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

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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
- Nanotube: rolled graphene
- Graphite: stacked graphene
- Fullerene: wrapped graphene
Graphene phenomenology II: a promising material for applied physics ...

Graphene-based gate-controlled current switch ...

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

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 ...

\[
\begin{align*}
1s^2 & \quad 2s^2 \quad 2p^2 \\
\downarrow & \\
3 \; \text{sp}^2 + p & \\
\downarrow & \\
\text{lattice} & \quad \text{free electron}
\end{align*}
\]

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


Figure: A.H. Castro Neto, Materials Today 13, 1 (2010).
Graphene phenomenology VI: theory of the electronic band structure ...  

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

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

Conical dispersion around two “valleys”, centered around the “Dirac points” (K,K’) ...

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

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":

\[ E_k \simeq \nu k \]
\[ \nu \simeq c/300 \]

Velocity of quasiparticles

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**Fermions (in 2+1 dimensions)**

Dirac flavors, \( N_f = 2 \) describes a graphene monolayer ...

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

\[
D = \gamma_0 \partial_0 + \nu \gamma_i \partial_i, \quad i = 1, 2
\]

\[
\gamma^\mu, \mu = 0, 1, 2 \quad \{\gamma^\mu, \gamma^\nu\} = 2\delta^{\mu\nu}
\]
Graphene at low energies II: quasiparticles with instantaneous Coulomb interactions ...

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

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

Gauge field (in 3+1 dimensions)

Electrostatic Coulomb interaction ...

\[ A_0 \rightarrow A_0 + \alpha(t) \quad \psi \rightarrow \exp \left\{ i \int \! dt \alpha(t) \right\} \psi \]

Gauge invariance

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

\[ g^2 = \frac{e^2}{\epsilon_0} \]

\[ \alpha_g \equiv \frac{e^2}{4\pi\epsilon_0 \hbar v} \approx 300\alpha \sim 1 \]

Fine-structure constant of graphene
The massless quasiparticles possess **chiral symmetry**, which can be spontaneously broken ... 

\[ U(2N_f) \rightarrow U(N_f) \times U(N_f) \]

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

- **Semimetal**: chiral symmetry **unbroken**, quasiparticles remain **massless**. 
- **Insulator**: chiral symmetry **spontaneously broken**, quasiparticles **massive**.

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G.W. Semenoff, Phys. Rev. Lett. 54, 2449 (1984),
Lattice Monte Carlo simulation I: evaluating the condensate ...


Integrate out the fermion fields ...

\[ Z = \int DA_0 \exp(-S_{\text{eff}}[A_0]) \quad S_{\text{eff}}[A_0] = -N_f \ln \det(D[A_0]) + S_{E}^{q}[A_0] \]

Positive definite probability measure for MC calculation

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

\[ \sigma = \frac{1}{VZ} \int DA_0 \text{Tr}(D^{-1}[A_0]) \exp(-S_{\text{eff}}[A_0]) \]

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

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

\[ \beta = \frac{\epsilon_0 v}{e^2} \]
Lattice Monte Carlo simulation II:
finding the transition ... 

- 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) ...

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

- 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 ...

Continuum physics is recovered in the vicinity of the second-order transition.
Lattice Monte Carlo simulation III: discretized theory ...

Non-compact gauge action ...

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

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


\[ S^f_E[\bar{\chi}, \chi, U] = -\sum_{n,m} \bar{\chi}(n) D_s[U, n, m] \chi(m) \]

\[ D_s[U, n, m] = \frac{1}{2} (\delta_{n+e_0,m} U(n) - \delta_{n-e_0,m} U^\dagger(m)) + \frac{\nu}{2} \sum_i \eta^i(n) (\delta_{n+e_i,m} - \delta_{n-e_i,m}) + m_0 \delta_{n,m} \]

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

\[ U(n) = \exp \{ i\theta(n) \} \]
Lattice Monte Carlo simulation IV:
generation of gauge configurations, Hybrid Monte Carlo ...


