Electronic instabilities on the honeycomb lattice with electron-phonon interactions

Laura Classen[1]

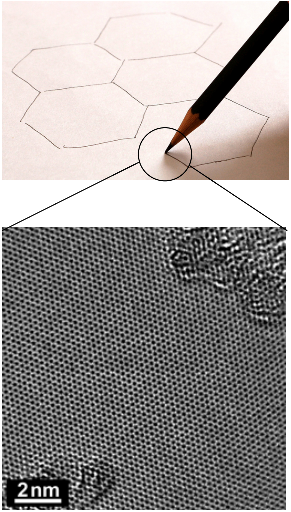
Carsten Honerkamp[2], Michael Scherer[1]

[1]Institute for Theoretical Physics, Heidelberg University
[2]Institute for Theoretical Solid State Physics, RWTH Aachen University

Lefkada, September 2014

Overview

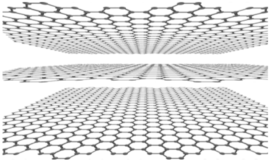
- Ordering tendencies in graphene?
- With phonons:
  Superconductivity? Something else?
- Interplay with short-ranged Coulomb repulsions

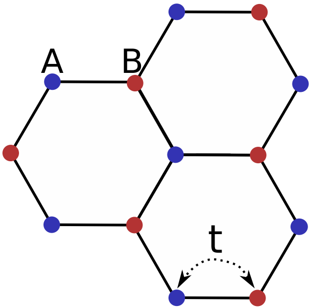


Graphene

- 1 layer of graphite
- Bipartite lattice
- Hopping of free electrons:

$$H = -t \sum_{\langle i,j \rangle, s} c^{\dagger}_{i,A,s} c_{j,B,s} + \text{h.c.}$$

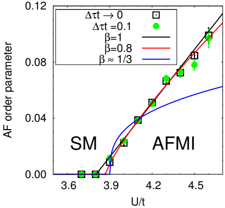




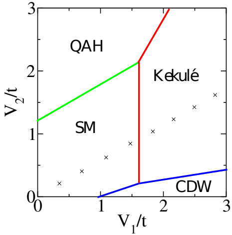
- At zero energy: 2 bands touching at Dirac points
- DOS $\propto$ energy
- Interaction effects suppressed

Induced ordering tendencies from e^-- e^- interactions

Interaction Strength



S. Sorella *et al*
arxiv:1207.1783 (2012)



C. Weeks & M. Franz
PRB **81** (2010)

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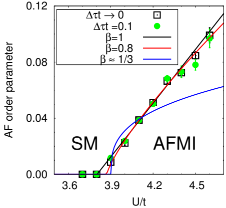

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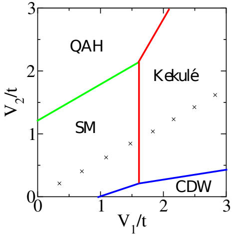

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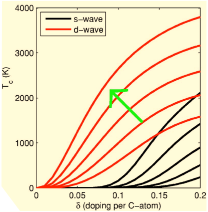
Doping



A.M. Black-Schaffer
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PRB **75**(2007)

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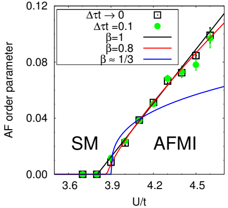

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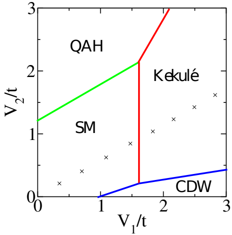

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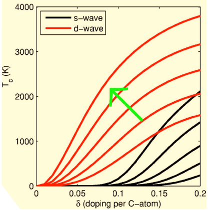

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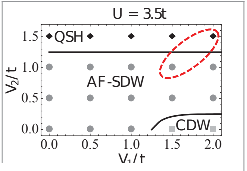
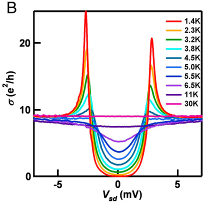
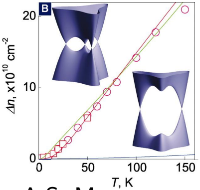


