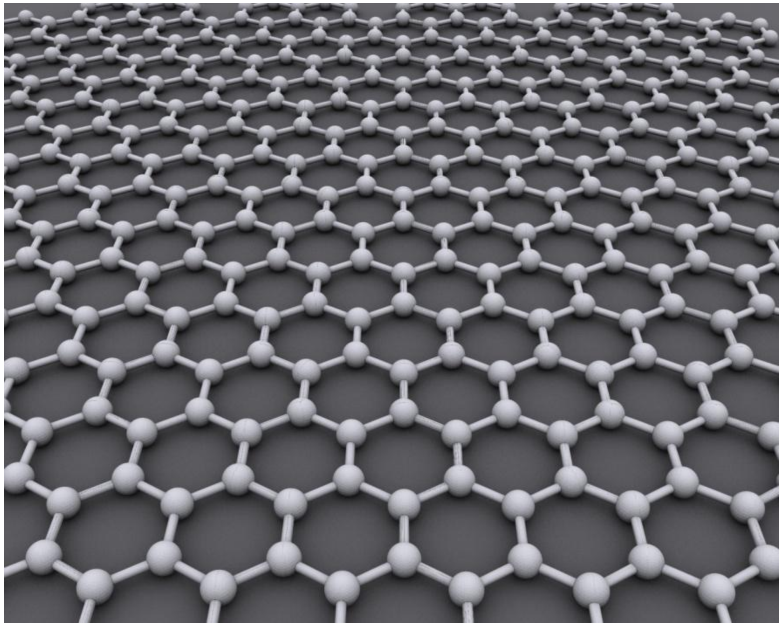
グラフェン状の系における秩序現象と相構造

Competiton of orders and phase structure in graphene-like systems



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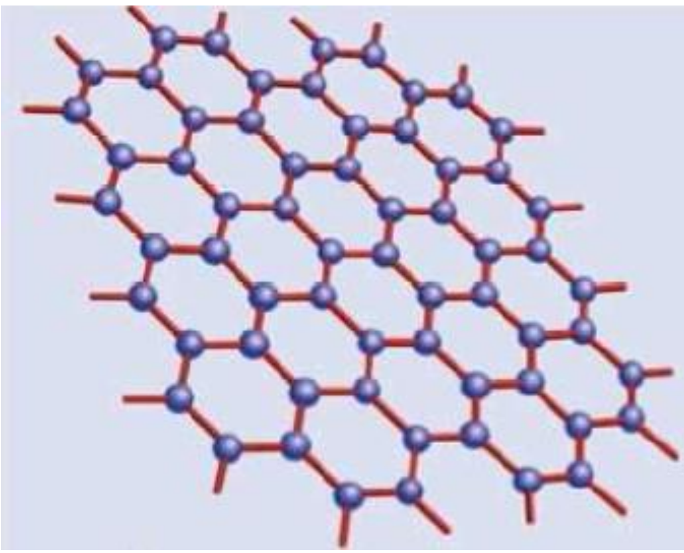
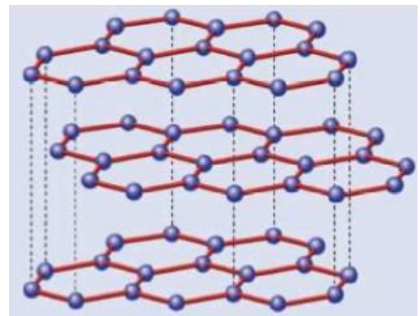
Aug. 22-24, 基研研究会「熱場の量子論とその応用」2012

What is “graphene”?

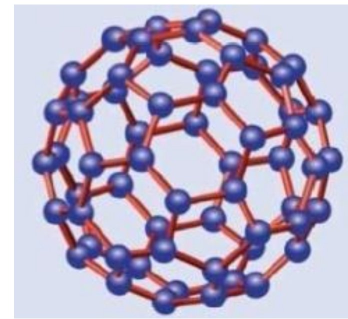
Monoatomic layer material of carbon atoms

Honeycomb lattice structure in 2-dim plane.



