Monte-Carlo simulations of the electronic properties of graphene

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Graphene: strongly coupled fermionic field theory

- Large effective coupling constant $\alpha \sim 1/137$, $1/v_F \sim 2$
- Experimental data are not always clean
- Numerical methods are required
- Massless Dirac fermions at low energies
- Spontaneous breaking of chiral symmetry???
- Numerical studies of effective low energy theory using lattice QCD techniques (staggered fermions)
  [J. Drut, T. Lahde, S. Hands, ITEP Group]
- Numerical studies directly on the hexagonal lattice
  [ITEP Group, C. Rebbi, R. Brower, D. Schaich]
Geometry of hexagonal lattice

Periodic boundary conditions on the Euclidean torus:

\[ (\xi_1 + L_x, \xi_2) \rightarrow (\xi_1, \xi_2), \]
\[ (\xi_1, \xi_2 + L_y) \rightarrow (\xi_1 + L_y/2, \xi_2). \]
The “Tight-binding” Hamiltonian

\[ \hat{H}_{tb} = -\kappa \sum_{\sigma=\uparrow, \downarrow} \sum_{<XY>} \left( \hat{a}_{\sigma,X}^\dagger \hat{a}_{\sigma,Y} + \hat{a}_{\sigma,Y}^\dagger \hat{a}_{\sigma,X} \right) \]

\[ \{ \hat{a}_{\sigma,X}^\dagger, \hat{a}_{\sigma',Y} \} = \delta_{\sigma \sigma'} \delta_{X,Y} \]

\[ \hat{H}_I = \sum_{X,Y} \frac{e^2}{r(X,Y)} \hat{q}_X \hat{q}_Y, \]
• Each lattice site can be occupied by two electrons (with opposite spin)

• The ground states is electrically neutral

• One electron (for instance) at each lattice site

• «Dirac Sea»: hole = absence of electron in the state
Hamiltonian: particles and holes

\[
\hat{H}_{tb} = -\kappa \sum_{\sigma=\uparrow,\downarrow} \sum_{<XY>} \left( \hat{\psi}^\dagger_{\sigma,X} \exp \left( \pm i \hat{\theta}_{XY} \right) \hat{\psi}_{\sigma,Y} + \hat{\psi}^\dagger_{\sigma,Y} \exp \left( \pm i \hat{\theta}_{YX} \right) \hat{\psi}_{\sigma,X} \right) + \\
+ \sum_{\sigma=\uparrow,\downarrow} \sum_{X_1} m \hat{\psi}^\dagger_{\sigma,X_1} \hat{\psi}_{\sigma,X_1} - \sum_{\sigma=\uparrow,\downarrow} \sum_{X_2} m \hat{\psi}^\dagger_{\sigma,X_2} \hat{\psi}_{\sigma,X_2} \tag{9}
\]

Redefinition of creation/annihilation operators

\[
\hat{\psi}_{\uparrow,X} = \hat{a}^\dagger_{\uparrow,X}, \quad \hat{\psi}_{\downarrow,X} = \pm \hat{a}^\dagger_{\downarrow,X},
\]

Charge operator

\[
\hat{q}_X = \hat{\psi}^\dagger_{\uparrow,X} \hat{\psi}_{\uparrow,X} - \hat{\psi}^\dagger_{\downarrow,X} \hat{\psi}_{\downarrow,X}.
\]
Spectrum of quasiparticles in graphene

Consider the non-Interacting tight-binding model!!!

Eigenmodes are just the plain waves:

\[
\psi_{\zeta} (\alpha, \xi; q) = N_{\alpha,\zeta} (q) \exp (i q \xi), \\
\psi_{\zeta} (\beta, \xi; q) = N_{\beta,\zeta} (q) \exp (i q \xi),
\]

Eigenvalues:

\[
E_{\zeta} (q) \equiv \zeta E (q) = \zeta \sqrt{m^2 + \kappa^2 |\Phi (q)|^2},
\]

Wave function normalization:

\[
N_{\alpha,\zeta} (q) = \sqrt{\frac{E (q) + \zeta m}{2 E (q) L_x L_y}}, \\
N_{\beta,\zeta} (q) = -\zeta e^{-i\varphi(q)} \sqrt{\frac{E (q) - \zeta m}{2 E (q) L_x L_y}},
\]

\[
\Phi (k) = \sum_{a=1}^{3} e^{i \mathbf{k} \cdot \mathbf{e}_a}
\]
Spectrum of quasiparticles in graphene

