Competing order in the fermionic Hubbard model on the hexagonal graphene lattice

Southampton, 27 July 2016

Pavel Buividovich, Maksim Ulybyshev
(Regensburg)

Dominik Smith, Lorenz von Smekal
(Giessen)

DFG Deutsche Forschungsgemeinschaft

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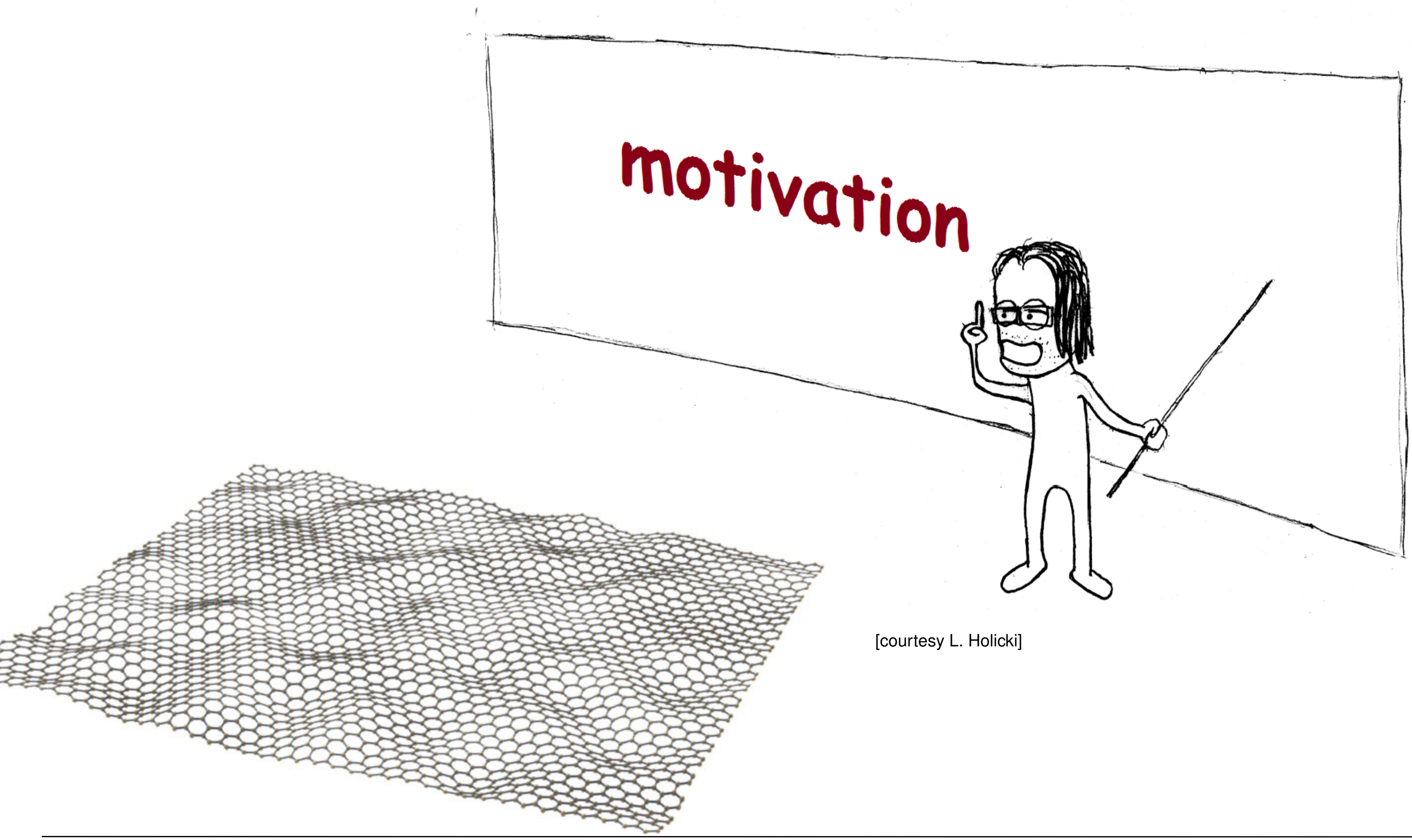
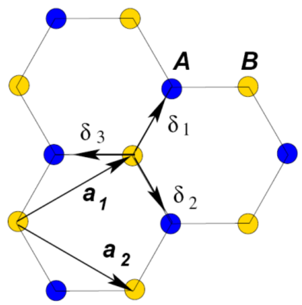
Introduction

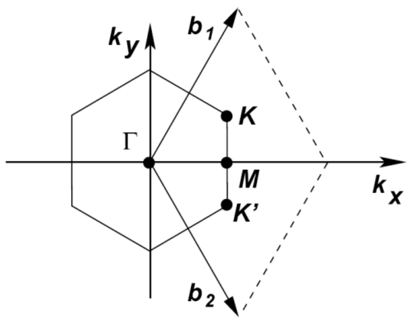


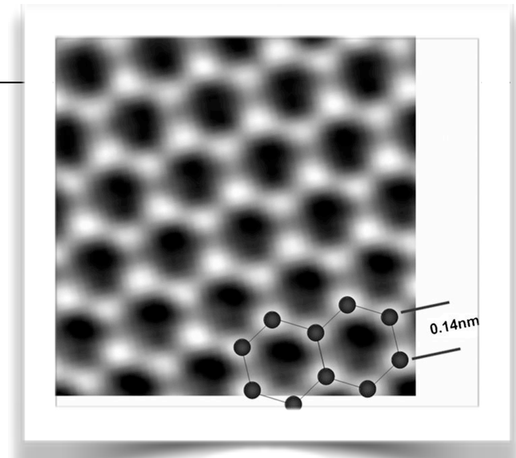
[courtesy L. Holicki]

Honeycomb Lattice

- triangular lattice – hexagonal Brillouin zone
  (2 atoms per unit cell)







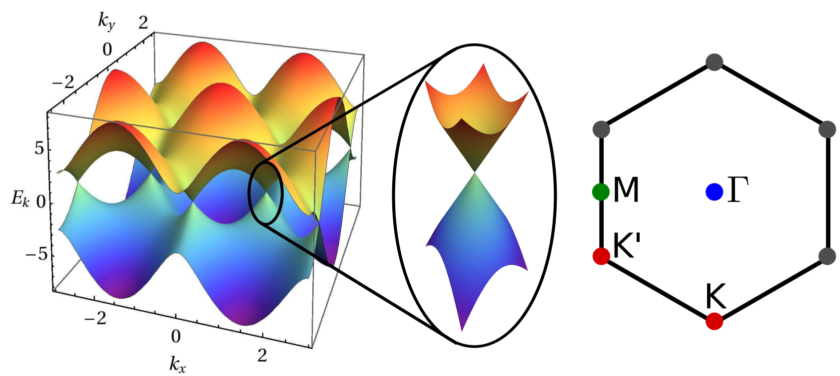
graphene

- single-particle energy bands

$$E_\pm(\mathbf{k}) = \pm\,|\Phi(\mathbf{k})|$$

structure factor:

$$\boldsymbol{\Phi}(\mathbf{k}) = t\sum_i e^{i\mathbf{k}\cdot\boldsymbol{\delta}_i}$$



- massless dispersion around Dirac points $K_\pm$

[Wallace, 1947]

$$E(\mathbf{p}) = \pm\hbar v_f|\mathbf{p}|\,, \qquad v_f = 3ta/2 \simeq 1\times 10^6\mathrm{m/s} \simeq c/300$$

Honeycomb Lattice

- **mass terms (gaps)**

Graphene Gets a Good Gap on SiC
Nevis *et al.*, PRL 115 (2015) 136802

$$\mathcal{H}_m = \frac{1}{N^2} \sum_{\boldsymbol{k},\sigma} m_\sigma \left(a^\dagger_{\boldsymbol{k},\sigma} a_{\boldsymbol{k},\sigma} - b^\dagger_{\boldsymbol{k},\sigma} b_{\boldsymbol{k},\sigma} \right)$$

(pseudo-spin) staggered on-site potential

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- **spin (flavor) dependence**

$$m_{\text{cdw}} = \frac{1}{2} (m_u + m_d)$$
$$m_{\text{sdw}} = \frac{1}{2} (m_u - m_d)$$