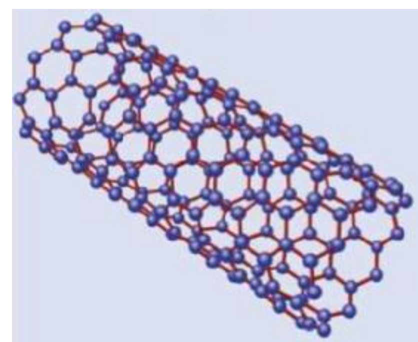


graphite



fullerene

Building block of carbon materials.



nanotube

For review:

A. Castro Neto *et al.*, RMP **81**, 109 (2009).

Interaction and gap formation in graphene

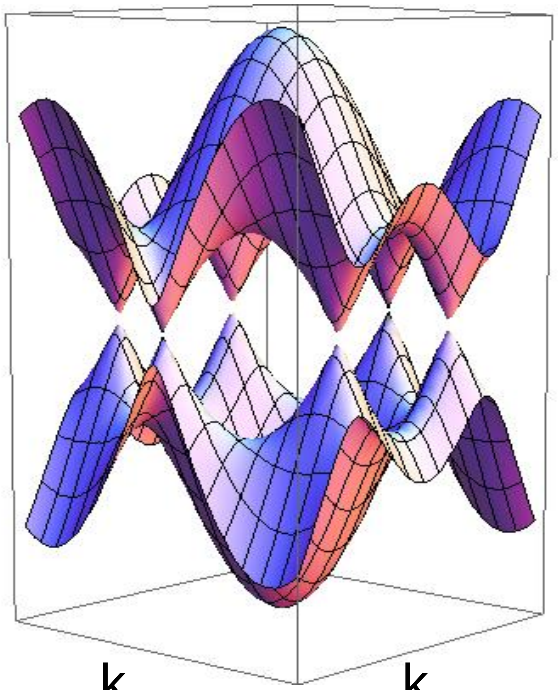
Electronic spectrum of monolayer graphene:

linear dispersion around two “Dirac points”.

$$E(\mathbf{K}_\pm + \mathbf{k}) \simeq v_F |\mathbf{k}|$$

Wallace(1947)
Semenoff(1984)

(Fermi velocity v_F = (3/2)*ah* ~ *c*/300)



- Effective Coulomb interaction strength:

“Fine structure const.”

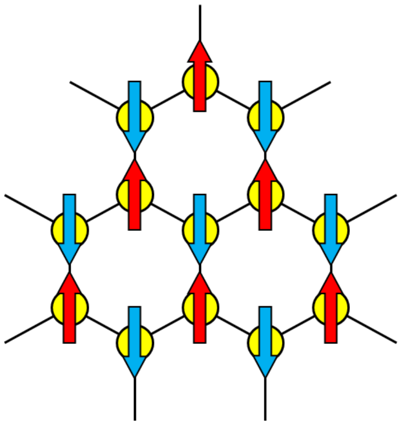
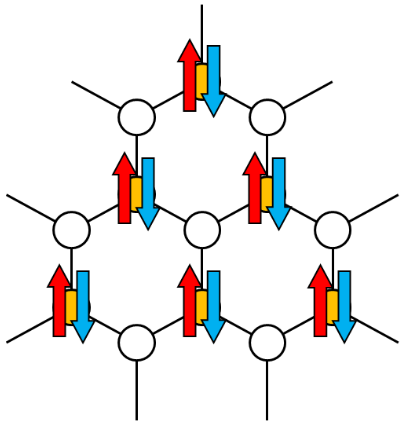
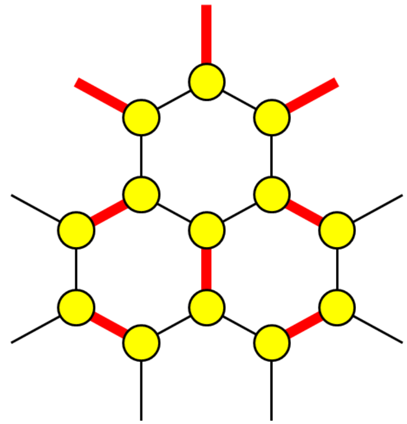
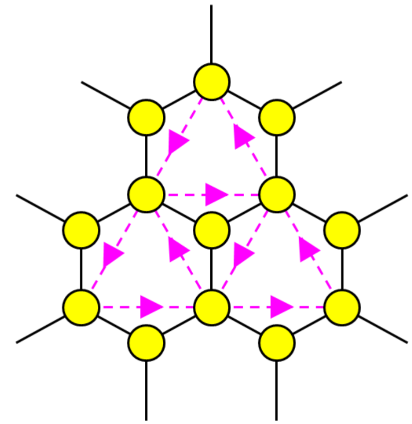
$$\alpha_{\mathrm{eff}} = \frac{e^2}{4\pi\epsilon v_F} \quad (\gg \alpha_{\mathrm{QED}})$$

