

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

## Pavel Buividovich, Maksim Ulybyshev

 (Regensburg)Dominik Smith, Lorenz von Smekal (Giessen)

DFG
Deutsche
Forschungsgemeinschaft

Plymouth, 1 August 2016


## Outline

- Intro \& Motivation, Graphene
- Extended Hubbard Model, Hartree-Fock
- HMC on Hexagonal Lattice, Geometric Mass
- Improved Fermion Action, Exact Sublattice Symmetry
- Phase-Diagram Scan
- Conclusion


## Introduction



## Honeycomb Lattice

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

- single-particle energy bands

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

structure factor:

$$
\Phi(\mathbf{k})=t \sum_{i} e^{i \mathbf{k} \cdot \delta_{i}}
$$



[Wallace, 1947]

- massless dispersion around Dirac points $K_{ \pm}$

graphene

$$
E(\mathbf{p})= \pm \hbar v_{f}|\mathbf{p}|, \quad v_{f}=3 t a / 2 \simeq 1 \times 10^{6} \mathrm{~m} / \mathrm{s} \simeq c / 300
$$

## Honeycomb Lattice

- mass terms (gaps)

$$
\mathcal{H}_{m}=\frac{1}{N^{2}} \sum_{\boldsymbol{k}, \sigma} m_{\sigma}\left(a_{\boldsymbol{k}, \sigma}^{\dagger} a_{\boldsymbol{k}, \sigma}-b_{\boldsymbol{k}, \sigma}^{\dagger} b_{\boldsymbol{k}, \sigma}\right)
$$

(pseudo-spin) staggered on-site potential

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

| eXtreme QCD 2016 | 1 August $2016 \mid$ Lorenz von Smekal $\mid$ p. 5 | JUSTUS-LIEBIG- |
| :--- | :---: | :---: | :---: |
| UNIVERSITAT |  |  |

## Honeycomb Lattice

- mass terms (gaps)

$$
\mathcal{H}_{m}=\frac{1}{N^{2}} \sum_{\boldsymbol{k}, \sigma} m_{\sigma}\left(a_{\boldsymbol{k}, \sigma}^{\dagger} a_{\boldsymbol{k}, \sigma}-b_{\boldsymbol{k}, \sigma}^{\dagger} b_{\boldsymbol{k}, \sigma}\right)
$$

(pseudo-spin) staggered on-site potential

- spin (flavor) dependence

$$
\begin{aligned}
m_{\mathrm{cdw}} & =\frac{1}{2}\left(m_{u}+m_{d}\right) \\
m_{\mathrm{sdw}} & =\frac{1}{2}\left(m_{u}-m_{d}\right)
\end{aligned}
$$

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

## Honeycomb Lattice

- mass terms (gaps)

$$
\mathcal{H}_{m}=\frac{1}{N^{2}} \sum_{\boldsymbol{k}, \sigma} m_{\sigma}\left(a_{\boldsymbol{k}, \sigma}^{\dagger} a_{\boldsymbol{k}, \sigma}-b_{\boldsymbol{k}, \sigma}^{\dagger} b_{\boldsymbol{k}, \sigma}\right)
$$

(pseudo-spin) staggered on-site potential

- spin (flavor) dependence

$$
\begin{aligned}
m_{\mathrm{cdw}} & =\frac{1}{2}\left(m_{u}+m_{d}\right) \\
m_{\mathrm{sdw}} & =\frac{1}{2}\left(m_{u}-m_{d}\right)
\end{aligned}
$$

- Coulomb interaction

$$
\alpha_{g}=\frac{e^{2}}{4 \pi \varepsilon \hbar v_{f}}
$$

effective coupling

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

## Honeycomb Lattice

- mass terms (gaps)

$$
\mathcal{H}_{m}=\frac{1}{N^{2}} \sum_{\boldsymbol{k}, \sigma} m_{\sigma}\left(a_{\boldsymbol{k}, \sigma}^{\dagger} a_{\boldsymbol{k}, \sigma}-b_{\boldsymbol{k}, \sigma}^{\dagger} b_{\boldsymbol{k}, \sigma}\right)
$$

Graphene Gets a Good Gap on SiC Nevis et al., PRL 115 (2015) 136802
(pseudo-spin) staggered on-site potential

- spin (flavor) dependence
with strong interactions:

$$
m \rightarrow 0 \quad \text { Mott-insulator transition }
$$

$m_{\mathrm{cdw}}=\frac{1}{2}\left(m_{u}+m_{d}\right) \quad \longrightarrow \quad$ charge-density wave (CDW)
$m_{\mathrm{sdw}}=\frac{1}{2}\left(m_{u}-m_{d}\right) \quad \longrightarrow \quad$ AF spin-density wave (SDW)