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- **Coulomb interaction**

$$\alpha_g = \frac{e^2}{4\pi\varepsilon \, \hbar v_f}$$

effective coupling

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- **spin (flavor) dependence**

with strong interactions:
Mott-insulator transition

$$m_{\mathrm{cdw}} = \frac{1}{2}(m_u + m_d) \quad \xrightarrow{m \to 0} \quad \text{charge-density wave (CDW)}$$

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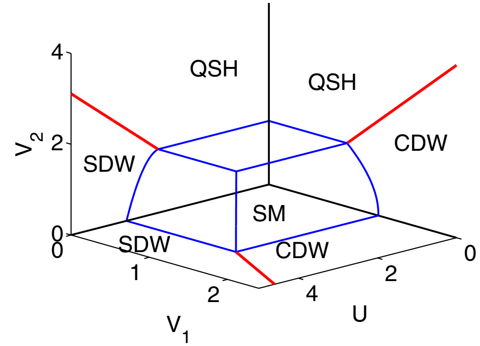

Raghu *et al.*, PRL 100 (2008) 156401

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$$m \to 0$$

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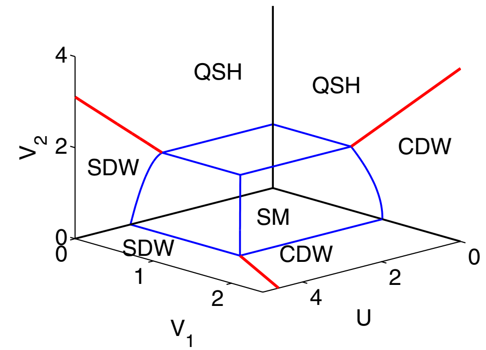
effective coupling

- **sign-problem in HMC** with $m_{\rm cdw} > 0$



Raghu *et al.*, PRL 100 (2008) 156401

Potentially Strong Interactions

- **suspended graphene**

  $\varepsilon \to 1$

$$\alpha_g = \frac{e^2}{4\pi\,\hbar v_f} \approx \frac{300}{137} \approx 2.19$$

remains conducting, semimetal
Elias *et al.*, Nature Phys. 2049 (2011)

- **puzzle**

  predictions at the time $\alpha_{\rm crit} \sim 1$

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  predictions at the time $\alpha_{\rm crit} \sim 1$

- **screening at short distances**

  from σ-band electrons and localised higher energy states

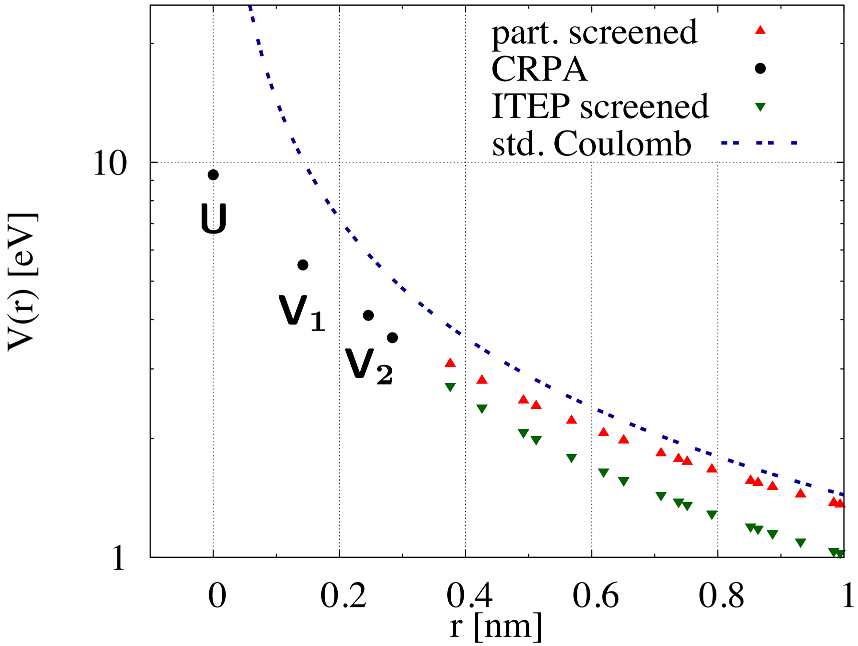
- **interpolate at intermediate distances**

  with dielectric thin-film model

$$\epsilon^{-1}(\vec{k}) = \frac{1}{\epsilon_1}\,\frac{\epsilon_1 + 1 + (\epsilon_1 - 1)e^{-kd}}{\epsilon_1 + 1 - (\epsilon_1 - 1)e^{-kd}}$$

(ϵ_1 = 2.4 and d = 2.8Å)

