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

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Introduction
Honeycomb Lattice

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

- single-particle energy bands

\[ E_{\pm}(k) = \pm |\Phi(k)| \]

structure factor:

\[ \Phi(k) = t \sum_{i} e^{i k \cdot \delta_i} \]

- massless dispersion around Dirac points \( K_{\pm} \)

\[ E(p) = \pm \hbar v_{f} |p|, \quad v_{f} = 3ta/2 \approx 1 \times 10^6 \text{m/s} \approx c/300 \]
Honeycomb Lattice

- mass terms (gaps)

\[ \mathcal{H}_m = \frac{1}{N^2} \sum_{\mathbf{k}, \sigma} m_\sigma \left( a_{\mathbf{k}, \sigma}^\dagger a_{\mathbf{k}, \sigma} - b_{\mathbf{k}, \sigma}^\dagger b_{\mathbf{k}, \sigma} \right) \]

(pseudo-spin) staggered on-site potential

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

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(pseudo-spin) staggered on-site potential

- 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
Honeycomb Lattice

- **mass terms (gaps)**

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(pseudo-spin) staggered on-site potential

- **spin (flavor) dependence**

\[ m_{\text{cdw}} = \frac{1}{2} (m_u + m_d) \quad \text{with strong interactions:} \quad m \to 0 \]

charge-density wave (CDW)

\[ m_{\text{sdw}} = \frac{1}{2} (m_u - m_d) \quad \text{AF spin-density wave (SDW)} \]

- **Coulomb interaction**

\[ \alpha_g = \frac{e^2}{4\pi\varepsilon \hbar \nu_f} \]

effective coupling
Honeycomb Lattice

- mass terms (gaps)

\[ H_m = \frac{1}{N^2} \sum_{\mathbf{k}, \sigma} m_\sigma (a_\mathbf{k,\sigma}^\dagger a_{\mathbf{k,\sigma}} - b_\mathbf{k,\sigma}^\dagger b_{\mathbf{k,\sigma}}) \]

(pseudo-spin) staggered on-site potential

- spin (flavor) dependence

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

\[ m \rightarrow 0 \quad \text{with strong interactions:} \quad \text{Mott-insulator transition} \]
\[ \text{charge-density wave (CDW)} \]
\[ \text{AF spin-density wave (SDW)} \]

- Coulomb interaction

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effective coupling

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Raghu et al., PRL 100 (2008) 156401
Honeycomb Lattice

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effective coupling

• sign-problem in HMC with \( m_{\text{cdw}} > 0 \)

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

Raghu et al., PRL 100 (2008) 156401
• suspended graphene
\[ \varepsilon \rightarrow 1 \]
\[ \alpha_g = \frac{e^2}{4\pi \hbar v_f} \approx \frac{300}{137} \approx 2.19 \]

• puzzle
predictions at the time
\[ \alpha_{\text{crit}} \sim 1 \]

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

- suspended graphene
  \[ \varepsilon \to 1 \]
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- puzzle
  predictions at the time
  \[ \alpha_{\text{crit}} \sim 1 \]

- screening at short distances
  from \( \sigma \)-band electrons and localised higher energy states

- interpolate at intermediate distances
  with dielectric thin-film model

  \[ \varepsilon^{-1}(\vec{k}) = \frac{1}{\varepsilon_1 + 1 + (\varepsilon_1 - 1)e^{-kd}} \]

  \[ \varepsilon_1 = 2.4 \text{ and } d = 2.8 \text{ Å} \]

remains conducting, semimetal

Elias et al., Nature Phys. 2049 (2011)

Wehling et al., PRL 106 (2011) 236805
HMC on Hexagonal Lattice

- **chiral extrapolation**

  \[ m_{sdw} \to 0 \]

- **semimetal-insulator transition in unphysical regime**

  \[ \alpha_{crit} \approx 3 > 2.19 \]

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

Smith, LvS, PRB 89 (2014) 195429
Dyson-Schwinger Equations

- hexagonal lattice, screened Coulomb

\[ \alpha = 1.0 \]

Manon Bischoff, MSc, TU Da (2015)
Katja Kleeberg, MSc, JLU Gi (2015)
Dyson-Schwinger Equations

- hexagonal lattice, screened Coulomb

\[ \alpha = 2.0 \]

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Dyson-Schwinger Equations

- hexagonal lattice, screened Coulomb

\[ \alpha = 3.0 \]

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Katja Kleeberg, MSc, JLU Gi (2015)
Dyson-Schwinger Equations

- hexagonal lattice, screened Coulomb

\[ \alpha = 4.0 \]

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Dyson-Schwinger Equations

- hexagonal lattice, screened Coulomb

graphene’s single-particle band structure

\[ \alpha_{\text{crit}} \approx 1.5 \]

\[ \Pi(\omega, \vec{q}) = \begin{array}{c}
\text{from } \pi\text{-band electrons}
\end{array} \]

- no Lindhard screening

- 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

\[ i \Sigma(p) = \frac{1}{\text{green}} - \frac{1}{\text{black}} \]

fermion self-energy
Dyson-Schwinger Equations

- hexagonal Hubbard model, Hartree-Fock

\[
i \Sigma(p) = \frac{1}{\mathcal{G} - \mathcal{Z} - \mathcal{W} \mathcal{Z}^{-1}}
\]

