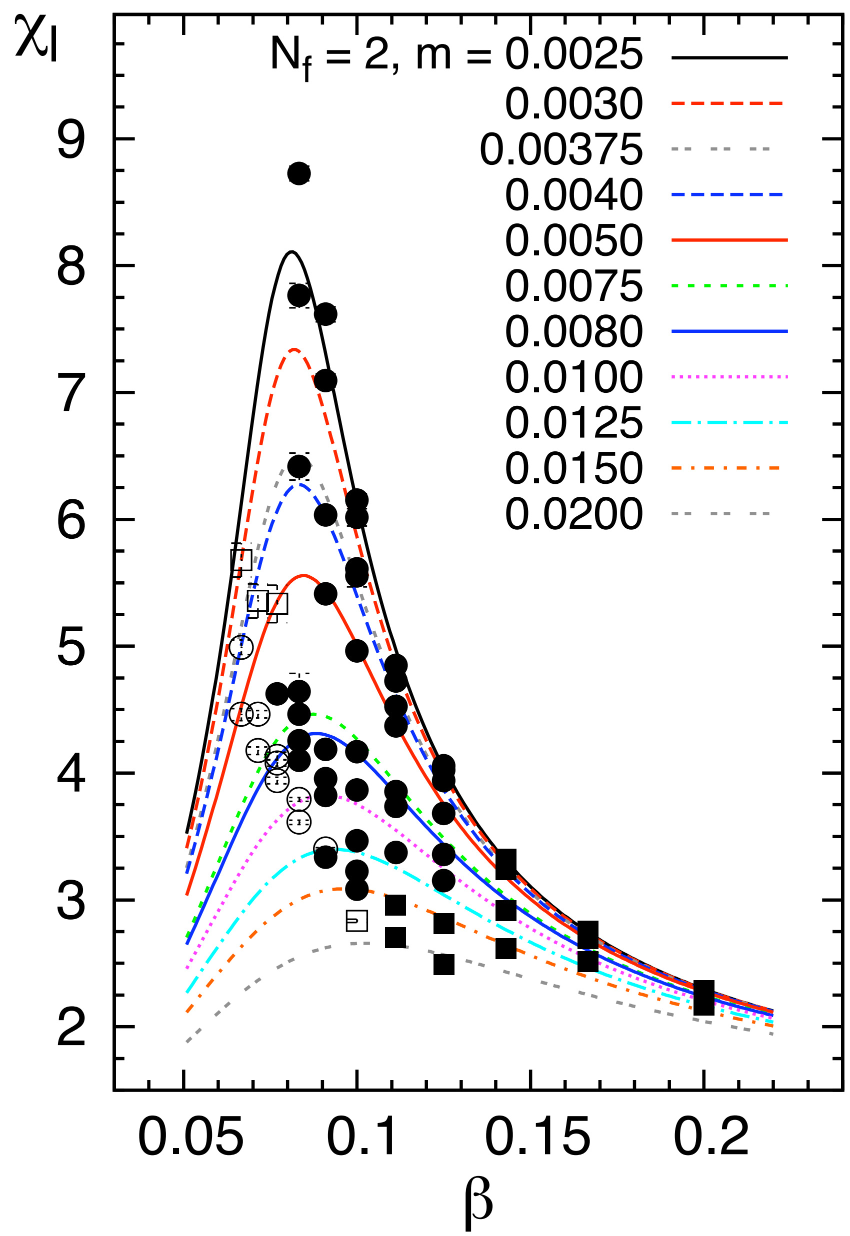
Lattice artifacts V:
unimproved results for the non-compact theory ...

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

$\beta_c \sim 0.074 \pm 0.001$

- Data at strong coupling cannot be fitted, "scaling violations" ...