- Coulomb interaction

$$
\alpha_{g}=\frac{e^{2}}{4 \pi \varepsilon \hbar v_{f}}
$$

effective coupling

| eXtreme QCD 2016 | 1 August $2016 \mid$ Lorenz von Smekal \| p. 5 | JUSTUS-LIEBIG- |
| :--- | :--- | :--- |
| UNIVERSITAT |  |  |

## Honeycomb Lattice

- mass terms (gaps)

$$
\mathcal{H}_{m}=\frac{1}{N^{2}} \sum_{\boldsymbol{k}, \sigma} m_{\sigma}\left(a_{\boldsymbol{k}, \sigma}^{\dagger} a_{\boldsymbol{k}, \sigma}-b_{\boldsymbol{k}, \sigma}^{\dagger} b_{\boldsymbol{k}, \sigma}\right)
$$

Graphene Gets a Good Gap on SiC Nevis et al., PRL 115 (2015) 136802
(pseudo-spin) staggered on-site potential

- spin (flavor) dependence

> with strong interactions:
$\begin{array}{lll}m_{\mathrm{cdw}}=\frac{1}{2}\left(m_{u}+m_{d}\right) & \longrightarrow 0 & \begin{array}{l}\text { Mott-insulator transition } \\ \text { charge-density wave (CDW) }\end{array} \\ m_{\mathrm{sdw}}=\frac{1}{2}\left(m_{u}-m_{d}\right) & \longrightarrow & \text { AF spin-density wave (SDW) }\end{array}$

- Coulomb interaction

$$
\alpha_{g}=\frac{e^{2}}{4 \pi \varepsilon \hbar v_{f}}
$$

effective coupling


Raghu et al., PRL 100 (2008) 156401

## Honeycomb Lattice

- mass terms (gaps)

$$
\mathcal{H}_{m}=\frac{1}{N^{2}} \sum_{\boldsymbol{k}, \sigma} m_{\sigma}\left(a_{\boldsymbol{k}, \sigma}^{\dagger} a_{\boldsymbol{k}, \sigma}-b_{\boldsymbol{k}, \sigma}^{\dagger} b_{\boldsymbol{k}, \sigma}\right)
$$

Graphene Gets a Good Gap on SiC Nevis et al., PRL 115 (2015) 136802
(pseudo-spin) staggered on-site potential

- spin (flavor) dependence

> with strong interactions:
$\begin{array}{lll}m_{\mathrm{cdw}}=\frac{1}{2}\left(m_{u}+m_{d}\right) & \longrightarrow 0 & \text { Mott-insulator transition } \\ m_{\mathrm{Sdw}}=\frac{1}{2}\left(m_{u}-m_{d}\right) & \longrightarrow & \text { charge-density wave (CDW) } \\ & & \end{array}$

- Coulomb interaction

$$
\alpha_{g}=\frac{e^{2}}{4 \pi \varepsilon \hbar v_{f}}
$$

effective coupling

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


Raghu et al., PRL 100 (2008) 156401

## Potentially Strong Interactions

- suspended graphene

$$
\varepsilon \rightarrow 1 \quad \alpha_{g}=\frac{e^{2}}{4 \pi \hbar v_{f}} \approx \frac{300}{137} \approx 2.19
$$

- puzzle
predictions at the time $\quad \alpha_{\text {crit }} \sim 1$

$$
\alpha_{\text {crit }} \sim 1
$$

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

## Potentially Strong Interactions

- suspended graphene

$$
\varepsilon \rightarrow 1 \quad \alpha_{g}=\frac{e^{2}}{4 \pi \hbar v_{f}} \approx \frac{300}{137} \approx 2.19
$$

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

- puzzle
predictions at the time $\quad \alpha_{\text {crit }} \sim 1$
- screening at short distances

Wehling et al., PRL 106 (2011) 236805 from o-band electrons and localised higher energy states

- interpolate at intermediate distances with dielectric thin-film model

$$
\epsilon^{-1}(\vec{k})=\frac{1}{\epsilon_{1}} \frac{\epsilon_{1}+1+\left(\epsilon_{1}-1\right) e^{-k d}}{\epsilon_{1}+1-\left(\epsilon_{1}-1\right) e^{-k d}}
$$

$$
\left(\epsilon_{1}=2.4 \text { and } d=2.8 \AA\right)
$$

## HMC on Hexagonal Lattice

- chiral extrapolation

$$
m_{\text {sdw }} \rightarrow 0
$$




- semimetal-insulator transition in unphysical regime

$$
\alpha_{\text {crit }} \approx 3>2.19 \quad \begin{aligned}
& \text { Ulybyshev, Buividovich, Katsnelson, Polikarpov, } \\
& \\
& \\
& \\
& \\
& \text { PRL 111 (2013) } 056801 \\
& \text { Smith, LvS, PRB } 89(2014) 195429
\end{aligned}
$$

## Dyson-Schwinger Equations

- hexagonal lattice, screened Coulomb

$$
\alpha=1.0
$$



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

## Dyson-Schwinger Equations

- hexagonal lattice, screened Coulomb

$$
\alpha=2.0
$$



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

## Dyson-Schwinger Equations

- hexagonal lattice, screened Coulomb

$$
\alpha=3.0
$$



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

## Dyson-Schwinger Equations

- hexagonal lattice, screened Coulomb

$$
\alpha=4.0
$$



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

## Dyson-Schwinger Equations

- hexagonal lattice, screened Coulomb
graphene's single-particle band structure


- no Lindhard screening

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


$\bullet$ what about CDW and the other insulating phases?