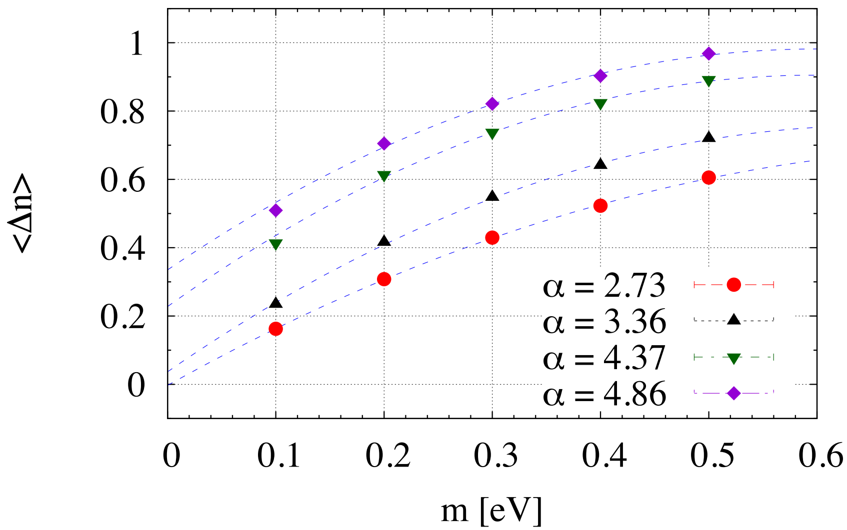
Wehling *et al.*, PRL 106 (2011) 236805

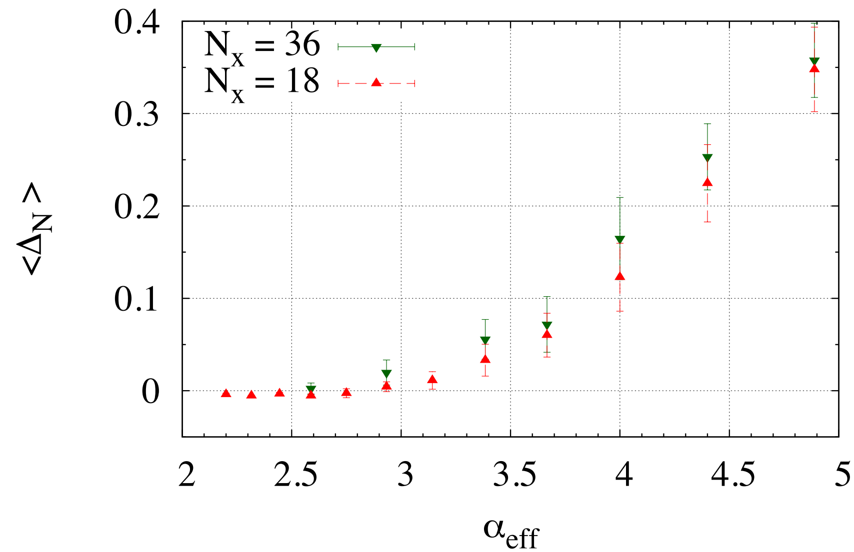


HMC on Hexagonal Lattice

- chiral extrapolation

$$m_{\mathbf{sdw}} \to 0$$





- semimetal-insulator transition in unphysical regime

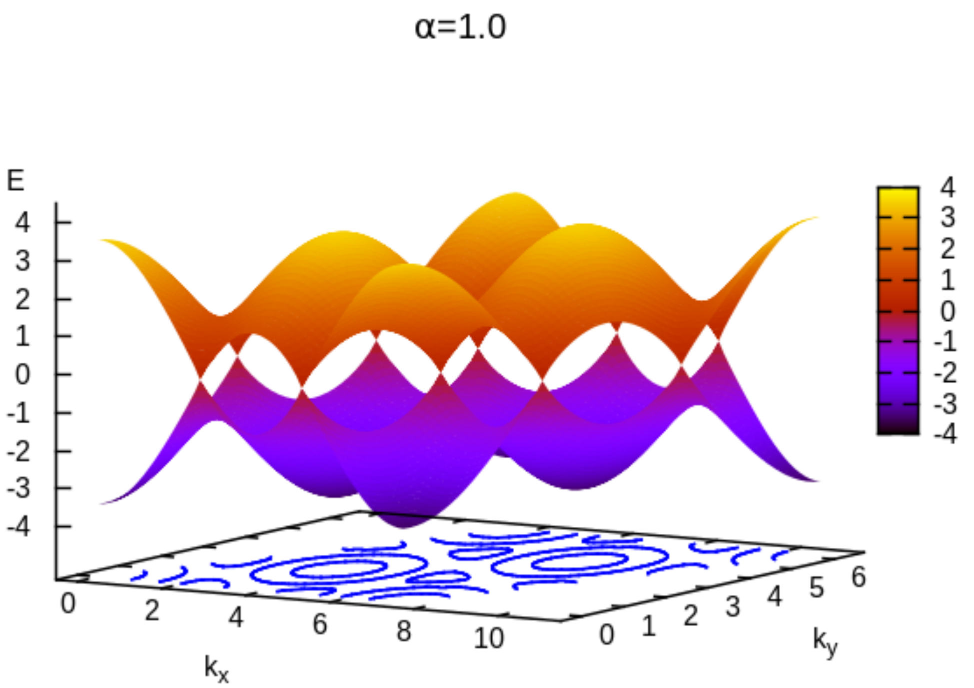
$$\alpha_{\mathrm{crit}} \approx 3 > 2.19$$

Ulybyshev, Buividovich, Katsnelson, Polikarpov, PRL 111 (2013) 056801

Smith, LvS, PRB 89 (2014) 195429

Dyson-Schwinger Equations

- **hexagonal lattice, screened Coulomb**



Manon Bischoff, MSc, TU Da (2015)
Katja Kleeberg, MSc, JLU Gi (2015)

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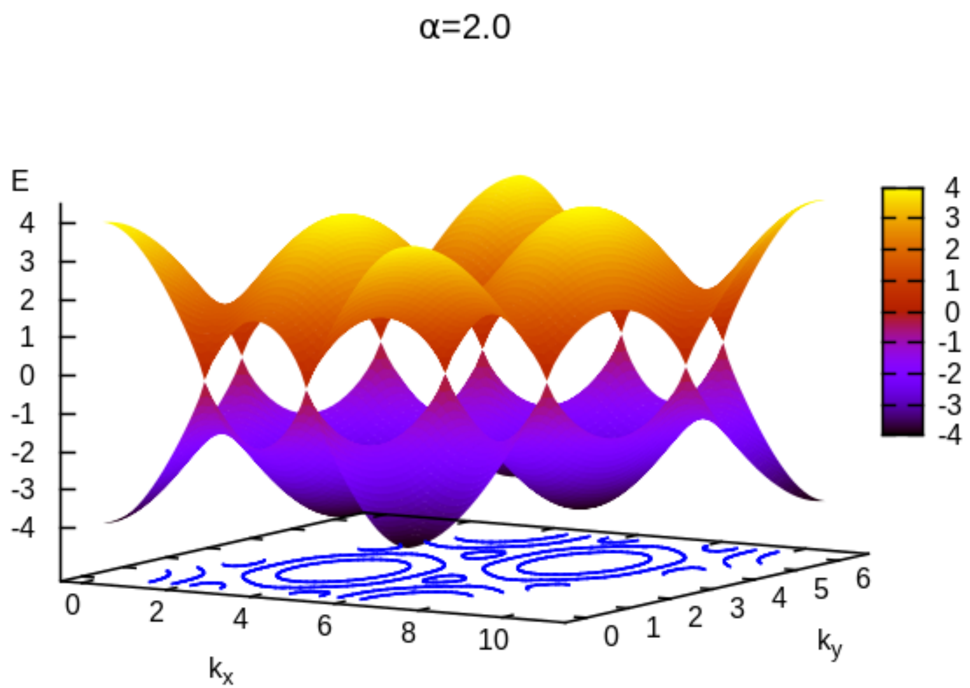

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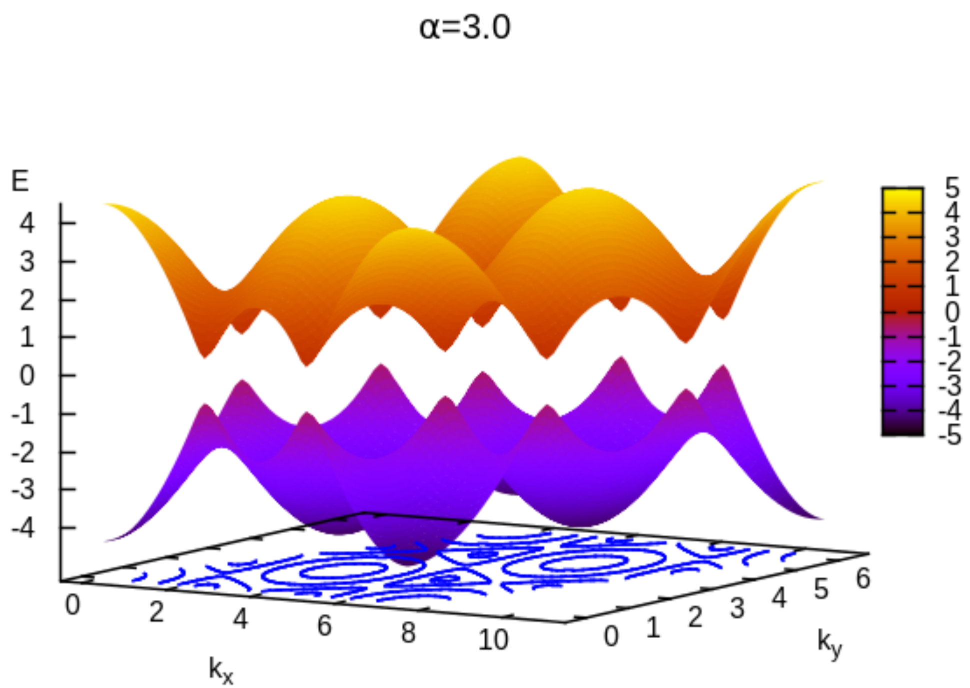

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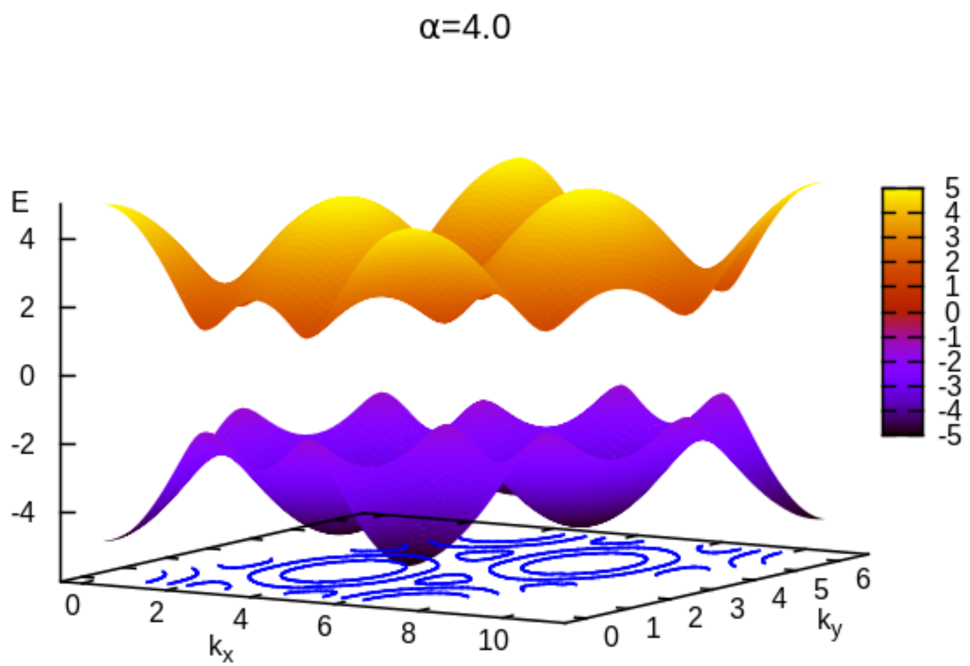

