ITEP Lattice

Lattice simulations of graphene on the hexagonal lattice

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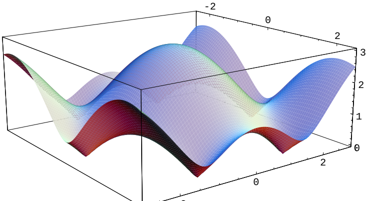
Tight-binding model of graphene

- The simplest model: hopping of charge carriers between neighboring atoms

$$\hat{H}_0 = -\kappa \sum_{<xy>} \sum_{s=\uparrow\downarrow} \left(\hat{\psi}^\dagger_s(x) \hat{\psi}_s(y) + \hat{\psi}^\dagger_s(y) \hat{\psi}_s(x) \right)$$

- $\left\{ \hat{\psi}^\dagger_s(x), \hat{\psi}_{s'}(y) \right\} = \delta(x,y)\,\delta(s,s')$ - Fermi statistics
- $\kappa = 2.7\,eV$ - characteristic energy scale



Tight-binding model: ground state

- 1 free charge carrier per atom.
- Assume: all carriers have spin $s = \uparrow$ (highly degenerate ground state).
- Ground state:

$$\hat{\psi}_{\downarrow}(x)\,|0\rangle = 0, \quad \hat{\psi}^{\dagger}_{\uparrow}(x)\,|0\rangle = 0,$$

- $\Rightarrow s = \downarrow$ - particles, $s = \uparrow$ - holes

Tight-binding model: electromagnetic interactions

- Characteristic speed of charge carriers $v_F \approx c/300$
- Magnetic interactions: $\alpha_M \sim v_F e^2 \sim 1/(137 \times 300)$
- Electric interactions: $\alpha_E \sim e^2/v_F \sim 300/137$ - STRONG COUPLING
- Coulomb interaction in the tight-binding model:

$$\hat{H}_I = \sum_{x \neq y} \hat{q}(x)\, \hat{q}(y)\, \frac{2e^2}{(1+\epsilon)\,|x-y|}$$

- $\hat{q}(x) = \hat{\psi}^\dagger_\downarrow \hat{\psi}_\downarrow - \hat{\psi}_\uparrow \hat{\psi}^\dagger_\uparrow$ - charge operator

Our model: tight-binding model + Coulomb interaction

- Coulomb interaction: introduce scalar field which propagates in 3D

$$\hat{H} = \hat{H}_0 + \sum_{x} \hat{q}(x)\,\hat{\phi}(x) + \frac{1+\epsilon}{2e^2} \int d^2x dz \left(\partial \hat{\phi}(x,z)\right)^2$$

- Phonon interactions, lattice distortions etc. are NOT taken into account

Lattice discretization for tight-binding model

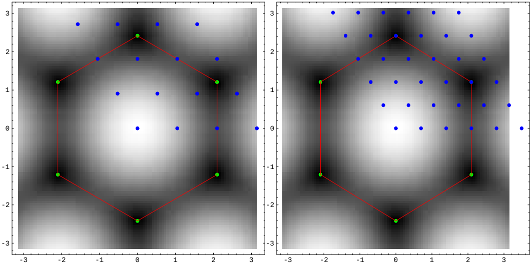
- Two dimensions are discretized by definition
- Spacing of hexagonal lattice: $a = 1.42 \cdot 10^{-10} m$.
- Spacing in z direction: $\Delta z \sim a$, no sense to take smaller values
- L_t discrete time steps of size Δt:

$$\hbar^{-1} \kappa \Delta t \ll 1, \quad \hbar^{-1} \kappa \Delta t \, L_t \gg 1$$