Close to the «Dirac points»: $E = v_F k$
Spectrum of quasiparticles in graphene

Dirac points are only covered by discrete lattice momenta if the lattice size is a multiple of three
Symmetries of the free Hamiltonian

- 2 Fermi-points \times 2 sublattices = 4 components of the Dirac spinor

- Chiral U(4) symmetry (massless fermions): right ↔ left

- Discrete \( \mathbb{Z}_2 \) symmetry between sublattices

- U(1) x U(1) symmetry: conservation of currents with different spins
Coulomb interactions

\[ V(r) = \frac{2e^2}{(\varepsilon + 1)r} \]

\[ \alpha \rightarrow \frac{2\alpha}{\varepsilon + 1} \]

Dielectric permittivity:

- Suspended graphene
  \[ \varepsilon = 1.0 \]
- Silicon Dioxide SiO\(_2\)
  \[ \varepsilon \sim 3.9 \]
- Silicon Carbide SiC
  \[ \varepsilon \sim 10.0 \]

Coupling constant

\[ \alpha \sim \frac{1}{137} \quad \frac{1}{v_F} \sim 1 \]

Strongly coupled theory!!!
Numerical simulations using the Hybrid Monte-Carlo method

- Hexagonal lattice
- Noncompact $\text{U}(1)$ gauge field
- Algorithm can be accelerated outside of graphene plane
- Geometry: graphene on the substrate
Numerical simulations using the Hybrid Monte-Carlo method

Discretization of Laplacian on the hexagonal lattice reproduces Coulomb potential with a good precision.
Numerical simulations using the Hybrid Monte-Carlo method

Lattice action for fermions:

\[ S_{lb} [\eta(s, \xi, \tau)] = \sum_{s, \xi, \tau, s', \xi', \tau'} \bar{\eta}(s, \xi, \tau) M[s, \xi, \tau; s', \xi', \tau'] \eta(s', \xi', \tau') = \]
\[ = \sum_{s, \xi, \tau} \bar{\eta}(s, \xi, \tau) \left( \eta(s, \xi, \tau) - e^{i\phi(s, \xi, \tau)} \eta(s, \xi, \tau + \Delta\tau) \right) - \]
\[ -\kappa \Delta\tau \sum_{\xi, \tau, b} \bar{\eta}(\alpha, \xi, \tau) e^{i\phi(\alpha, \xi, \tau)} \eta(\beta, \xi + \rho_b, \tau + \Delta\tau) - \kappa \Delta\tau \sum_{\xi, \tau, b} \bar{\eta}(\beta, \xi, \tau) e^{i\phi(\beta, \xi, \tau)} \eta(\alpha, \xi - \rho_b, \tau + \Delta\tau) + \]
\[ + m \Delta\tau \sum_{\xi, \tau} \bar{\eta}(\alpha, \xi, \tau) e^{i\phi(\alpha, \xi, \tau)} \eta(\alpha, \xi, \tau + \Delta\tau) - m \Delta\tau \sum_{\xi, \tau} \bar{\eta}(\beta, \xi, \tau) e^{i\phi(\beta, \xi, \tau)} \eta(\beta, \xi, \tau + \Delta\tau), \]

Path integral weight:

\[ Z = \int D\phi(s, \xi, \tau, z) \left| \det (M[\phi(s, \xi, \tau, z = 0)]) \right|^2 \]
\[ \exp (-S_{em}[\phi(s, \xi, \tau, z)]) \]
Spontaneous sublattice symmetry breaking in graphene

Order parameter:
The difference between the number of particles on A and B sublattices

$$\Delta_N = N_A - N_B$$

“Mesons”: particle-hole bound state
Differences of particle numbers

Differences of particle numbers

Differences of particle numbers

Differences of particle numbers

Differences of particle numbers

Differences of particle numbers

Differences of particle numbers

Differences of particle numbers

Differences of particle numbers
Differences of particle numbers on lattices of different size
Extrapolation to zero mass

\[ \langle \Delta N \rangle \]

\[ \varepsilon \]

- Graph showing \( \langle \Delta N \rangle \) versus \( \varepsilon \) for different lattice sizes and temperatures.
- Data points for different lattice sizes and temperatures are marked with different symbols and colors.
- Trends indicate a decrease in \( \langle \Delta N \rangle \) with increasing \( \varepsilon \).
- Extrapolation to zero mass is suggested through the graph trend.
Susceptibility of particle number differences

\[
\chi_N = \left. \frac{\partial \Delta_N}{\partial m} \right|_{m \to 0}
\]
Conductivity of graphene