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Dyson-Schwinger Equations

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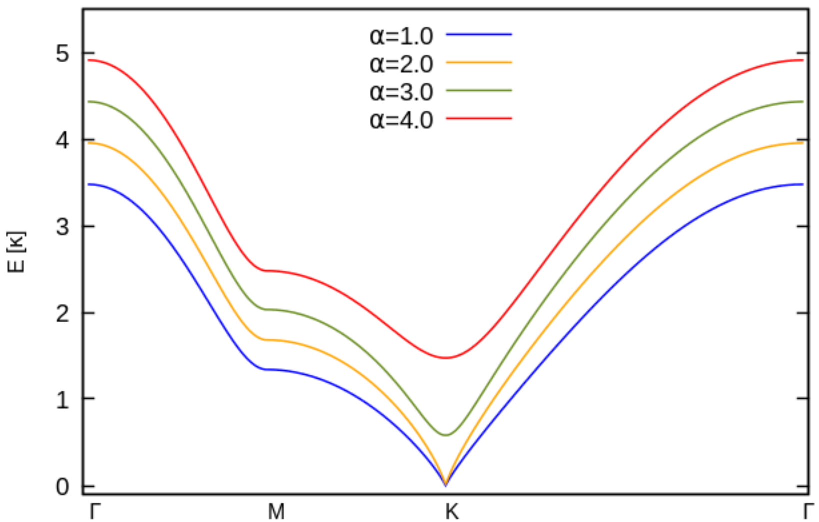
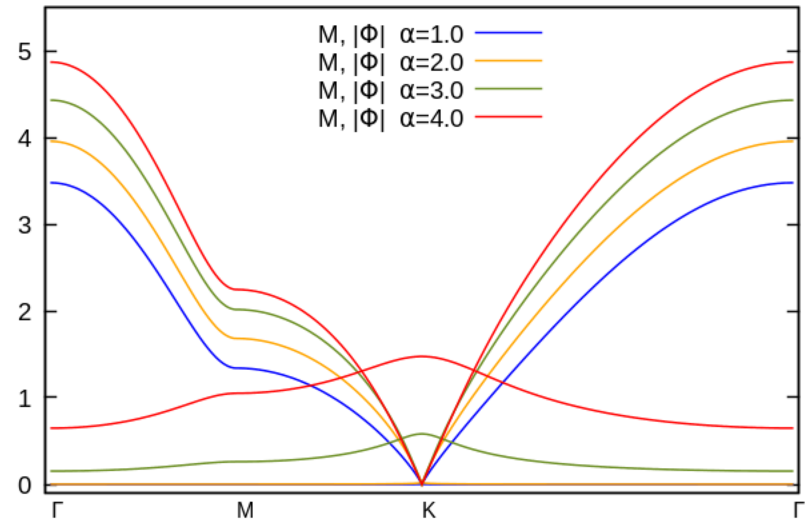
graphene's single-particle band structure

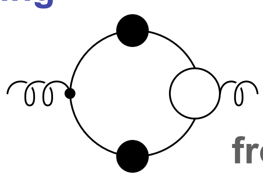




$$\alpha_{\text{crit}} \approx 1.5$$

- no Lindhard screening

$$\Pi(\omega, \vec{q}) =$$



from π-band electrons

Manon Bischoff, MSc, TU Da (2015)
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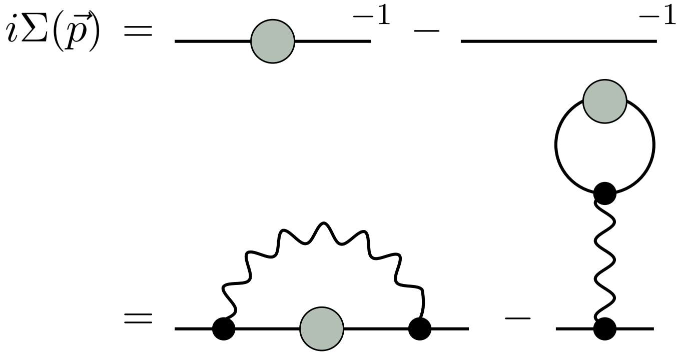
- what about CDW and the other insulating phases?