$$\left(\alpha_{\mathrm{QED}} = \frac{e^2}{4\pi\epsilon_0 c} = \frac{1}{137}\right)$$

⇒ Effectively strong coupling (in vacuum-suspended graphene).

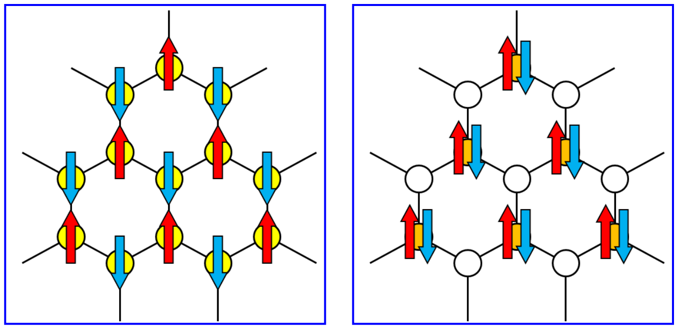
Spontaneous symmetry breaking (ordering) ⇒ Gap generation?

Possible orders on honeycomb lattice

Spin density wave (SDW)	Charge density wave (CDW)	Kekulé distortion (KD)	Quantum anomalous Hall
			
Sublattice (inversion) symmetry is broken.		Translational symmetry is broken.	(Time-reversal symm. is broken)
	Induced explicitly by substrates (BN, SiC, …) “mass term”	Induced explicitly by adatoms (Ca, Al, …)	(Model of topo-logical insulators) Haldane(1988)