Lattice discretization for tight-binding model

- In realistic simulations $\hbar^{-1}\kappa\Delta t \sim 2$, $L_t \sim 20$
- Time step is much larger than spatial spacing (nonrelativistic system): $\delta t \approx a/v_F$
- Effective temperature $T \sim \frac{\hbar}{k\Delta t L_t} \sim 10^3 K$
- Temperature dependence of the electronic properties should be small
- Extrapolation to smaller temperatures should be easy
- Model can be studied by Monte-Carlo methods common for lattice QCD
- BUT: only equilibrium properties

Lattice discretization: periodic boundary conditions on the torus



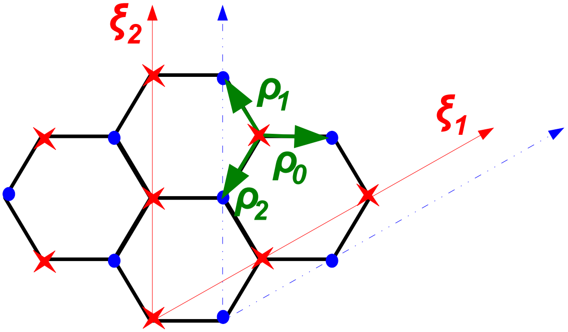
$\Rightarrow$ Dirac points are covered only if torus size $L_s = 3n$, $n \in \mathbb{Z}$.

Technical details: lattice discretization

- Start with a Feynman-Kac formula:

$$\mathrm{Tr}\,\exp\left(-\hat{H}/kT\right) = \mathrm{Tr}\prod_{n}\exp\left(-\Delta t\,\hat{H}\right) =$$
$$= \int \mathcal{D}\bar{\psi}\left(\xi,t\right)\mathcal{D}\psi\left(\xi,t\right)D\phi\left(\xi,z,t\right)$$
$$\exp\left(-S_F\left(\bar{\psi},\psi,\phi\right) - S_P\left(\phi\right)\right)$$

Technical details: Coordinates on hexagonal lattice



Technical details: lattice action for fermions

$$
\begin{aligned}
S_F = \sum_{\xi,t} & \bar{\psi}_A(\xi,t)\, e^{-i\phi_A(t-\Delta t)} \psi_A(\xi, t-\Delta t) - \bar{\psi}_A(\xi,t)\,\psi_A(\xi,t) \\
& + \bar{\psi}_B(\xi,t)\, e^{-i\phi_B(t-\Delta t)} \psi_B(\xi, t-\Delta t) - \bar{\psi}_B(\xi,t)\,\psi_B(\xi,t) \\
& + \kappa \Delta t \sum_{a=1}^{3} \bar{\psi}_A(\xi,t)\, e^{-i\phi_A(t-\Delta t)} \psi_B(\xi+\rho_a, t-\Delta t) \\
& + \kappa \Delta t \sum_{a=1}^{3} \bar{\psi}_B(\xi,t)\, e^{-i\phi_B(t-\Delta t)} \psi_A(\xi-\rho_a, t-\Delta t)
\end{aligned}
$$

Technical details: lattice action for "photons"

$$S_P = \sum_{\xi,z,t} \frac{\beta_{hex}}{2}\sum_{a}\left(\phi_A\left(\xi,z,t\right)-\phi_B\left(\xi+\rho_a,z,t\right)\right)^2 + \frac{\beta_z}{2}\left(\phi_A\left(\xi,z,t\right)-\phi_A\left(\xi,z+\Delta z,t\right)\right)^2 + \frac{\beta_z}{2}\left(\phi_B\left(\xi,z,t\right)-\phi_B\left(\xi,z+\Delta z,t\right)\right)^2$$

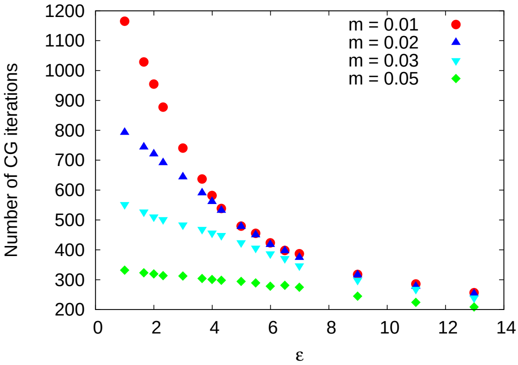
Technical details: path integral in terms of photons