Dyson-Schwinger Equations

- hexagonal Hubbard model, Hartree-Fock

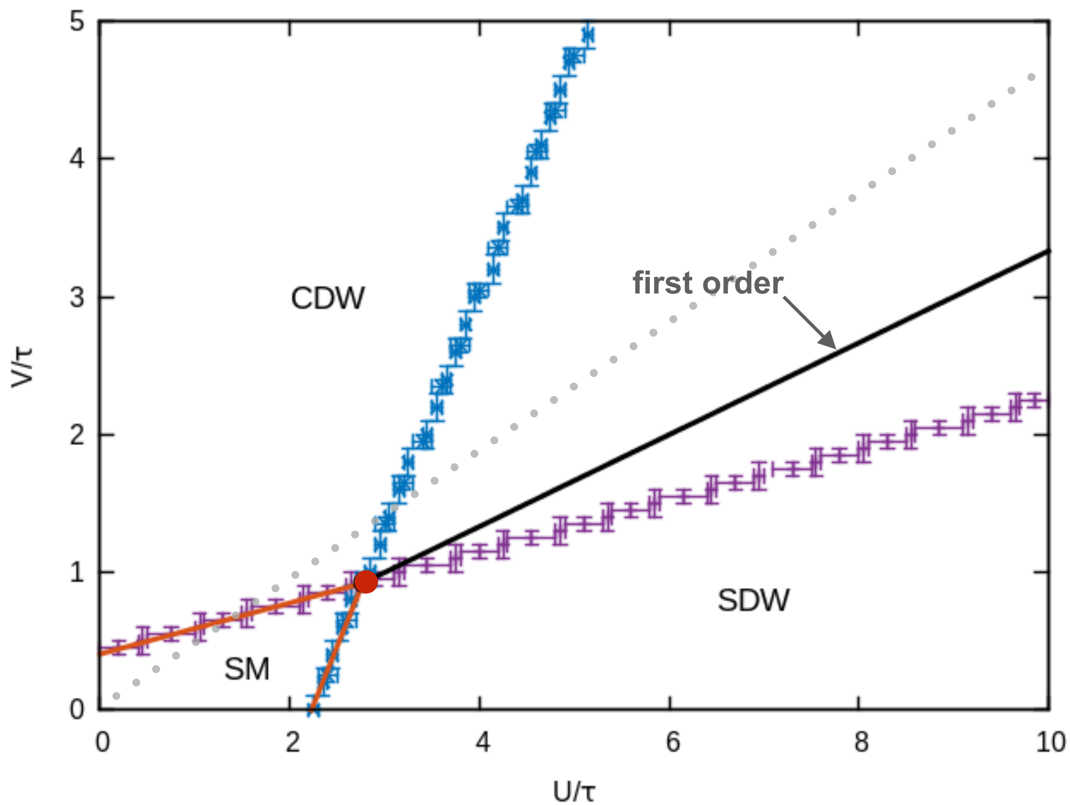


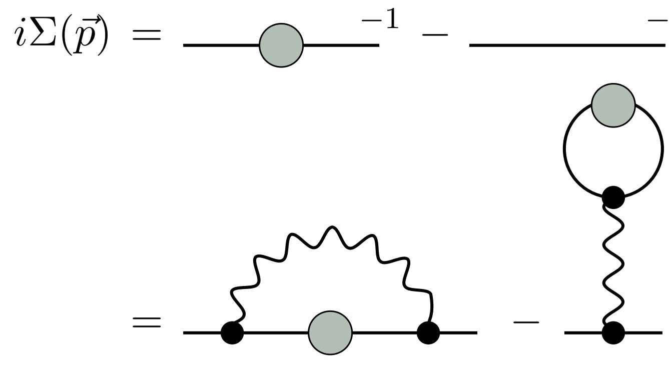
fermion self-energy

Dyson-Schwinger Equations

- hexagonal Hubbard model, Hartree-Fock

with on-site U and nearest-neighbor V





fermion self-energy

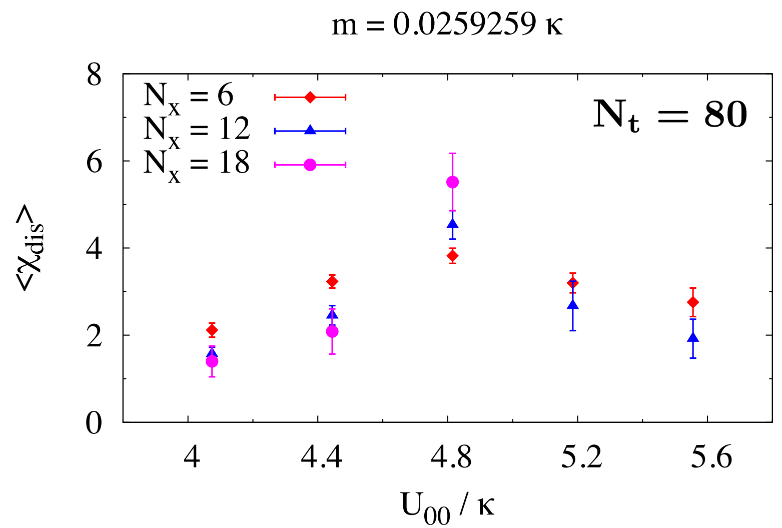
Katja Kleeberg *et al.*, in preparation

Araki and Semenoff, PRB 86 (2012) 121402(R)

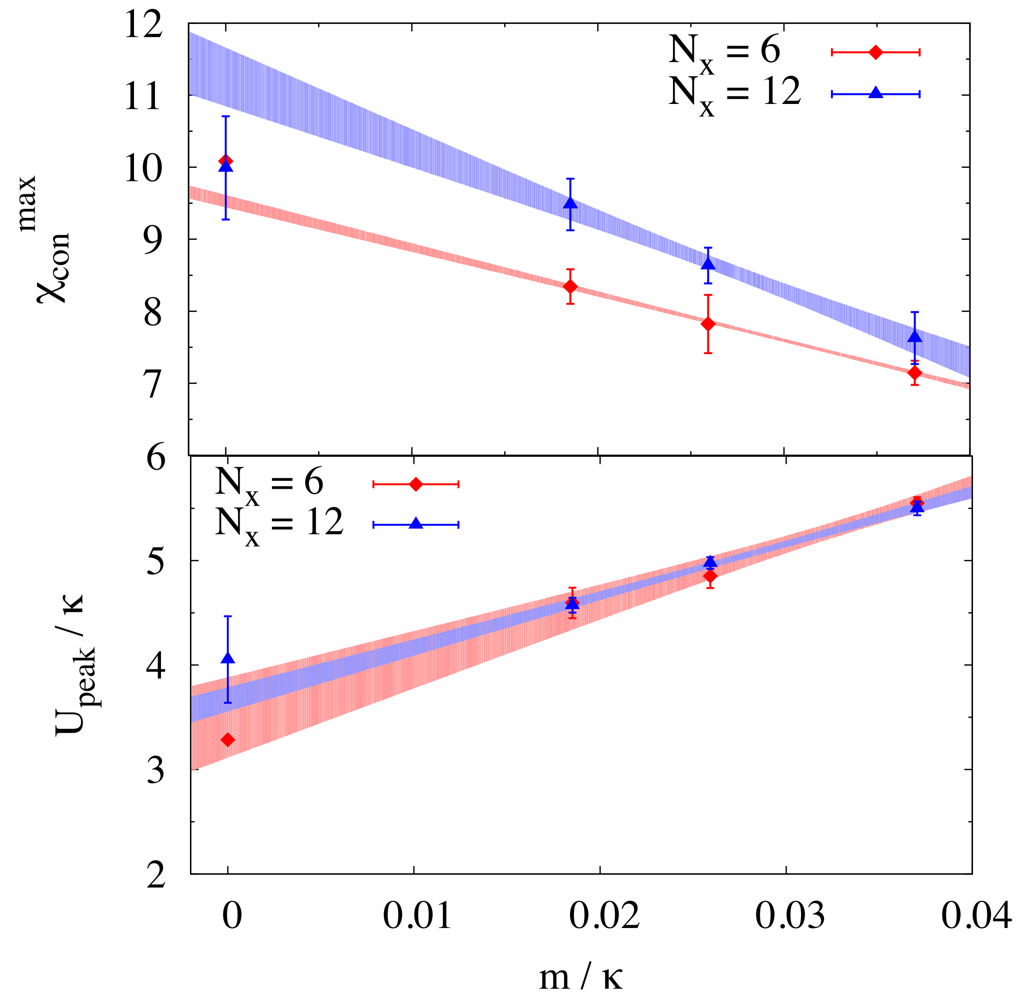
HMC on Hexagonal Lattice

- **chiral extrapolation, SDW**

  only on-site U first



$m_{\rm sdw} \to 0$



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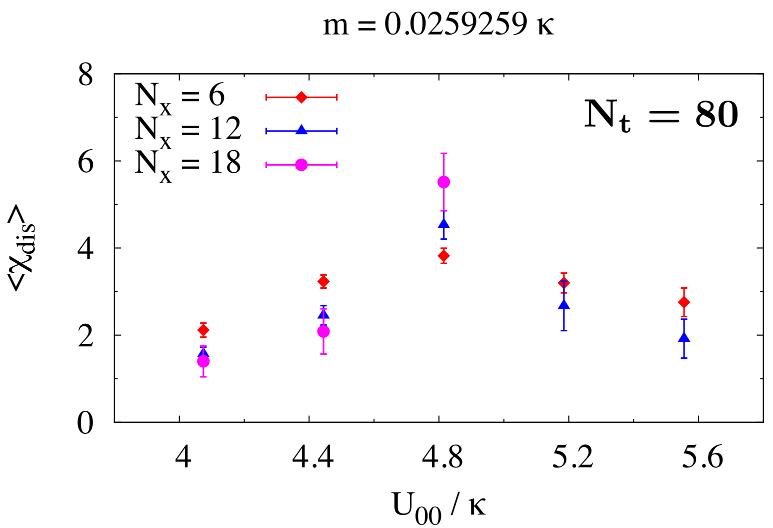
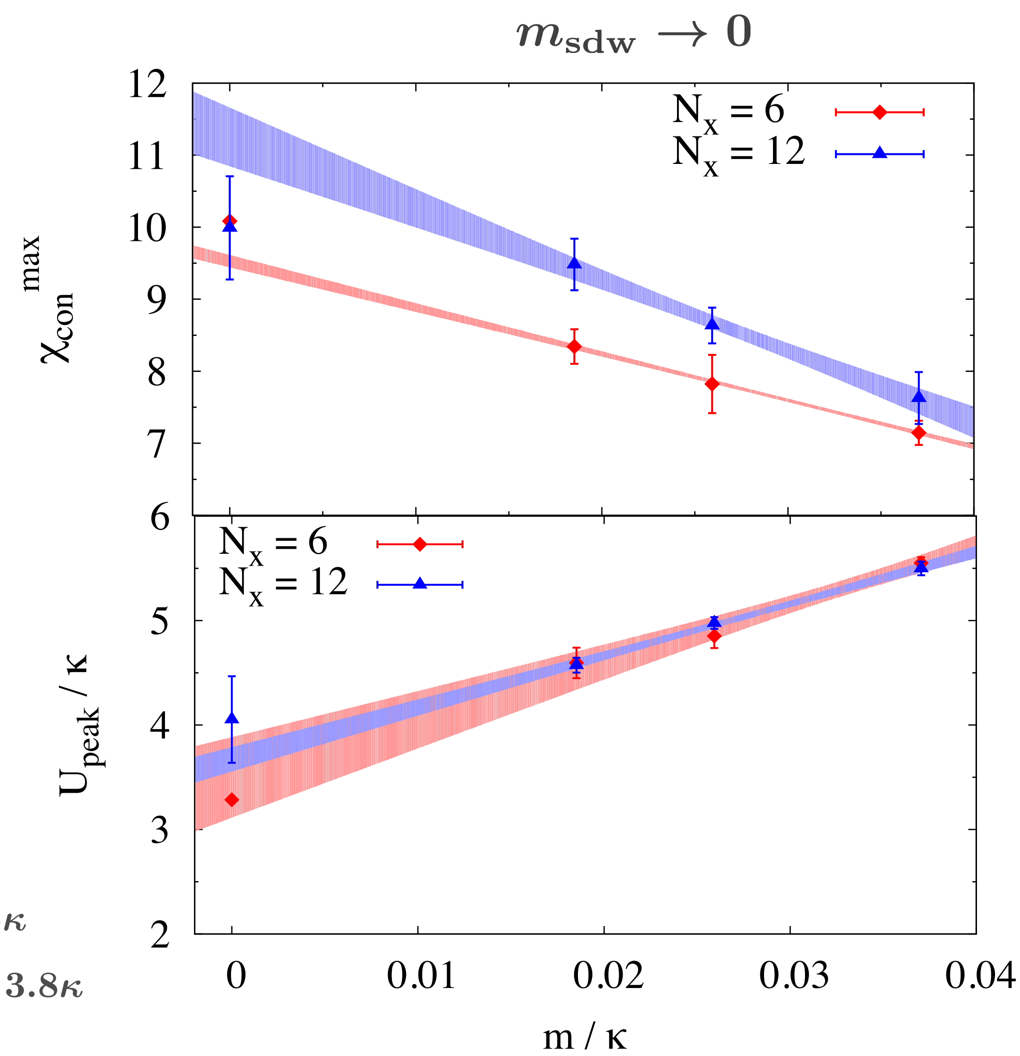