Katja Kleeberg et al., in preparation

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

with on-site U and nearest-neighbor V
• chiral extrapolation, SDW
  only on-site U first

$$m = 0.0259259 \kappa$$

$N_t = 80$

$N_x = 6$
$N_x = 12$
$N_x = 18$

$N_t = 80$

$m_{sdw} \rightarrow 0$

$N_x = 6$
$N_x = 12$

$\langle \chi_{\text{dis}} \rangle$

$U_{00} / \kappa$

$U_{\text{peak}} / \kappa$

$\chi_{\text{con}} \max$

$m / \kappa$

$0$
$0.01$
$0.02$
$0.03$
$0.04$

$0$
$2$
$4$
$6$
$8$

$0$
$2$
$4$
$6$
$8$

$0$
$4.4$
$4.8$
$5.2$
$5.6$

$0$
$4.4$
$4.8$
$5.2$
$5.6$
HMC on Hexagonal Lattice

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\[ m = 0.0259259 \kappa \]

\[ \langle \chi_{\text{dis}} \rangle \]

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\[ U_{\text{peak}} / \kappa \]

\[ \chi_{\text{con}} \]

\[ m_{\text{sdw}} \rightarrow 0 \]

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

8 × 8 lattice

12 × 12 lattice

- removes Dirac points
- preserves symmetries
- improves invertibility
Suitable Order Parameters

for zero(geometric)-mass simulations, use

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

with
Suitable Order Parameters

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with

- spin-density wave:

\[ O_i \rightarrow \vec{S}_i = \sum_{\sigma, \sigma'} c_{i, \sigma}^\dagger \vec{\sigma}_{\sigma \sigma'} \frac{c_{i, \sigma'}}{2} \]

\[ c_i = \begin{cases} a_i, & i \in A \\ b_i, & i \in B \end{cases} \]
Suitable Order Parameters

for zero(geometric)-mass simulations, use

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

with

- spin-density wave:

\[
O_i \rightarrow \vec{S}_i = \sum_{\sigma, \sigma'} c_{i,\sigma}^\dagger \vec{\sigma}_{\sigma\sigma'} c_{i,\sigma'}
\]

\[
c_i = \begin{cases} 
  a_i, & i \in A \\
  b_i, & i \in B 
\end{cases}
\]

- charge-density wave:

\[
O_i \rightarrow Q_i = \sum_{\sigma} (c_{i,\sigma}^\dagger c_{i,\sigma} - 1)
\]
HMC with Geometric Mass

- pure on-site $U$, SDW

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

$U = 2.96 \, \kappa$
$= 3.33 \, \kappa$
$= 3.70 \, \kappa$
$= 4.07 \, \kappa$
$= 4.44 \, \kappa$
$= 4.81 \, \kappa$

$S_x^\wedge$, $V_{00} = 2.96 \, \kappa$
$S_x^\wedge$, $V_{00} = 3.33 \, \kappa$
$S_x^\wedge$, $V_{00} = 3.70 \, \kappa$
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$S_x^\wedge$, $V_{00} = 4.44 \, \kappa$
$S_x^\wedge$, $V_{00} = 4.81 \, \kappa$

as before: $U_c \approx 3.8 \kappa$

$T = 0.046 \, \kappa$, $dt = 0.27$, $V_{01} = 0$
violation of spin symmetry!

\[ L = 8, 14, 20, 26 \]

\[ N_t = 80 \]
violation of spin symmetry!

lower temperatures don’t help
• violation of spin symmetry!

\begin{align*}
S_x, U = 4.07 \\
S_z, U = 3.33
\end{align*}

continuum limit in time does
**Perfect Action**

- time-discretisation breaks sublattice symmetry already in non-interacting tight-binding theory

\[ 1 - H_{tb} \Delta \tau \rightarrow e^{-H_{tb} \Delta \tau} \]

\[
\begin{align*}
\langle S_x \rangle, & \quad V_{00} = 3.33 \kappa, \text{ lattice } 8x8 \\
\langle S_z \rangle, & \quad V_{00} = 4.07 \kappa, \text{ lattice } 8x8 \\
\langle S_x \rangle, & \quad V_{00} = 3.33 \kappa, \text{ ExpLattice } 8x8 \\
\langle S_z \rangle, & \quad V_{00} = 4.07 \kappa, \text{ ExpLattice } 8x8 \\
\end{align*}
\]

\[ U = 4.07 \kappa \]

\[ U = 3.33 \kappa \]

\[ L = 8 \]

\[ N_t: \quad 320 \quad 160 \quad 80 \quad 40 \]

with exponential for continuous time-evolution in fermion matrix
Phase Diagram

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

![Phase Diagram Graph]

- Preliminary
- T = 0.046 \kappa
- Phase coexistence?
- \( V = U/3 \)
- CDW?
- SDW
- SM

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

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  - screened Coulomb interactions $\rightarrow$ suspended graphene in semimetal phase

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  - no explicit symmetry breaking $\rightarrow$ study competition between various insulating phases

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  - $U_c \approx 3.8 \kappa$ confirmed for anti-ferromagnetic Mott insulator transition (SDW)
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Thank you for your attention!