Lattice artifacts VI:

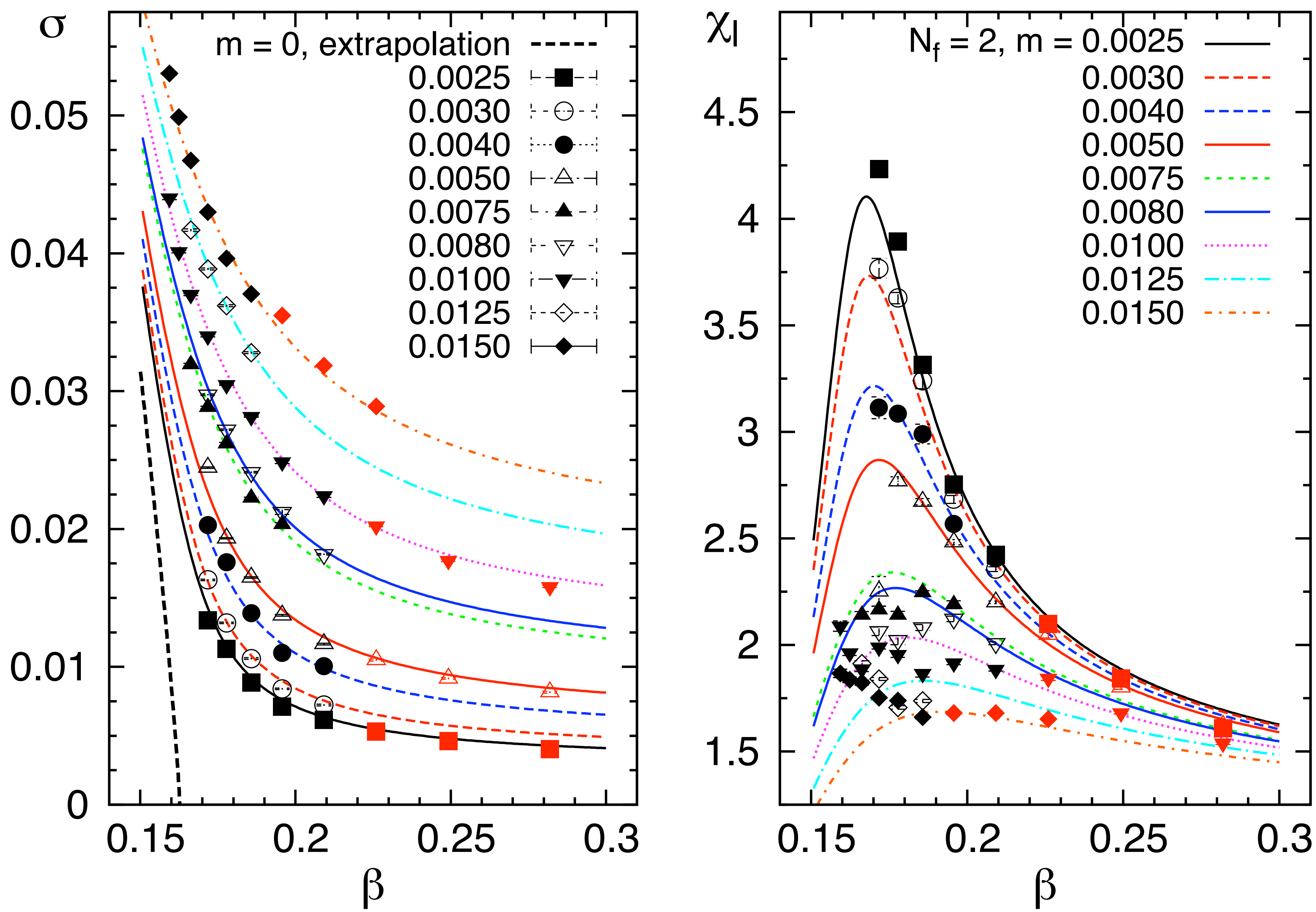
tadpole-improved non-compact theory ...

$$\beta \equiv \frac{v}{g^2} = \frac{v'/u_0}{g'^2} = \frac{\beta'}{u_0}$$

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

$\beta_c \sim 0.165 \pm 0.001$ ← Significant effect, insulating phase more likely!

- Fit range and stability much improved ...