M. Scherer *et al*
PRB **85** (2012)

Number of Layers

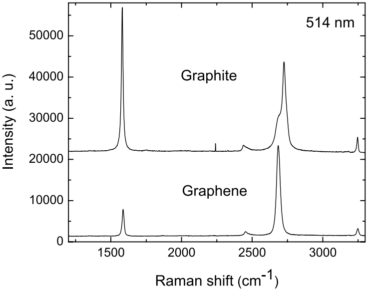


W. Bao *et al*
arxiv:1202.3212 (2012)

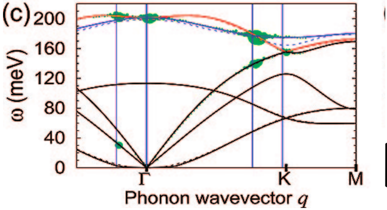


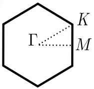
A.S. Mayorov *et al*
Science **333** (2011)

Lattice vibrations



A. C. Ferrari *et al.* PRL **97** (2006)





C. Park *et al.* NL **8** (2008)

PHYSICAL REVIEW B **84**, 214508 (2011)

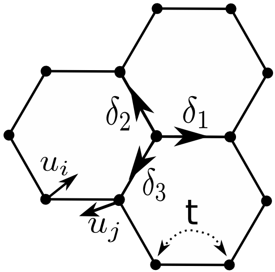
Possibility of superconductivity due to electron-phonon interaction in graphene

Matthias Einenkel and Konstantin B. Efetov
Institut für Theoretische Physik III, Ruhr-Universität Bochum, DE-44780 Bochum, Germany
(Received 20 September 2011; published 6 December 2011)

From lattice displacements to electron-phonon interactions

- Tight-binding Hamiltonian

$$H = -t \sum_{\langle i,j \rangle, \sigma} \left(c^{\dagger}_{i,A,\sigma} c_{j,B,\sigma} + h.c. \right)$$



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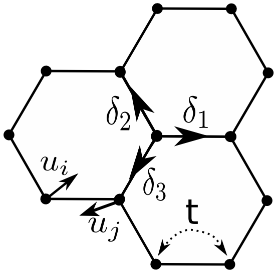
- Lattice distortion changes hopping parameter

$$\boxed{t \to t - \alpha_{||} (\mathbf{u}_i - \mathbf{u}_j) \cdot \hat{\boldsymbol{\delta}}}$$



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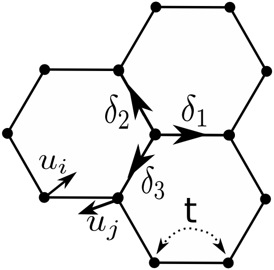

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$$\boxed{t \to t - \alpha_{||}(\mathbf{u}_i - \mathbf{u}_j) \cdot \hat{\boldsymbol{\delta}}}$$

  - Quantization of displacement fields $\mathbf{u}_i \to b_{\lambda,\mathbf{q}} + b^\dagger_{\lambda,-\mathbf{q}}$

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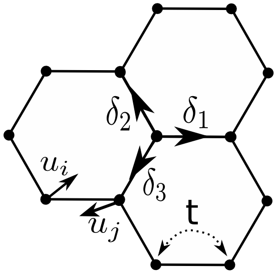

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$$\delta H = \sum_{\mathbf{k},\mathbf{q},s,\lambda} \left[g^\lambda_{\mathbf{k}}(\mathbf{q}) c^\dagger_{\mathbf{k},A,s} c_{\mathbf{k}-\mathbf{q},B,s} \left(b_{\lambda,\mathbf{q}} + b^\dagger_{\lambda,-\mathbf{q}} \right) + \mathrm{h.c.} \right]$$

$$g^\lambda_{\mathbf{k}}(\mathbf{q}) = \frac{\alpha_{||}}{\sqrt{2MN\Omega_{\lambda,\mathbf{q}}}} \sum_{\delta} \left(e^{i\mathbf{q}\cdot\boldsymbol{\delta}} + 1 \right) e^{-i\mathbf{k}\cdot\boldsymbol{\delta}} \mathbf{e}^\lambda_{\mathbf{q}} \cdot \hat{\boldsymbol{\delta}}$$

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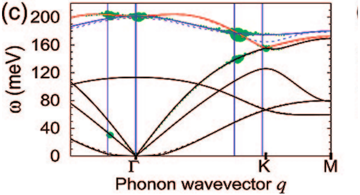