- Fermion action is bilinear: $S_F = \bar{\psi} M \psi$
- Fermions can be integrated out exactly:

$$\mathcal{Z} = \int \mathcal{D}\phi\left(\xi, z, t\right) \det\left(M\right) \det\left(M^{\dagger}\right) \exp\left(-S_P\left(\phi\right)\right)$$

- Monte-Carlo sampling of the field $\phi\left(\xi, z, t\right)$ with this weight
- $\Rightarrow$ Hybrid Monte-Carlo algorithm

Technical details: algorithm performance



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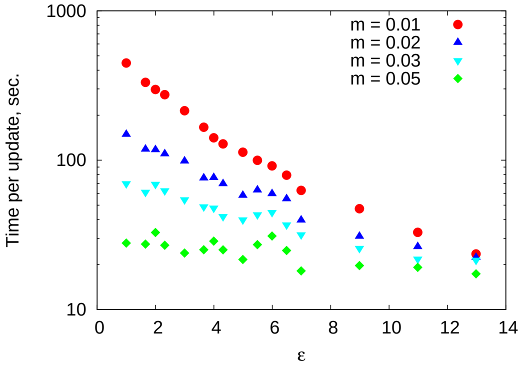
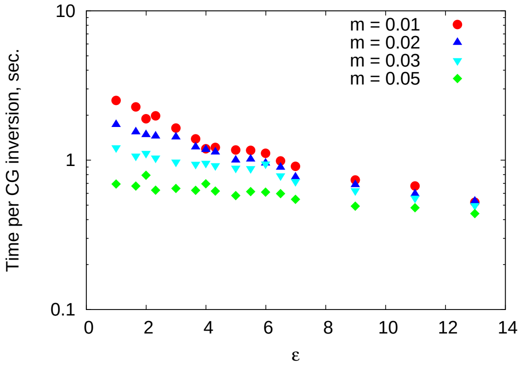
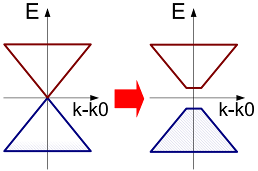


Technical details: algorithm performance

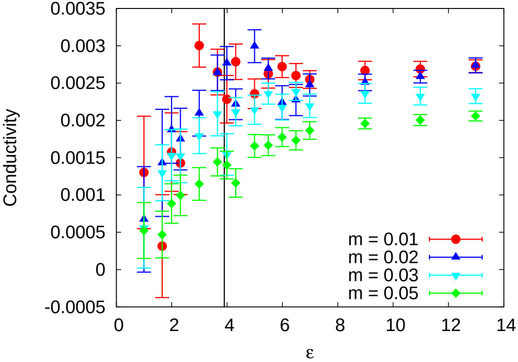


Conductivity of graphene

- "Non-interacting" graphene: conductor
- Interactions can induce a gap in the spectrum
- Strength of Coulomb interaction: controlled by substrate properties
- Critical ϵ: close to SiO_2 [Son, Semenoff, Araki, Drut, Lahde 2008-2012]



Conductivity of monolayer graphene: simulation results



20x20x20x20 lattice

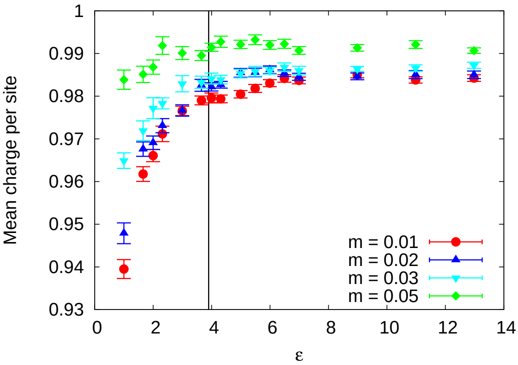
Spontaneous breaking of lattice symmetry