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

\[ H = \sum_n \frac{\pi_n^2}{2} + S_E[\theta] \]

Enables global updates of the lattice gauge potential

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

\[ \text{det}(Q) \propto \int \mathcal{D}\phi \phi^\dagger \Phi \exp(-S^p_E) \]

\[ S^p_E = \sum_{n,m} \phi_n^\dagger Q^{-1}_{n,m}[\theta] \phi_m = \sum_n \xi_n^\dagger \xi_n \]

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

\[ H = \sum_n \frac{\pi_n^2}{2} + S^g_E + S^p_E \]

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

\[ \dot{\theta}_n = \frac{\delta H}{\delta \pi_n} = \pi_n, \]

\[ \dot{\pi}_n = -\frac{\delta H}{\delta \theta_n} \equiv F^g_n + F^p_n \]
Lattice Monte Carlo simulation V: extrapolation to the critical point ...


"Equation of state" analysis ...

\[ m_0 = f(\sigma, \beta) \]

Trial function (also for QED4) ...

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

Dependence on \( \sigma \):
Information on critical exponents \( \delta, \beta_m \) !

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

Simultaneous fit to condensate and susceptibility

Dependence on \( \beta \):
Information on critical coupling \( \beta_c \)!

\[ X(\beta) = X_0 + X_1 (1 - \beta / \beta_c) \]
\[ Y(\beta) = Y_1 (1 - \beta / \beta_c) \]
Results I:
quantum phase transition into a gapped phase ...


$\beta_c \sim 0.073 \pm 0.002$

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:

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

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


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

\[ 4 < N_{\text{crit}} < 6 \]

J.E. Drut, T.A. Lähde,
Results IV:
supporting results by other groups (some examples) ...

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

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

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

- **Strong-coupling expansion of the lattice theory:**
  chiral EFT technique, transition to insulating phase confirmed ...
  
We chose arbitrarily to simulate the non-compact theory of graphene ...

\[ S_{E}^{g, nc}[\theta] = \frac{\beta}{2} \sum_{n} \left[ \sum_{i=1}^{3} \left( \theta_{n} - \theta_{n+e_{i}} \right)^{2} \right] \]

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

\[ S_{E}^{g, c}[\theta] = \beta \sum_{n} \left[ 3 - \sum_{i=1}^{3} \Re \left( U_{n} U_{n+e_{i}}^{\dagger} \right) \right] \]

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 ... 


- 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 ...


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

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 ...

\[ U_\mu \rightarrow u_0 e^{iagA_\mu^{IR}} \approx u_0 (1 + iagA_\mu^{IR}) \]

Renormalized gauge links give results closer to the continuum limit, estimate the correction \textit{a posteriori} ...

\[ u_0 \equiv \langle P \rangle^{1/2}, \quad P = \frac{1}{V} \sum_n U_n U_n^\dagger e_i \]
**Lattice artifacts IV: tadpole improvement of the non-compact theory ...**


\[ D_{n,n'}^I[\theta] = \frac{1}{2} \left[ \delta_{n+e_0,n'} U_n - \delta_{n-e_0,n'} U_{n'}^\dagger \right] \]
\[ + \frac{v'}{2} \sum_i \eta_{i,n} \left[ \delta_{n+e_i,n'} - \delta_{n-e_i,n'} \right] + m'_0 \delta_{n,n'} \]

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

\[ \sigma' \equiv \sigma/u_0, \quad v' \equiv u_0 v, \quad m'_0 \equiv u_0 m_0 \quad \chi \equiv \sqrt{u_0} \chi' \]

**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 ...


$$\beta_c \sim 0.074 \pm 0.001$$

Data at strong coupling cannot be fitted, “scaling violations” ...
Lattice artifacts VI:
tadpole-improved non-compact theory ...


\[ \beta_c \sim 0.165 \pm 0.001 \]  
Significant effect, insulating phase more likely!

Fit range and stability much improved ...

\[ \beta \equiv \frac{v}{g^2} = \frac{v'/u_0}{g'^2} = \frac{\beta'}{u_0} \]
Lattice artifacts VII: tadpole-improved compact theory?


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

\( \beta_c \sim 0.40 \xrightarrow{\text{TI}} \beta_c \sim 0.25 \)

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 ...

\[ \text{U(4) } \rightarrow \text{U(2) } \times \text{U(2)} \]

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

\[ \text{U(1) } \times \text{U(1)} \rightarrow \text{U(1)} \]


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.)

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

Future projects II: conductivity of graphene...

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

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

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