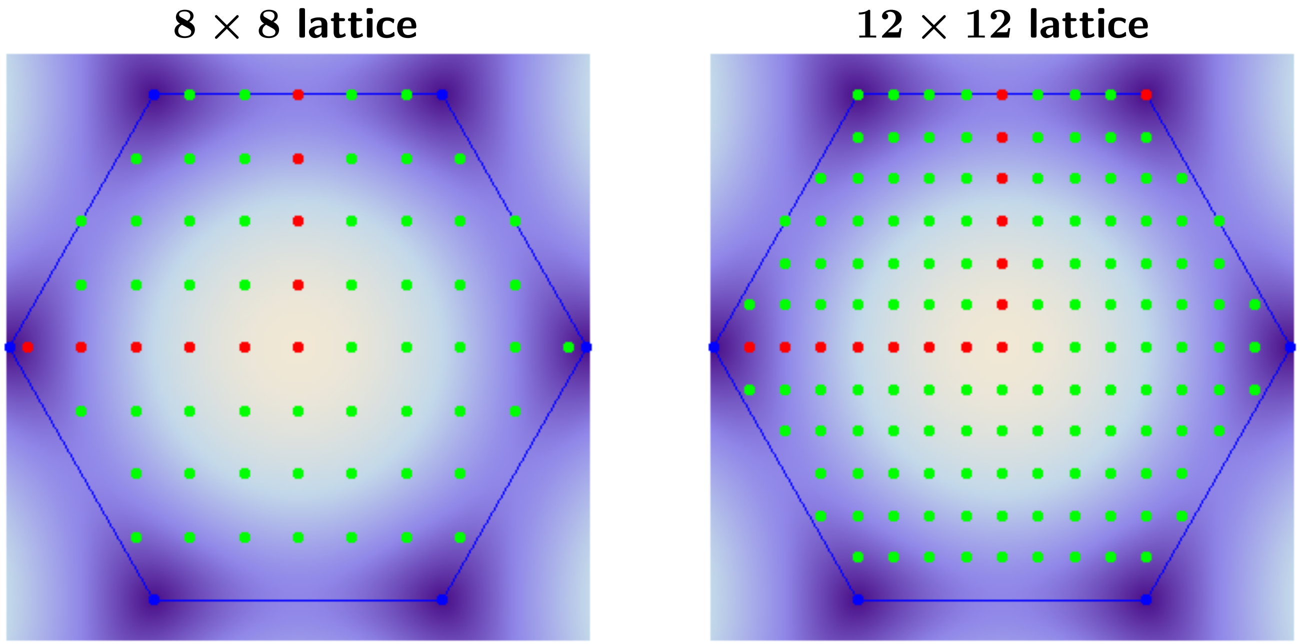


Sorella, Tosatti, EPL 19 (1992) 699: $U_c \approx 4.5\kappa$

Assaad, Herbut, PRX 3 (2013) 031010: $U_c \approx 3.8\kappa$

HMC with Geometric Mass

- hexagonal Brillouin zone



- removes Dirac points
- preserves symmetries
- improves invertibility

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Suitable Order Parameters

for zero(geometric)-mass simulations, use

$$O = \frac{1}{L^2}\sqrt{\Big\langle\Big(\sum_{i\in A} O_i\Big)^2\Big\rangle + \Big\langle\Big(\sum_{i\in B} O_i\Big)^2\Big\rangle}$$

with

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with

- **spin-density wave:**

$$O_i \to \vec{S}_i = \sum_{\sigma,\sigma'} c^\dagger_{i,\sigma} \frac{\vec{\sigma}_{\sigma\sigma'}}{2} c_{i,\sigma'} \qquad c_i = \begin{cases} a_i\,, & i \in A \\ b_i\,, & i \in B \end{cases}$$

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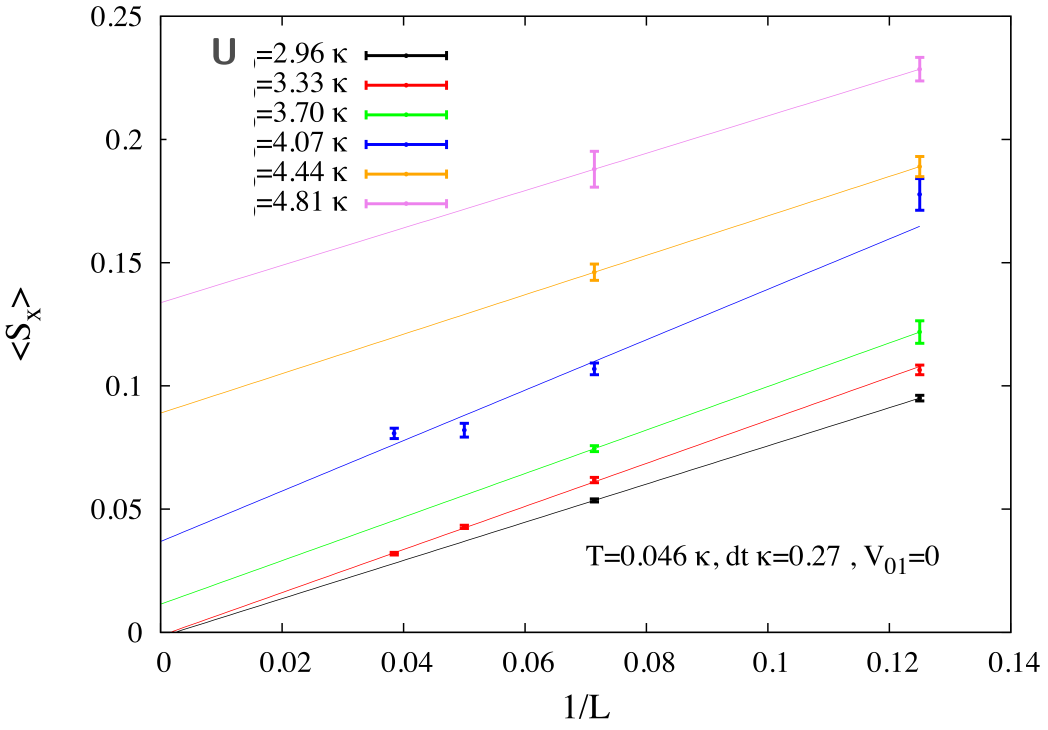
- **charge-density wave:**

$$O_i \to Q_i = \sum_{\sigma} \left(c^\dagger_{i,\sigma} c_{i,\sigma} - 1 \right)$$