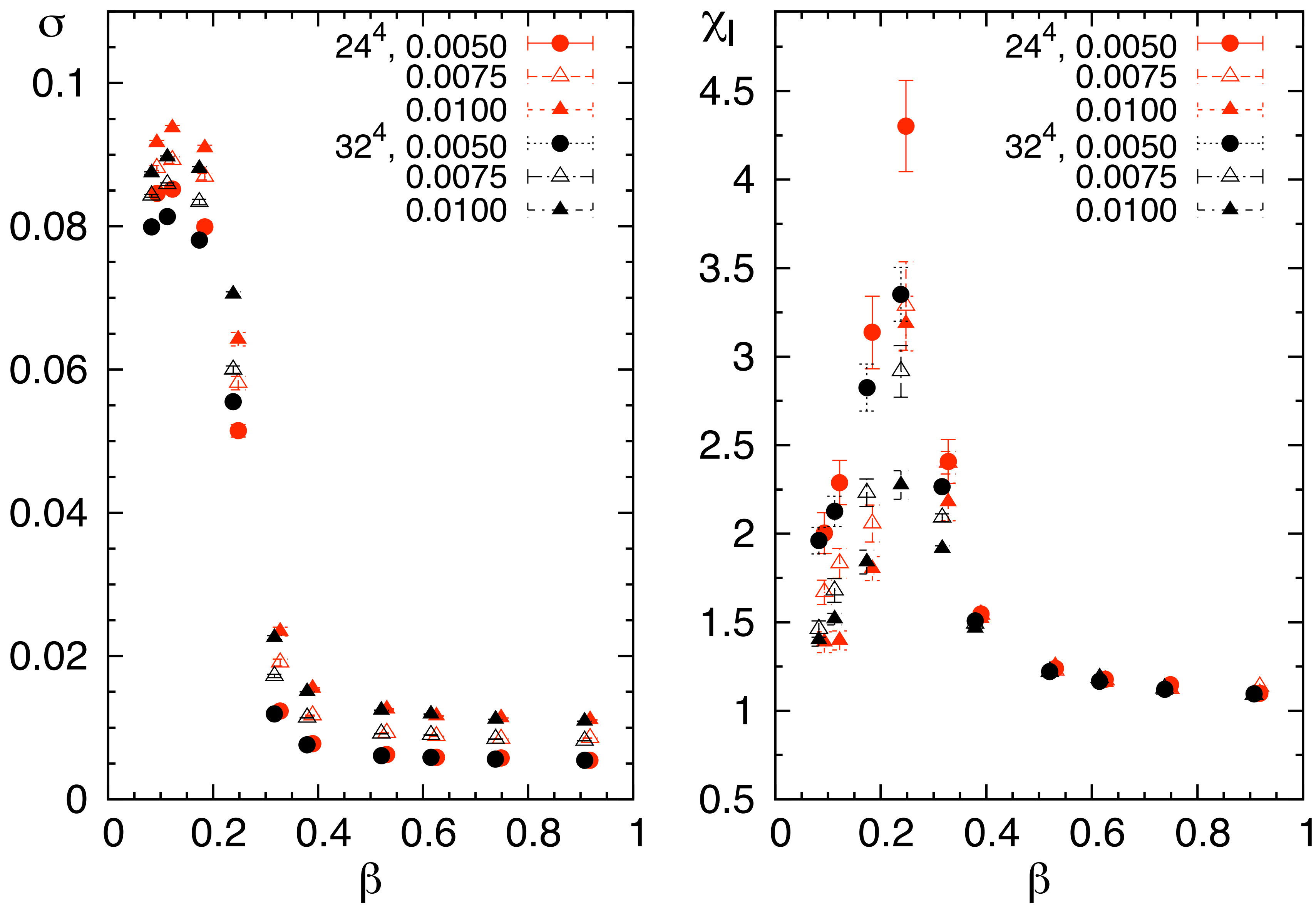
Lattice artifacts VII:
tadpole-improved compact theory?

$$\beta \equiv \frac{v}{g^2} = \frac{v'/u_0}{g'^2/u_0^2} = u_0\beta'$$

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

$\beta_c \sim 0.40$ $\xrightarrow{\text{TI}}$ $\beta_c \sim 0.25$

- Transition becomes less likely - effect of TI very different from the non-compact case!



Lattice artifacts VIII:
staggered fermions and chiral symmetry ...