- Symmetry between the two sublattices: similar to chiral symmetry in gauge theories:

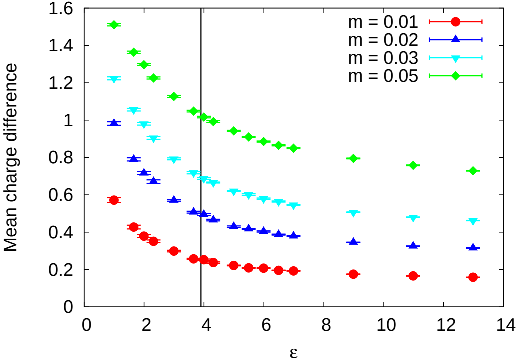
$$\hat{H} = \hat{\psi}^\dagger \begin{pmatrix} 0 & \hat{h}_{AB} \\ \hat{h}_{BA} & 0 \end{pmatrix} \hat{\psi}$$

- Order parameter: difference of charges Q_A and Q_B.
- This symmetry can be spontaneously broken by Coulomb interactions [Araki 2012]
- Also: nonzero density of particles and holes

Mean charge per site (particles)

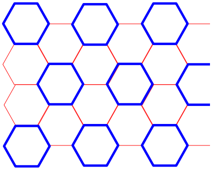


Difference of charges on sublattices A and B



Background magnetic field

- Paramagnetic effects: electron spins (might be difficult to simulate)
- Diamagnetic effects: Landau levels for free charge carriers
- More sophisticated patterns of symmetry breaking like Kekule distortion
- Spin-specific conductivity [Kharzeev 2007]

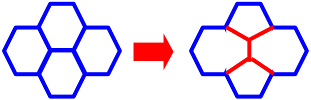


Conclusions

- Tight-binding model of graphene: good approximation for studying electromagnetic interactions in graphene
- Describes insulator-conductor phase transition
- Describes spontaneous breaking of sublattice symmetries and Kekule distortion [Araki 2012]
- Realistic lattice sizes: $\sim 10^1 \ldots 10^2$ crystal cells
- Realistic temperatures: $\sim 10^4 K$

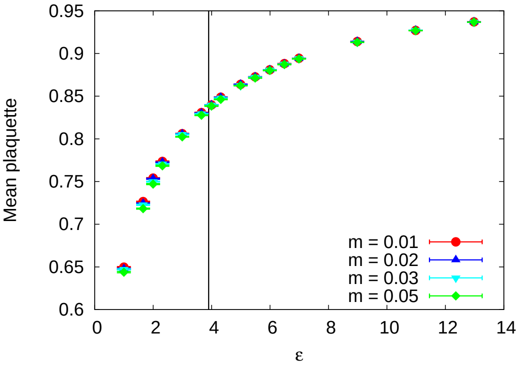
Further developments

- Multi-layer configurations with arbitrary tunneling rate
- Background magnetic field (also as an effective description of strain)
- Possibility to introduce lattice defects
- Phonons as additional dynamical field