HMC with Geometric Mass

- pure on-site U, SDW

$L\ =\ 8,\ 14,\ 20,\ 26$ $\quad\mathbf{N_t\ =\ 80}$



as before: $U_c \approx 3.8\kappa$

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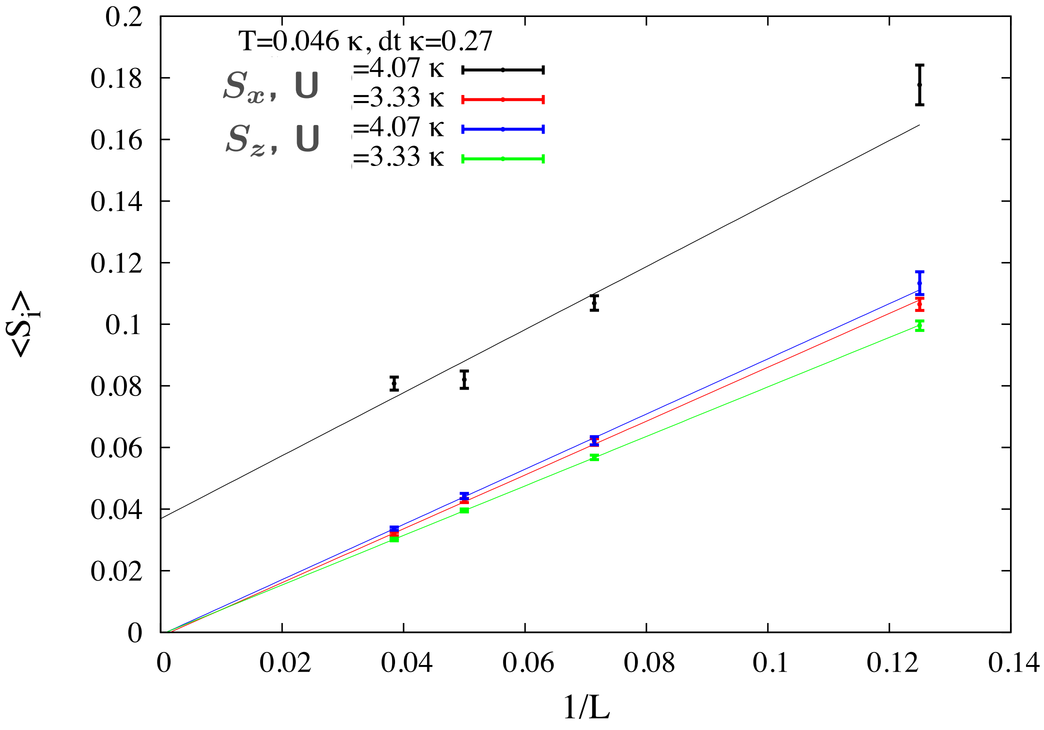
HMC with Geometric Mass

- violation of spin symmetry!

$L = 8, 14, 20, 26$ $\mathbf{N_t = 80}$



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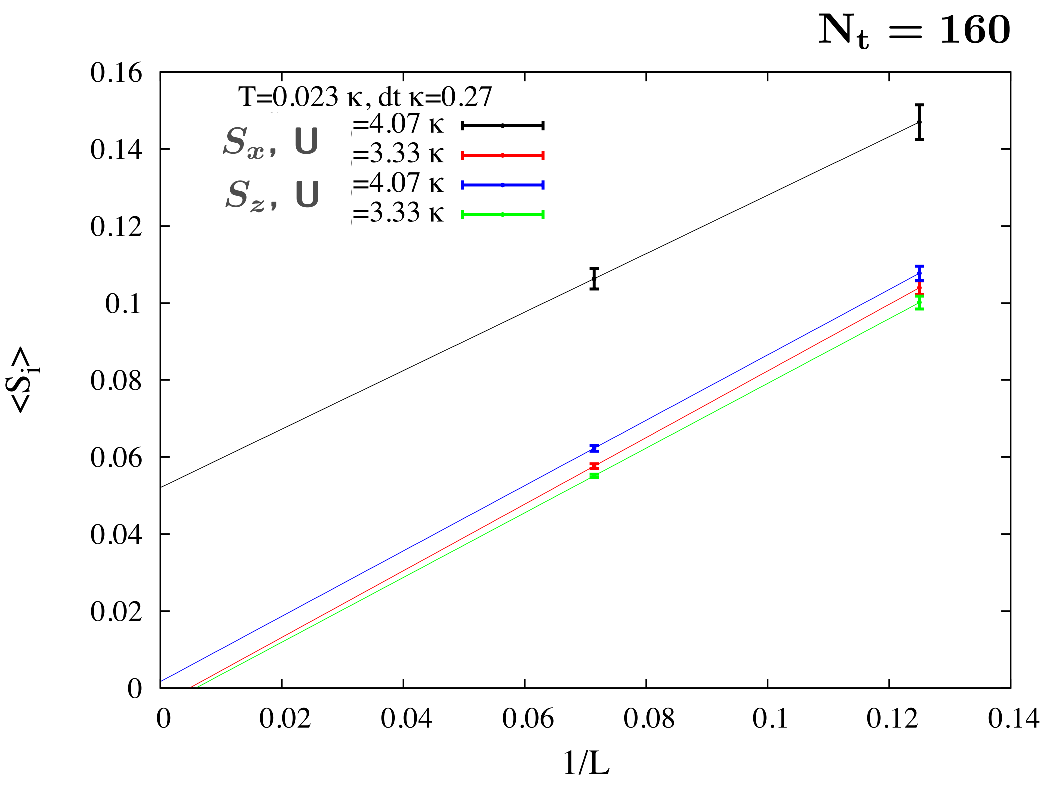

lower temperatures don't help

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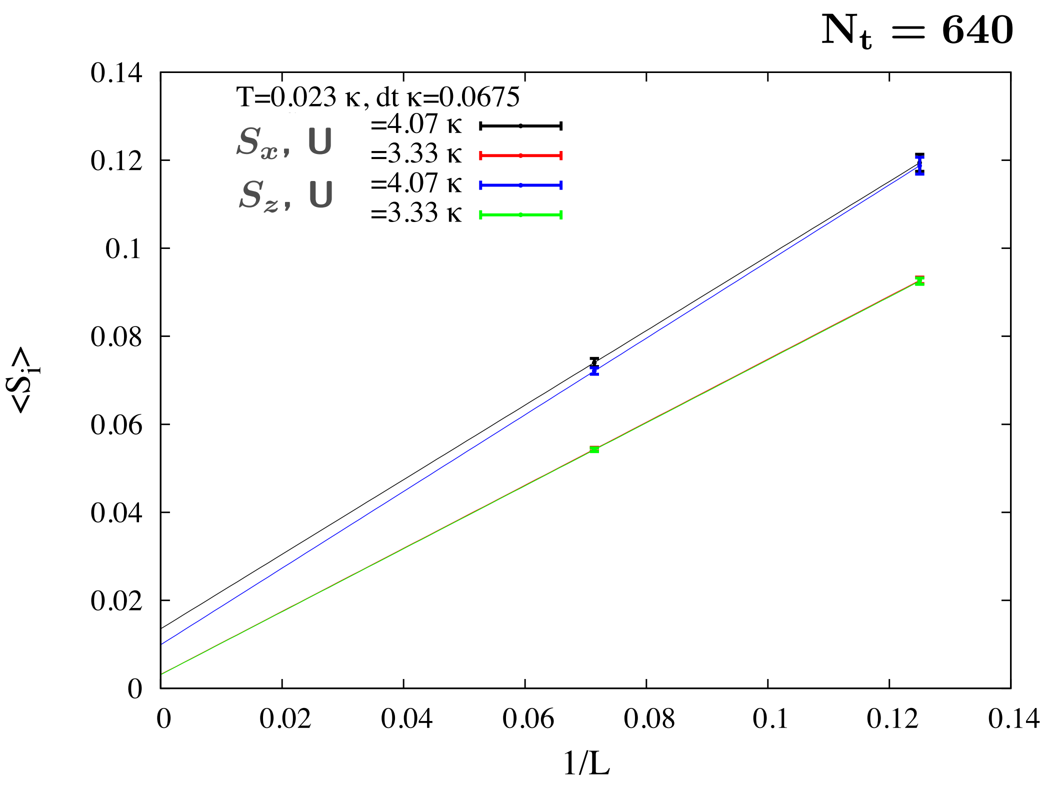