Current operator:

\[ \frac{\partial}{\partial t} \hat{q}(s, \xi) = \sum_a \hat{J}_a(s, \xi), \]

= charge, flowing through lattice links

\[ \hat{J}_a(\xi) = \hat{J}_{\uparrow,a}(\xi) - \hat{J}_{\downarrow,a}(\xi) \]

\[ \hat{J}_{\sigma,a}(\xi) = i \kappa \hat{\psi}_{\sigma}^\dagger(\beta, \xi + \rho_a) e^{\mp i \hat{\theta}_a(\xi)} \hat{\psi}_\sigma(\alpha, \xi) - \]

\[ - i \kappa \hat{\psi}_{\sigma}^\dagger(\alpha, \xi) e^{\pm i \hat{\theta}_a(\xi)} \hat{\psi}_\sigma(\beta, \xi + \rho_a), \]

\[ \hat{J}_a(\alpha, \xi) = \hat{J}_a(\xi), \quad \hat{J}_a(\beta, \xi) = \hat{J}_a(\xi - \rho_a). \]

Retarded propagator and conductivity:

\[ G_{Rab}(\xi, t; \xi', t') = i \theta(t - t') \times \]

\[ \times \text{Tr} \left( \left[ \hat{J}_a(\xi, t), \hat{J}_b(\xi', t') \right] e^{-\hat{H}/(kT)} \right) \]

\[ \sigma(w) = \frac{G_{Rbc}(w) T_{bc}}{3 \sqrt{3} w}, \]
Conductivity of graphene: Green-Kubo relations

Current-current correlators in Euclidean space:

\[
G(\tau) = \frac{1}{3\sqrt{3} L_x L_y} \sum_{\xi, \xi'} T_{bc} \times \nabla \times \text{Tr} \left( e^{\tau \hat{H}} \hat{J}_b(\xi) e^{-\tau \hat{H}} \hat{J}_c(\xi') e^{-\hat{H}/T} \right)
\]

Green-Kubo relations:

\[
G(\tau) = \int_0^{\infty} \frac{dw}{2\pi} K(w, \tau) \sigma(w),
\]

Thermal integral kernel:

\[
K(w, \tau) = \frac{2w \cosh \left( w \left( \tau - \frac{1}{2T} \right) \right)}{\sinh \left( \frac{w}{2T} \right)}.
\]
Conductivity of graphene

\( \sigma(\omega) \) – dimensionless quantity
(in a natural system of units), in SI: \( \sim e^2/h \)

Conductivity from Euclidean correlator:
an ill-posed problem

Maximal Entropy Method

Approximate calculation of \( \sigma(0) \):

\[
G(\beta/2) = \int_0^{+\infty} dw \frac{2w}{2\pi \sinh(\beta w / 2)} \sigma(w) \approx \pi (kT)^2 \sigma(0)
\]

AC conductivity, averaged over \( w \leq kT \)
Conductivity of graphene: free theory

For small frequencies (Dirac limit):

\[
\sigma^{(0)}(w) \approx \Xi \delta(w) + \theta(w - 2m) \left( 1 + \frac{4m^2}{w^2} \right) \tanh \left( \frac{\beta w}{4} \right),
\]

Threshold value \( w = 2m \)

Universal limiting value at \( \kappa >> w >> m \):

\[
\sigma_0 = \pi e^2/2 \ h=1/4 \ e^2/\hbar
\]

At \( w = 2m \):

\[
\sigma = 2\sigma_0
\]
Conductivity of graphene: Free theory
Current-current correlators: numerical results

\[ \kappa \Delta t = 0.15, \ m \Delta t = 0.01, \ \kappa/(kT) = 18, \ L_s = 24 \]
Conductivity of graphene $\sigma(0)$: numerical results (approximate definition)
Conclusions

• Electronic properties of graphene at half-filling can be studied using the Hybrid Monte-Carlo algorithm.

• Sign problem is absent due to the symmetries of the model.

• Signatures of insulator-semimetal phase transition for monolayer graphene.

• Order parameter:
  difference of particle numbers on two simple sublattices

• Spontaneous breaking of sublattice symmetry is accompanied by a decrease of conductivity

see ArXiv:1206.0619
Outlook

• **A puzzle**: according to lattice data, there should be spontaneous breaking of sublattice symmetry for suspended graphene

• **BUT** we observe rather mild decrease of conductivity

• Experimentally: suspended graphene is conducting, no signature of a gap in the spectrum [Elias et al. 2011]

• Confirmed by approximate analytical calculations [Talk by C. Popovici]