- Our objective is to study the following chiral symmetry breaking pattern ...

$$U(4) \rightarrow U(2) \times U(2)$$

- However, using one flavor of staggered fermions at finite lattice spacing, we have only a smaller symmetry ...

$$U(1) \times U(1) \longrightarrow U(1)$$

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

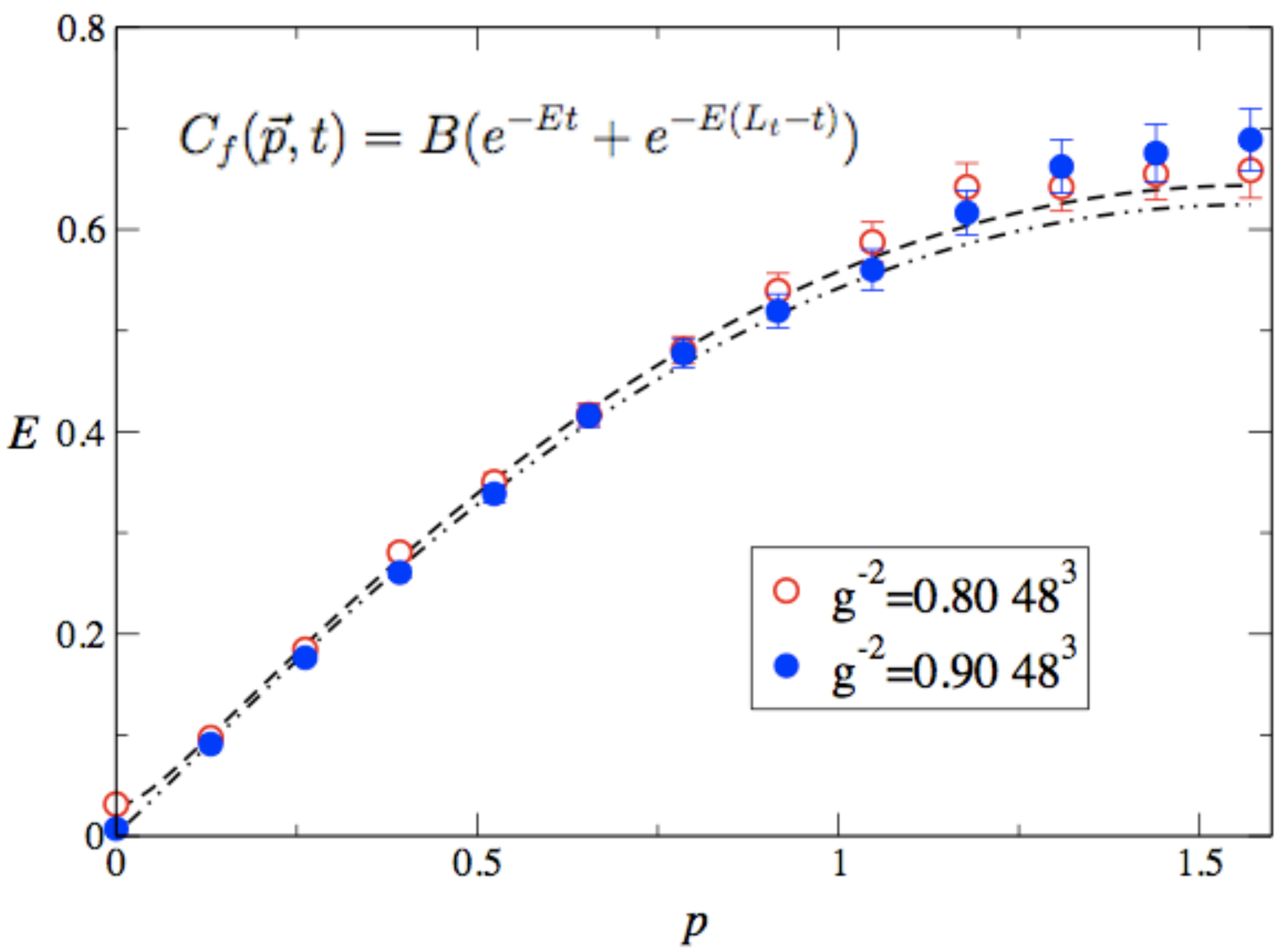
- The full symmetry is restored in the continuum limit, but is the extrapolation reliable?

