

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

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### 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







ÎHN

<del>un</del>iver Darms







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

structure factor:

$$\Phi({
m k}) = t \sum_i e^{i {
m k} \cdot \delta_i}$$

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

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





[Wallace, 1947]

0.14nn

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• 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



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#### • spin (flavor) dependence

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



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Coulomb interaction

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

0

effective coupling



 $\setminus \mathbf{0}$ 

m

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$$m \to 0$$

$$m_{\rm cdw} = \frac{1}{2} (m_u + m_d) \longrightarrow$$

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with strong interactions: Mott-insulator transition

charge-density wave (CDW)

AF spin-density wave (SDW)

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Raghu et al., PRL 100 (2008) 156401



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

### **Potentially Strong Interactions**

• suspended graphene

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

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

#### • puzzle

 $\varepsilon \to 1$ 

predictions at the time  $lpha_{
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#### screening at short distances

from σ-band electrons and localised higher energy states

 interpolate at intermediate distances with dielectric thin-film model

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

$$(\epsilon_1 = 2.4 \text{ and } d = 2.8 \text{\AA})$$



V(r) [eV]

Wehling et al., PRL 106 (2011) 236805



### **HMC on Hexagonal Lattice**

chiral extrapolation

 $m_{
m sdw} 
ightarrow 0$ 



• semimetal-insulator transition in unphysical regime

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

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

Smith, LvS, PRB 89 (2014) 195429



hexagonal lattice, screened Coulomb







hexagonal lattice, screened Coulomb

α=2.0





hexagonal lattice, screened Coulomb

α=3.0





 $\alpha = 4.0$ 

hexagonal lattice, screened Coulomb





#### hexagonal lattice, screened Coulomb



graphene's single-particle band structure

#### what about CDW and the other insulating phases?





• hexagonal Hubbard model, Hartree-Fock



fermion self-energy









### **HMC on Hexagonal Lattice**



**GIESSEN** 

### **HMC on Hexagonal Lattice**



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#### hexagonal Brillouin zone



 $8 \times 8$  lattice



12 imes 12 lattice

- removes Dirac points
- preserves symmetries
- improves invertibility



#### **Suitable Order Parameters**

for zero(geometric)-mass simulations, use

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

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• spin-density wave:

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



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• charge-density wave:

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



• pure on-site U, SDW



as before:  $U_c pprox 3.8\kappa$ 



#### • violation of spin symmetry!





#### • violation of spin symmetry!



lower temperatures don't help



#### • violation of spin symmetry!



continuum limit in time does



#### **Perfect Action**























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#### 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

 $U_c \approx 3.8 \text{ k}$  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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## Thank you for your attention!