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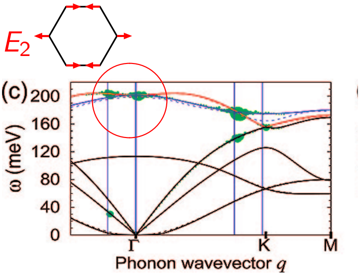

$$\mathbf{e}^\lambda_{\mathbf{q}} = \mathbf{e}^\lambda_{E_2}$$

- Quantization of displacement fields $\mathbf{u}_i \to b_{\lambda,\mathbf{q}} + b^\dagger_{\lambda,-\mathbf{q}}$
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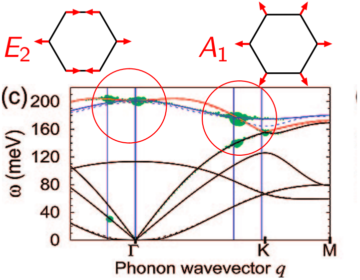

$\mathbf{e}^\lambda_\mathbf{q} = \mathbf{e}^\lambda_{E_2}$ or $\mathbf{e}^\lambda_\mathbf{q} = \mathbf{e}^\lambda_{A_1}$

- Quantization of displacement fields $\mathbf{u}_i \to b_{\lambda,\mathbf{q}} + b^\dagger_{\lambda,-\mathbf{q}}$
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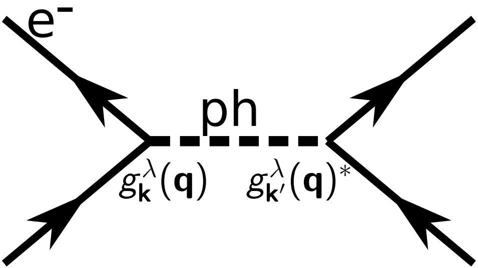
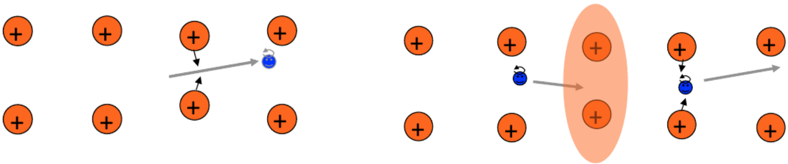
Phonon-mediated electronic interaction

- Integrate phonons out

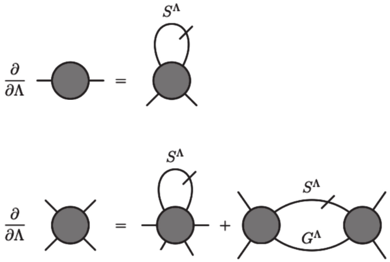


- Physical picture



Functional renormalization group

- Flow equations for 1PI vertices



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W. Metzner *et al*, RMP **84**,(2012)

Functional renormalization group

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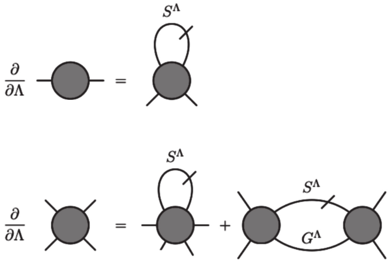

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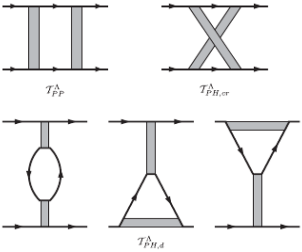
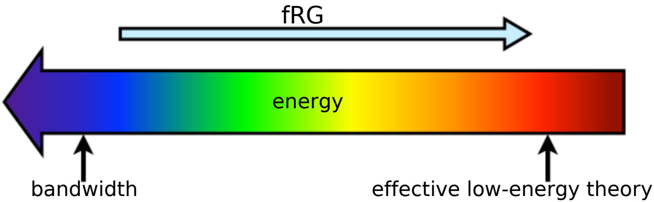
- Focus on 4-point vertex to find leading correlations



W. Metzner *et al*, RMP **84**,(2012)

From bare to effective interactions

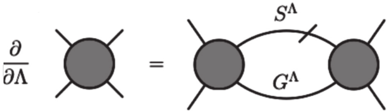


$$H_{bare} = U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \cdots \quad \longrightarrow \quad H_{eff} = \sum_{\substack{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3 \\ s,s'}} V(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) c^\dagger_{\mathbf{k}_3,s} c^\dagger_{\mathbf{k}_4,s'} c_{\mathbf{k}_2,s'} c_{\mathbf{k}_1,s}$$