Ultimately: simulate graphene with **overlap** fermions!!

Future projects I:
fermion velocity renormalization ...

Collaboration:
Lauri Suoranta (Aalto U.), master's thesis project
Joaquín Drut (Ohio State U.)

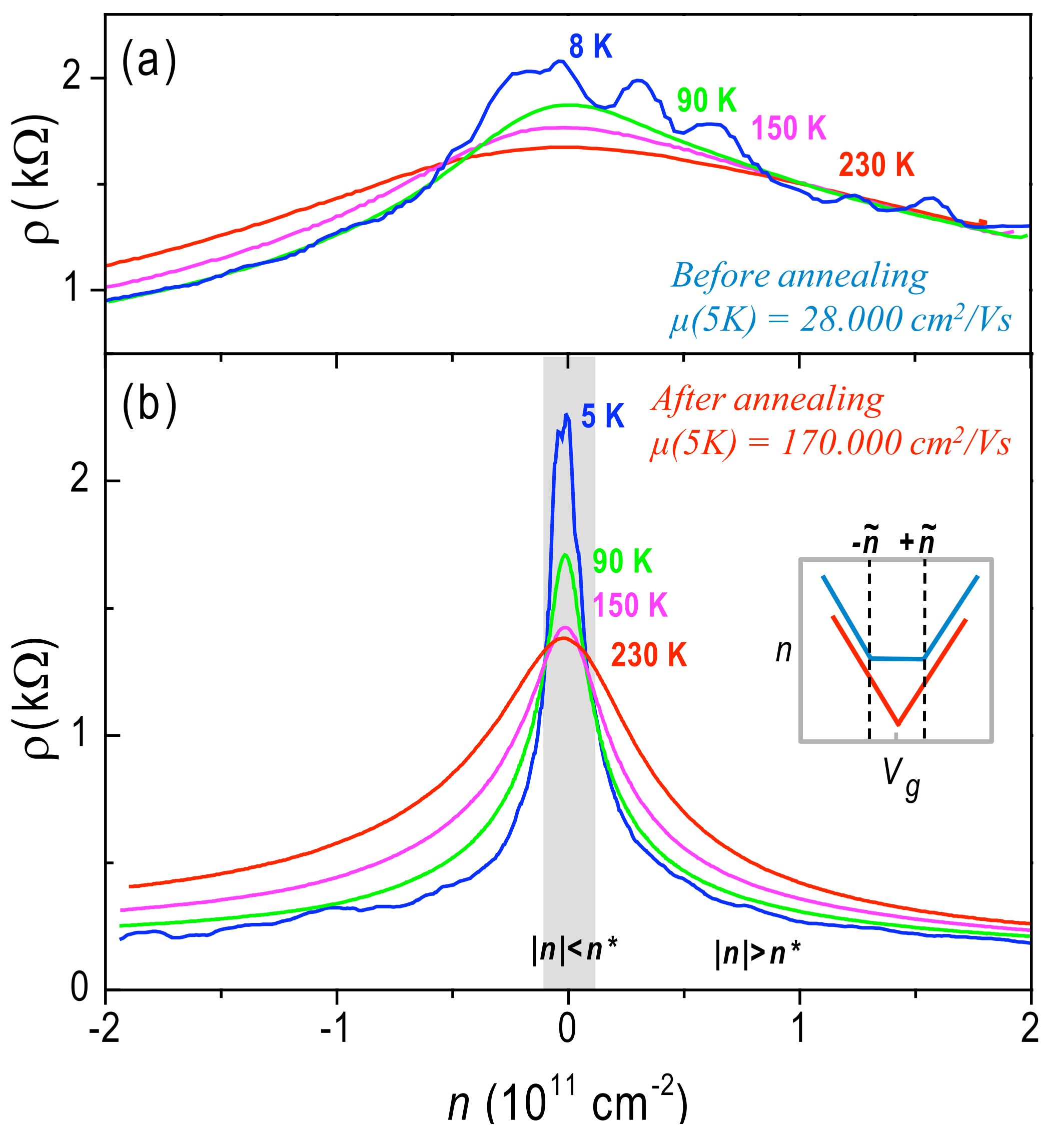
$$C_f(\vec{p},t) = \sum_{\vec{x}\ \text{even}} \langle \chi(\vec{0},0)\bar{\chi}(\vec{x},t)\rangle e^{-i\vec{p}.\vec{x}}$$