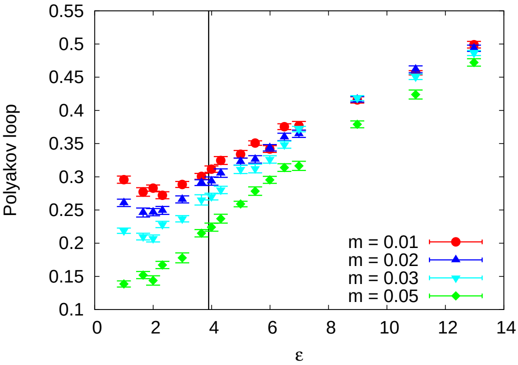


Back-up slides

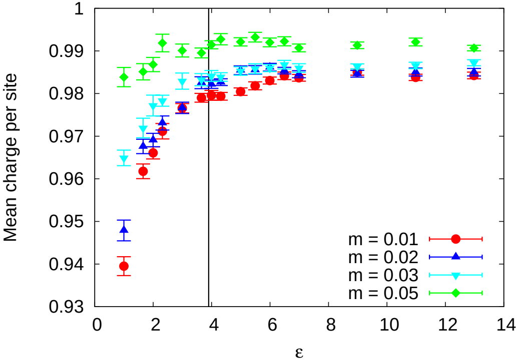
Mean plaquette



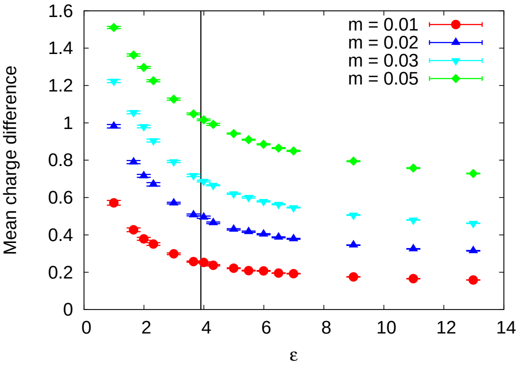
Polyakov loop



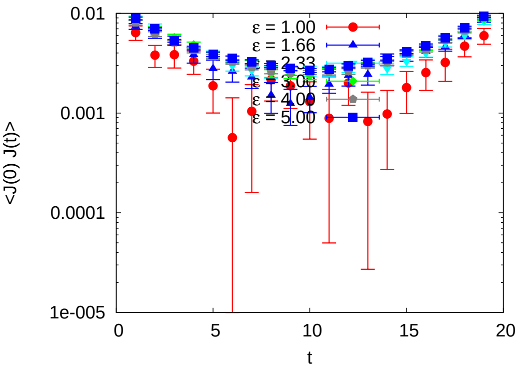
Mean charge per site



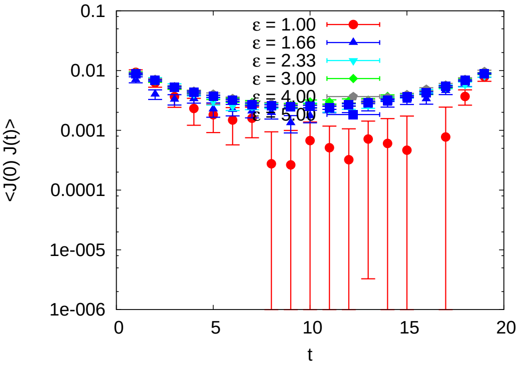
Difference of charges on sublattices A and B



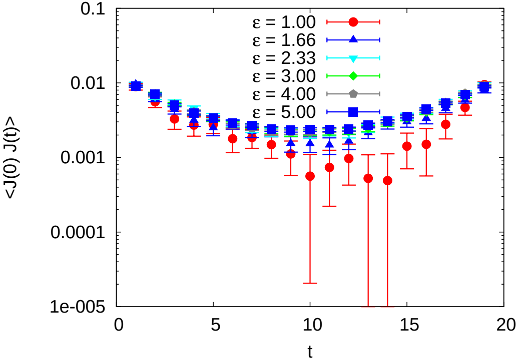
Current-current correlators at $m = 0.01$



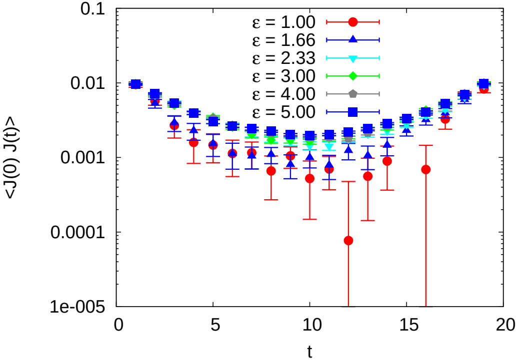
Current-current correlators at $m = 0.02$