- PP- and PH-channels on equal footing
- Unbiased
- Provides momentum structure at low energy $V(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)$
  $\rightarrow$ Extract ordering tendency
- Provides pseudocritical energy scales

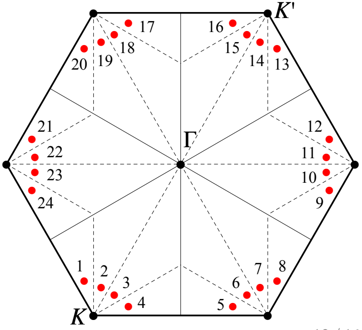
In practice: patching

- Two-particle interaction vertex

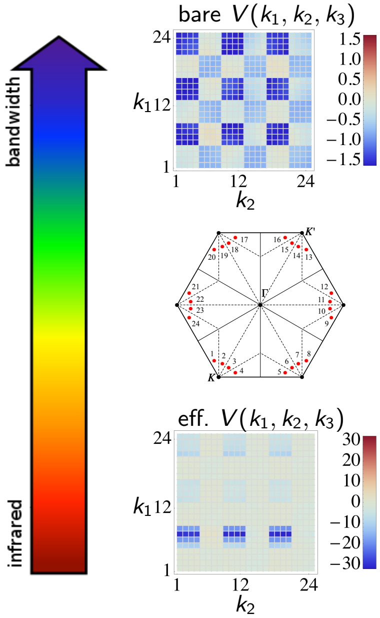


- Solve numerically: discretization through patching

- Representative momenta lie close to Fermi surface
- Interaction constant in one patch



Flow to strong coupling: ph-med interaction only



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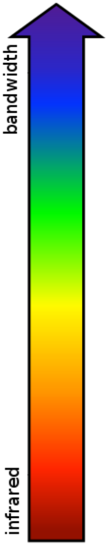
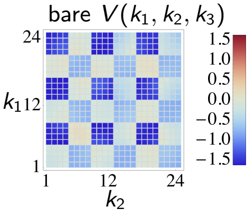
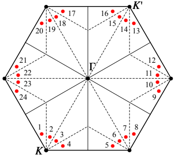
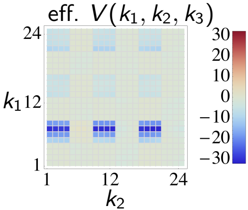
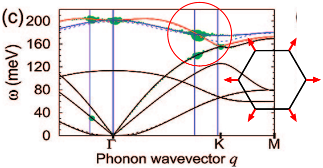




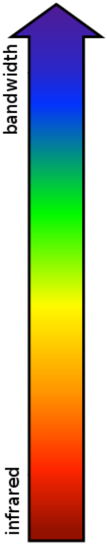


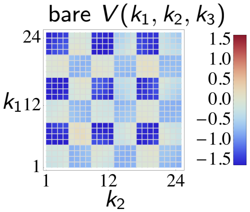


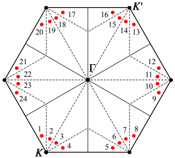
- At low energy: only momentum transfer **K**

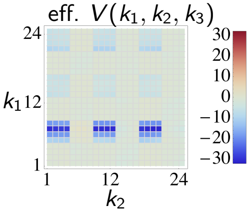


Flow to strong coupling: ph-med interaction only









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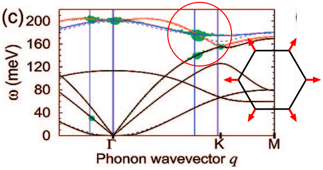
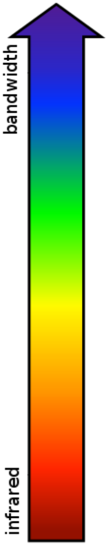
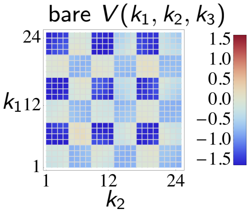
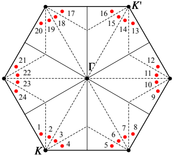