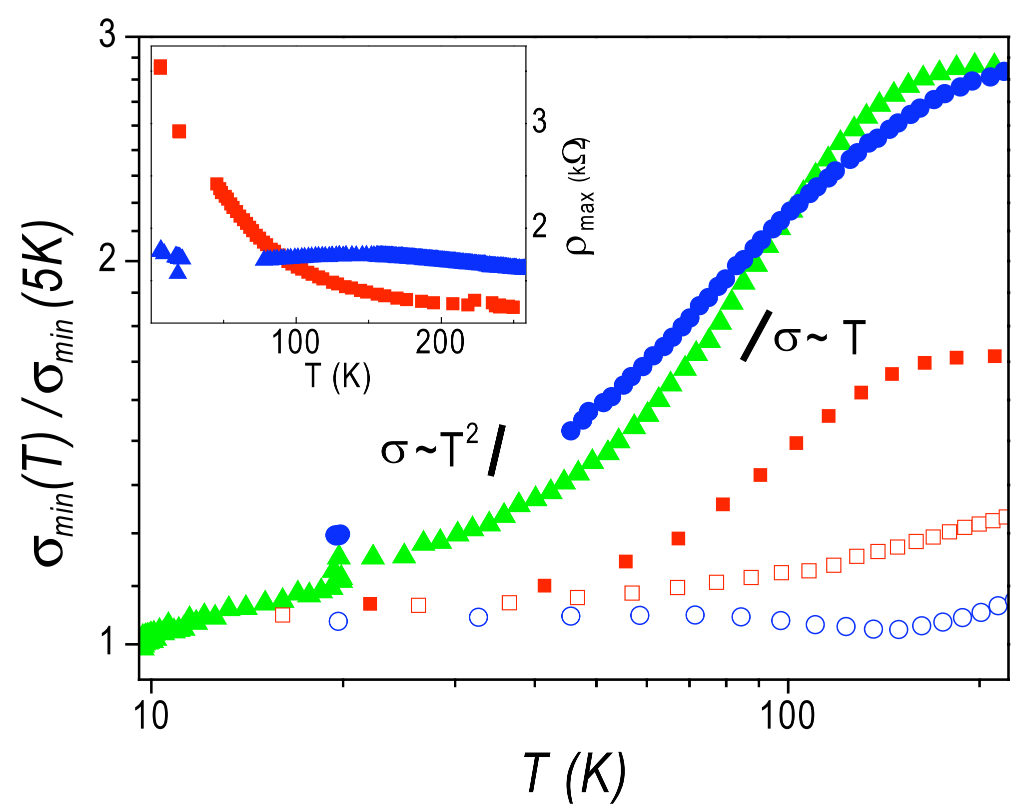


S.J. Hands, C. Strouthos, W. Armour, arXiv:0910.5646

Future projects II:
conductivity of graphene ...

Collaboration:
Eero Tölö, Lauri Suoranta (Aalto U.)
Joaquín Drut (Ohio State U.)