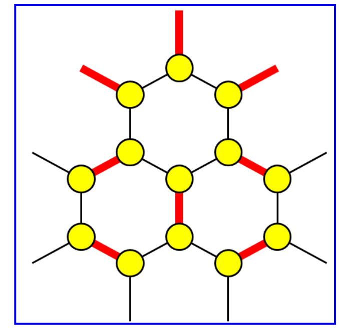
Competition of orders

e.g.) Sublattice symmetry breaking

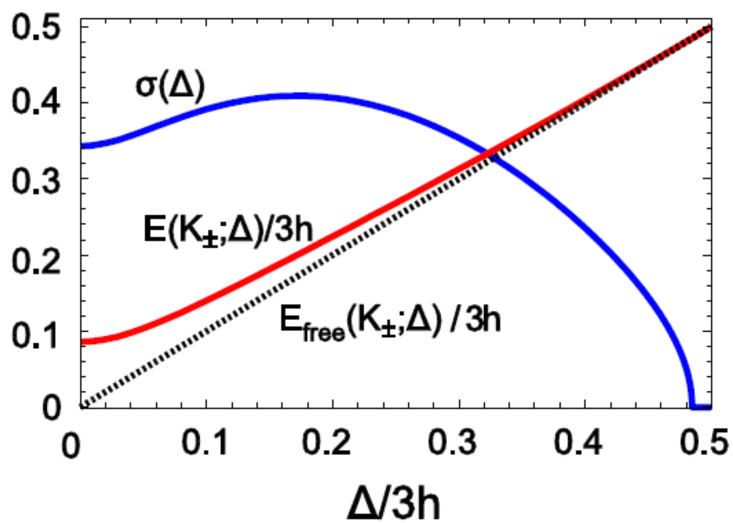


VS

Kekulé distortion

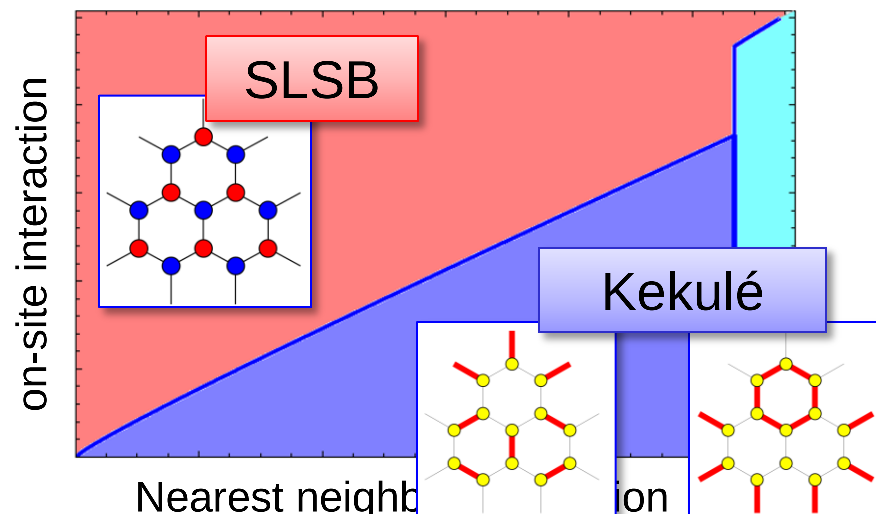


Spontaneous SLSB VS External Kekulé



YA, Phys. Rev. B **84**, 113402 (2011)

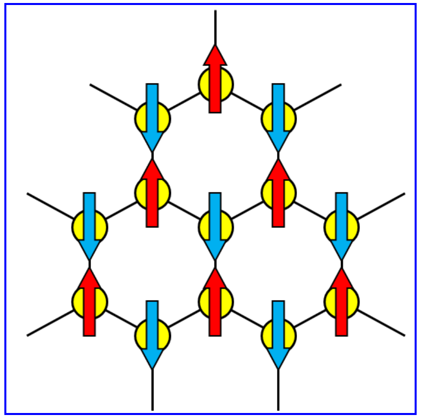
Spontaneous SLSB VS Spontaneous Kekulé



YA, Phys. Rev. B **85**, 125436 (2012)

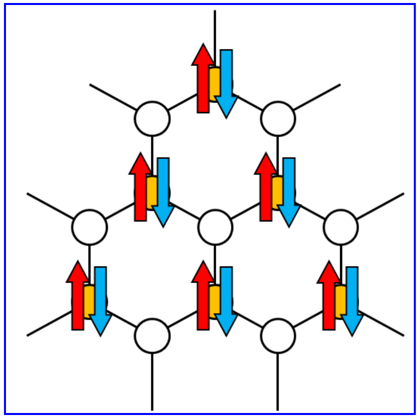
This talk

Spontaneous/External CDW



vs

Spontaneous SDW

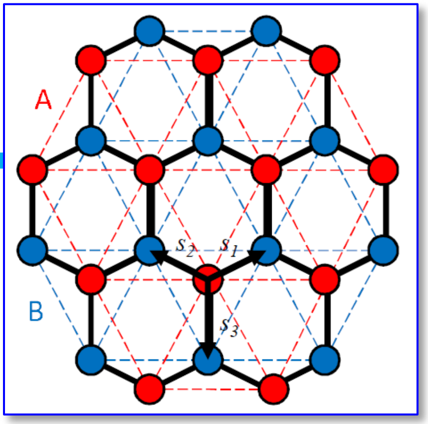


- Is there any interplay effect between these two orders?
- What may happen to the band structure and electronic properties of the system?