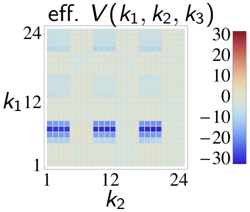
- Static: $\Omega \to 0$ to get diverging interaction ($V_{phmed} \propto \frac{1}{\Omega}$)

Flow to strong coupling: ph-med interaction only









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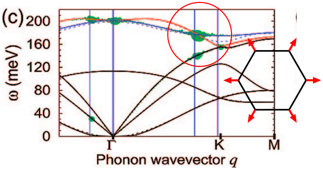
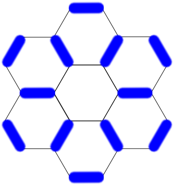
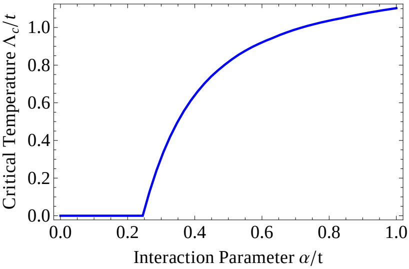


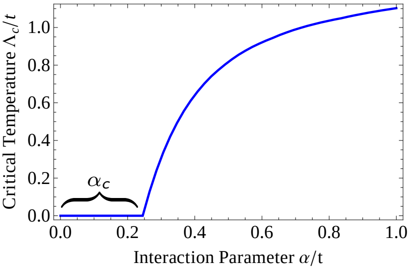
- Static: $\Omega \to 0$ to get diverging interaction ($V_{phmed} \propto \frac{1}{\Omega}$)
- Mean field decoupling: Kekulé distortion opens a gap



As function of the interaction strength

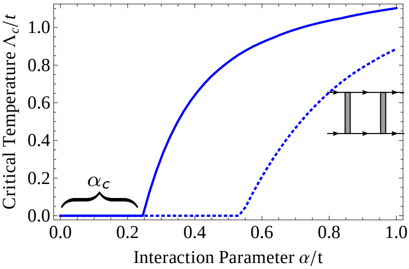


As function of the interaction strength



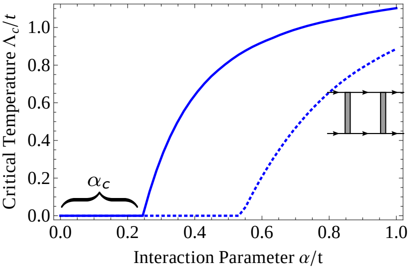
- Critical interaction needed (due to vanishing DOS)

As function of the interaction strength



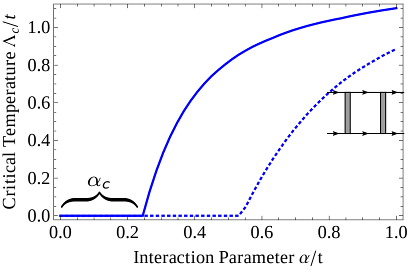
- Critical interaction needed (due to vanishing DOS)
- SC in pp channel

As function of the interaction strength

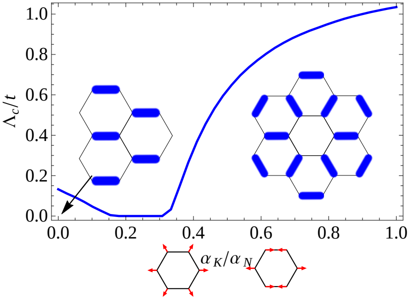


- Critical interaction needed (due to vanishing DOS)
- SC in pp channel
- Bond order in ph-direct favored instability

As function of the interaction strength

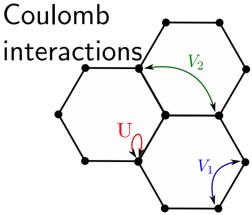


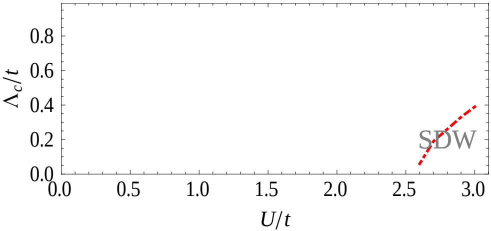
- Critical interaction needed (due to vanishing DOS)
- SC in pp channel
- Bond order in ph-direct favored instability