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

## Dyson-Schwinger Equations

- hexagonal Hubbard model, Hartree-Fock

fermion self-energy


## Dyson-Schwinger Equations

- hexagonal Hubbard model, Hartree-Fock


fermion self-energy

Katja Kleeberg et al., in preparation

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

## Dyson-Schwinger Equations

- hexagonal Hubbard model, Hartree-Fock



## HMC on Hexagonal Lattice



## HMC on Hexagonal Lattice



## HMC with Geometric Mass

- hexagonal Brillouin zone

- removes Dirac points
- preserves symmetries
- improves invertibility


## Suitable Order Parameters

for zero(geometric)-mass simulations, use

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

with

## Suitable Order Parameters

for zero(geometric)-mass simulations, use

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

with

- spin-density wave:

$$
O_{i} \rightarrow \vec{S}_{i}=\sum_{\sigma, \sigma^{\prime}} c_{i, \sigma}^{\dagger} \frac{\vec{\sigma}_{\sigma \sigma^{\prime}}}{2} c_{i, \sigma^{\prime}} \quad c_{i}= \begin{cases}a_{i}, & i \in A \\ b_{i}, & i \in B\end{cases}
$$

## Suitable Order Parameters

for zero(geometric)-mass simulations, use

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

with

- spin-density wave:

$$
O_{i} \rightarrow \vec{S}_{i}=\sum_{\sigma, \sigma^{\prime}} c_{i, \sigma}^{\dagger} \frac{\vec{\sigma}_{\sigma \sigma^{\prime}}}{2} c_{i, \sigma^{\prime}} \quad c_{i}= \begin{cases}a_{i}, & i \in A \\ b_{i}, & i \in B\end{cases}
$$

- charge-density wave:

$$
O_{i} \rightarrow Q_{i}=\sum_{\sigma}\left(c_{i, \sigma}^{\dagger} c_{i, \sigma}-1\right)
$$

## HMC with Geometric Mass

- pure on-site U, SDW

as before: $U_{c} \approx 3.8 \kappa$


## HMC with Geometric Mass

- violation of spin symmetry!



## HMC with Geometric Mass

- violation of spin symmetry!

lower temperatures don't help

| eXtreme QCD 2016 | 1 August $2016 \mid$ Lorenz von Smekal \| p. 20 | JUSTUS-LIEBIG- |
| :--- | :---: | :---: | :---: | :---: |
| GUNIVERSITAT |  |  |

## HMC with Geometric Mass

- violation of spin symmetry!

continuum limit in time does


## Perfect Action

- time-discretisation breaks sublattice symmetry already in non-interacting tight-binding theory
$\rightsquigarrow$ replace in fermion matrix $1-H_{\mathrm{tb}} \Delta \tau \rightarrow e^{-H_{\mathrm{tb}} \Delta \tau}$



## Phase Diagram

## - hexagonal Hubbard model

with on-site U and nearest-neighbor V



|  | eXtreme QCD 2016 | 1 August $2016 \mid$ Lorenz von Smekal $\mid$ p. 23 |
| :--- | :--- | :--- |

## Phase Diagram





## Phase Diagram



## Phase Diagram



## Phase Diagram



## Phase Diagram



## Phase Diagram

## - hexagonal Hubbard model

with on-site U and nearest-neighbor V



## Conclusions

- HMC on hexagonal graphene lattice
screened Coulomb interactions $" \rightarrow$ suspended graphene in semimetal phase
- geometric mass, no explicit sublattice symmetry breaking
no explicit symmetry breaking $" \rightarrow$ 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
$\mathrm{U}_{\mathrm{c}} \approx 3.8 \mathrm{k}$ confirmed for anti-ferromagnetic Mott insulator transition (SDW) extend results into U-V plane with first order transition to CDW (sign-problem)


## 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 $" \rightarrow$ 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
$\mathrm{U}_{\mathrm{c}} \approx 3.8 \mathrm{~K}$ confirmed for anti-ferromagnetic Mott insulator transition (SDW) extend results into U-V plane with first order transition to CDW (sign-problem)


## Thank you for your attention!