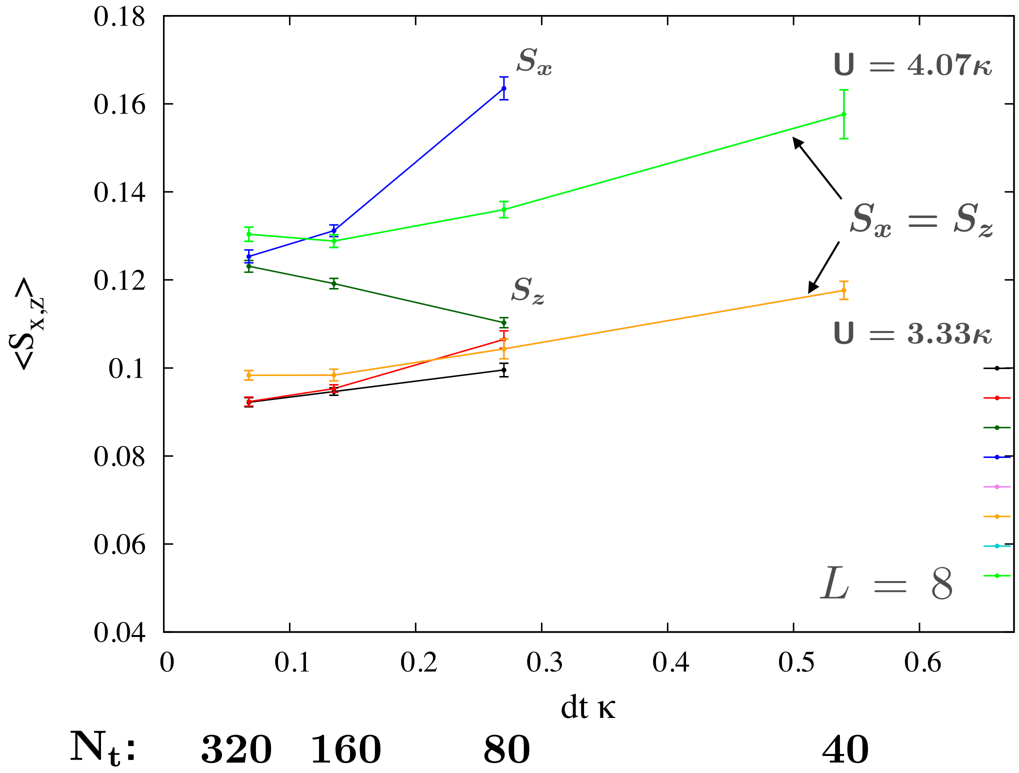
continuum limit in time does

Perfect Action

- **time-discretisation breaks sublattice symmetry**

  already in non-interacting tight-binding theory

  $\rightsquigarrow$ **replace in fermion matrix** $\quad 1 - H_{\rm tb}\,\Delta\tau \;\to\; e^{-H_{\rm tb}\,\Delta\tau}$

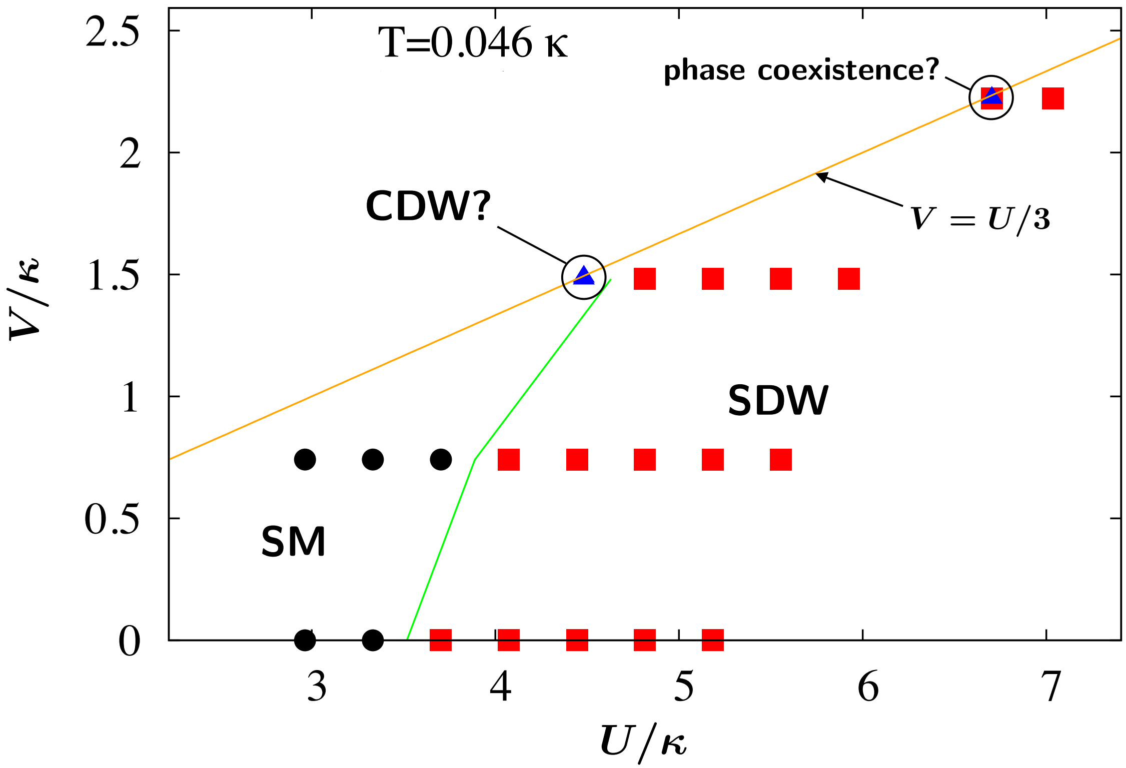


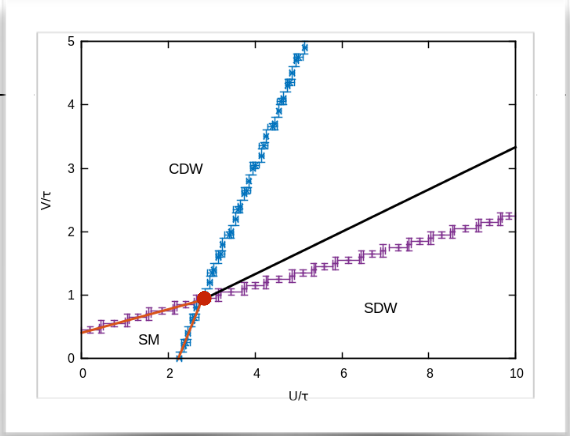
with exponential for continuous time-evolution in fermion matrix

Phase Diagram

- **hexagonal Hubbard model**
  with on-site U and nearest-neighbor V

preliminary





Hartree-Fock

Conclusions

- **HMC on hexagonal graphene lattice**

  screened Coulomb interactions ➟ suspended graphene in semimetal phase

- **geometric mass, no explicit sublattice symmetry breaking**

  no explicit symmetry breaking ➟ study competition between various insulating phases

- **continuous time-evolution in improved fermion matrix**

  maintain full spin and sublattice symmetries

- **study competing CDW/SDW order in extended Hubbard model**

  $U_c \approx 3.8\ \kappa$ confirmed for anti-ferromagnetic Mott insulator transition (SDW)
  extend results into U-V plane with first order transition to CDW (sign-problem)

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