- For strong zone center modes: nematic bond order
- Weakened by "Kekulé" phonons
- N-patch fRG detects these two ordering tendencies

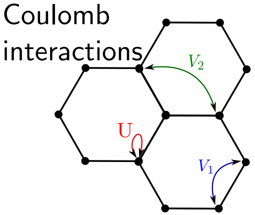
Inlcude short-ranged Coulomb interactions

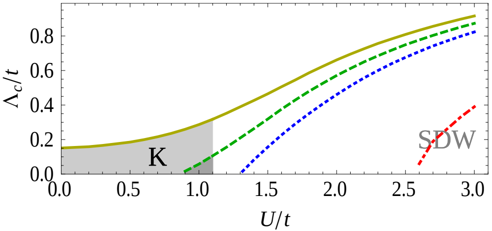




- On-site U induces SDW

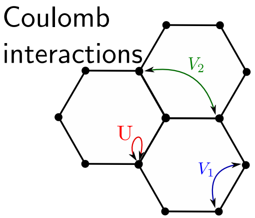
Inlcude short-ranged Coulomb interactions

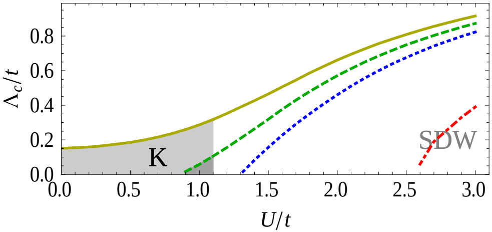


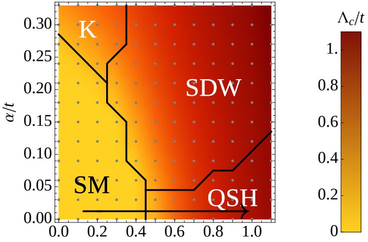


- On-site U induces SDW
- SDW benefits from inclusion of phonons

Inlcude short-ranged Coulomb interactions



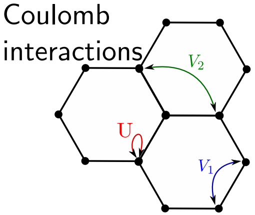


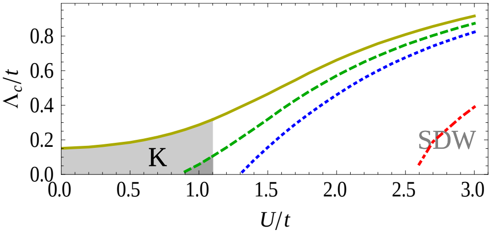


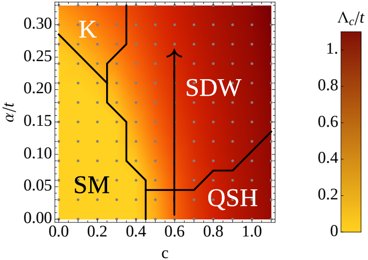
$\{U/t, V_1/t, V_2/t\} \approx \{3.3, 2.0, 1.5\}$
$\rightarrow c\,\{U/t, V_1/t, V_2/t\}$

- On-site U induces SDW
- SDW benefits from inclusion of phonons
- With $U, V_1 \& V_2$: QSH

Inlcude short-ranged Coulomb interactions







$\{U/t, V_1/t, V_2/t\} \approx \{3.3, 2.0, 1.5\}$
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- On-site U induces SDW
- SDW benefits from inclusion of phonons
- With $U, V_1 \& V_2$: QSH
- QSH suppressed by phonons

Summary

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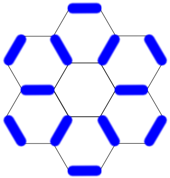
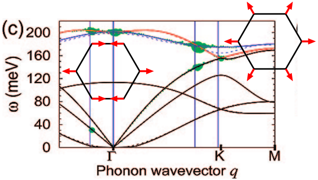
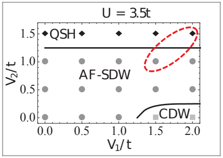
- Analytic e-ph coupling
- Effect of in-plane phonons on ordering tendencies





- Dominant instability in ph-channel
- Kekulé bond order favored over SC
- Small-q phonons drive nematic state

- With Coulomb: AF-SDW supported
- Extension to bilayer?



Thank you for your attention!