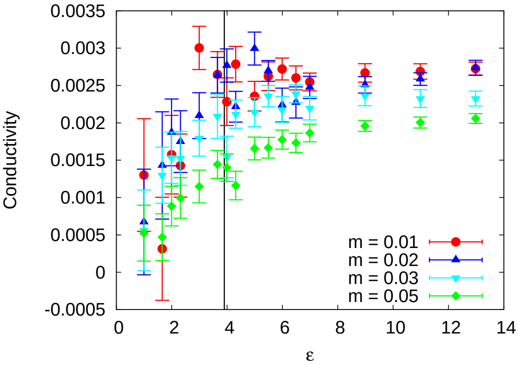
Current-current correlators at $m = 0.03$



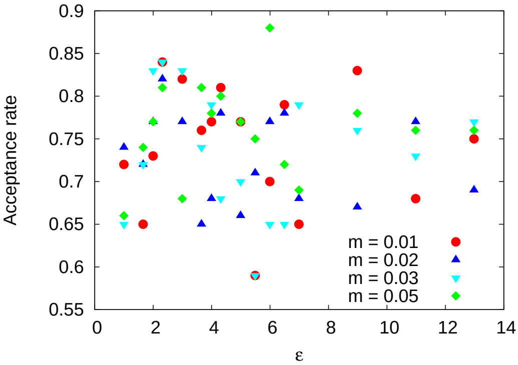
Current-current correlators at $m = 0.05$



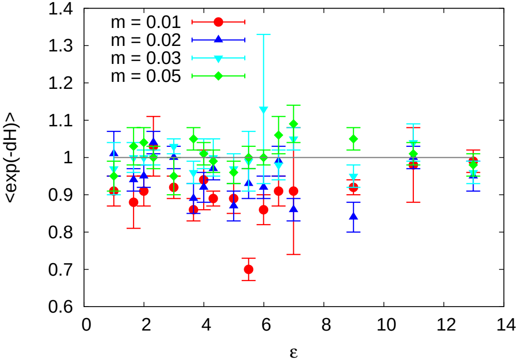
Conductivity of graphene monolayer



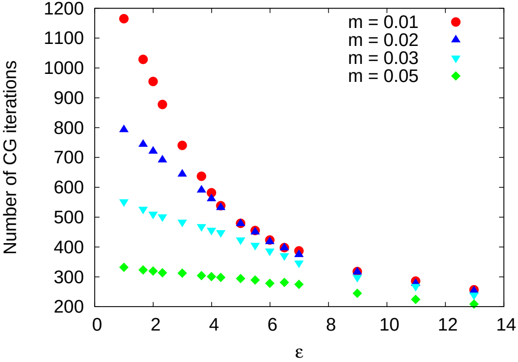
Acceptance rate



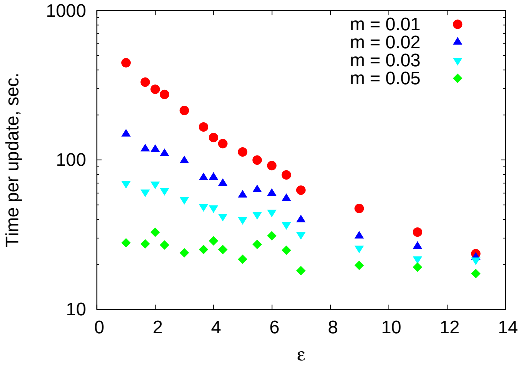
<exp(-dH)>


m = 0.01
m = 0.02
m = 0.03
m = 0.05
<exp(-dH)>
ε
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0
2
4
6
8
10
12
14

Average number of CG iterations (per inversion)



Average duration of a single HMC update



Average duration of a single CG inversion