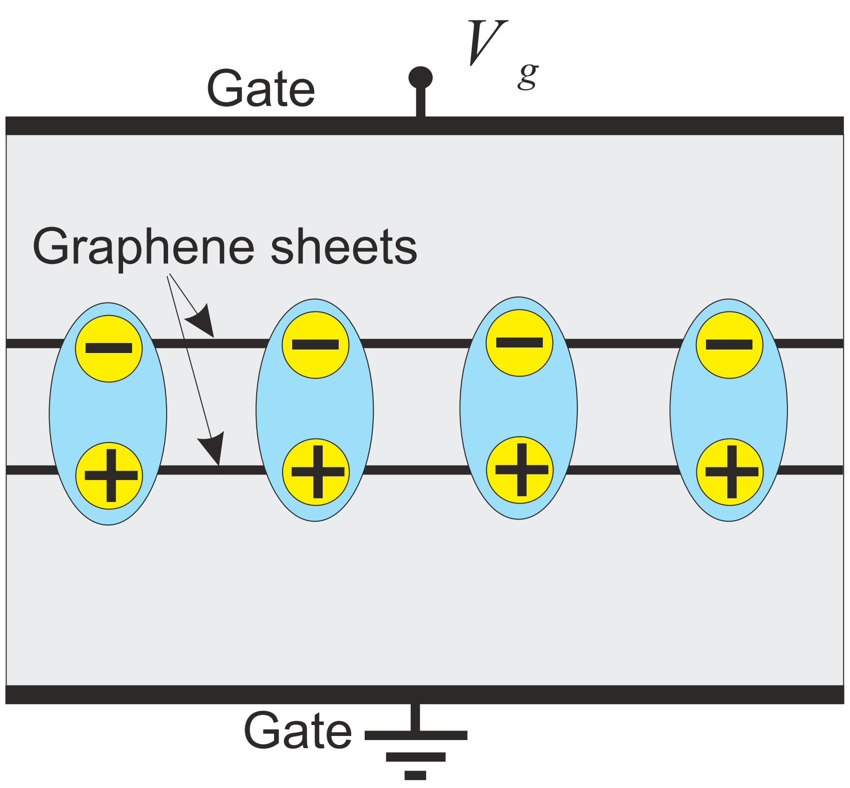


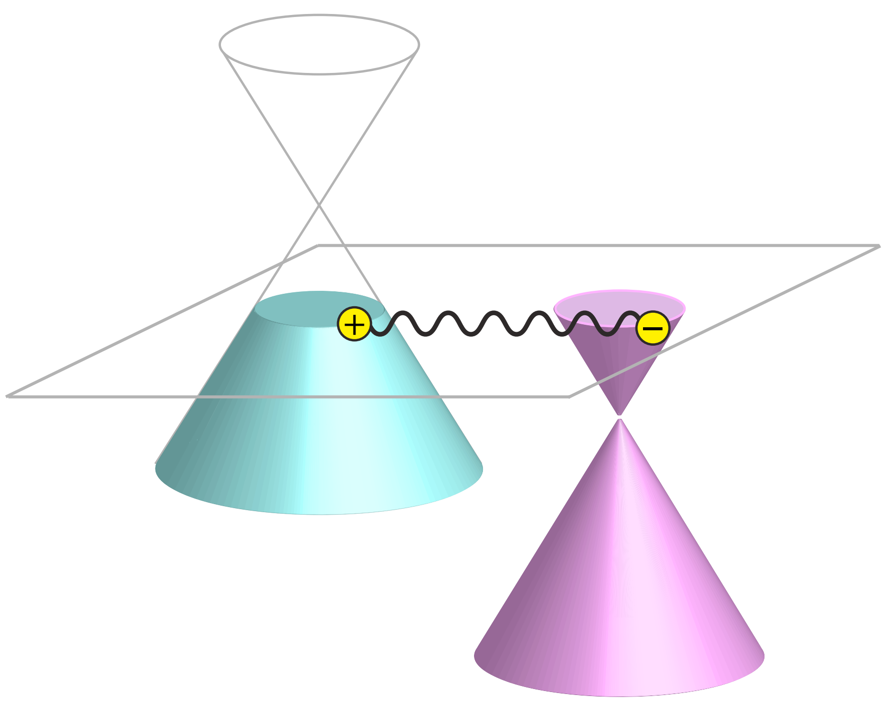


K.I. Bolotin et al., Phys. Rev. Lett. 101, 096802 (2008), V. Crespi, Physics 1, 15 (2008).

Future projects III:
exciton condensation in bilayer graphene ...

Collaboration:
Joaquín Drut (Ohio State U.)
Allan MacDonald (UT Austin) ...





M.Yu. Kharitonov, K. Efetov, arXiv:0903.4445