⇨ Solve by Hamiltonian variational method.

"Spin Versus Charge Density Wave Order in Graphene-like Systems",
Y. A. and G. W. Semenoff, arXiv:1204.4531[cond-mat.str-el].

Effective model



"Extended Hubbard model"

- Electron hopping (tight-binding model):

$$H_T = -t \sum_{\langle \mathbf{r}_A, \mathbf{r}_B \rangle} \left[a^\dagger_\sigma(\mathbf{r}_A) b_\sigma(\mathbf{r}_B) + b^\dagger_\sigma(\mathbf{r}_B) a_\sigma(\mathbf{r}_A) \right]$$

- On-site (Hubbard) repulsion:

$$H_U = U \left[\sum_{\mathbf{r}_A} n_\uparrow(\mathbf{r}_A) n_\downarrow(\mathbf{r}_A) + \sum_{\mathbf{r}_B} n_\uparrow(\mathbf{r}_B) n_\downarrow(\mathbf{r}_B) \right]$$

Favors SDW

- Nearest neighbor (NN) repulsion:

$$H_V = V \sum_{\langle r_A, \mathbf{r}_B \rangle} n(\mathbf{r}_A) n(\mathbf{r}_B)$$

Favors CDW

- Staggered potential:

$$H_M = m \left[\sum_{\mathbf{r}_A} a^\dagger_\sigma(\mathbf{r}_A) a_\sigma(\mathbf{r}_A) - \sum_{\mathbf{r}_B} b^\dagger_\sigma(\mathbf{r}_B) b_\sigma(\mathbf{r}_B) \right]$$

External CDW

Hamiltonian variational method

(1) Take a reference Hamiltonian H_0.

$$H_0^T = -\sum_\sigma Z_\sigma t \sum_{\mathbf{r}\in A,i} \left[a_\sigma^\dagger(\mathbf{r}) b_\sigma(\mathbf{r}+\mathbf{s}_i) + \mathrm{H.c.}\right]$$

$$H_0^M = \sum_\sigma \Delta_\sigma \sum_{\mathbf{r}} \left[a_\sigma^\dagger a_\sigma - b_\sigma^\dagger b_\sigma\right]$$

velocity renormalization

quasiparticle gap

⇨ dispersion: $E_\sigma(\mathbf{K}_\pm + \mathbf{k}) \simeq \sqrt{|Z_\sigma v_F \mathbf{k}|^2 + \Delta_\sigma{}^2}$

(2) Vary H_0 to approximate the original Hamiltonian H as much as possible.

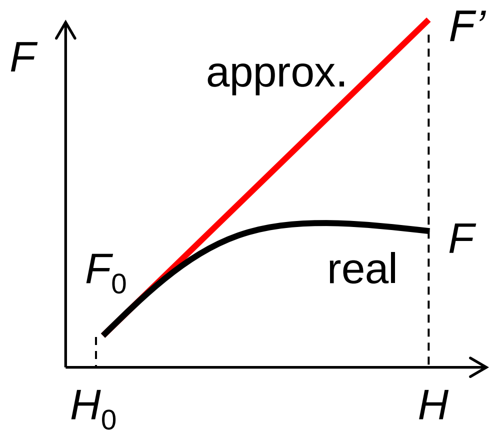
$$F \leq F' \equiv F_0 + \langle H - H_0 \rangle_0 \qquad (\langle A \rangle_0 \equiv \mathrm{Tr} A e^{-\beta H_0})$$

- "Jensen-Peierls inequality"

⇨ Minimize *F'* as much as possible.

i.e. $\dfrac{\delta F'}{\delta H_0} = 0$

(corresponds to the MF gap equation)



Phase structure

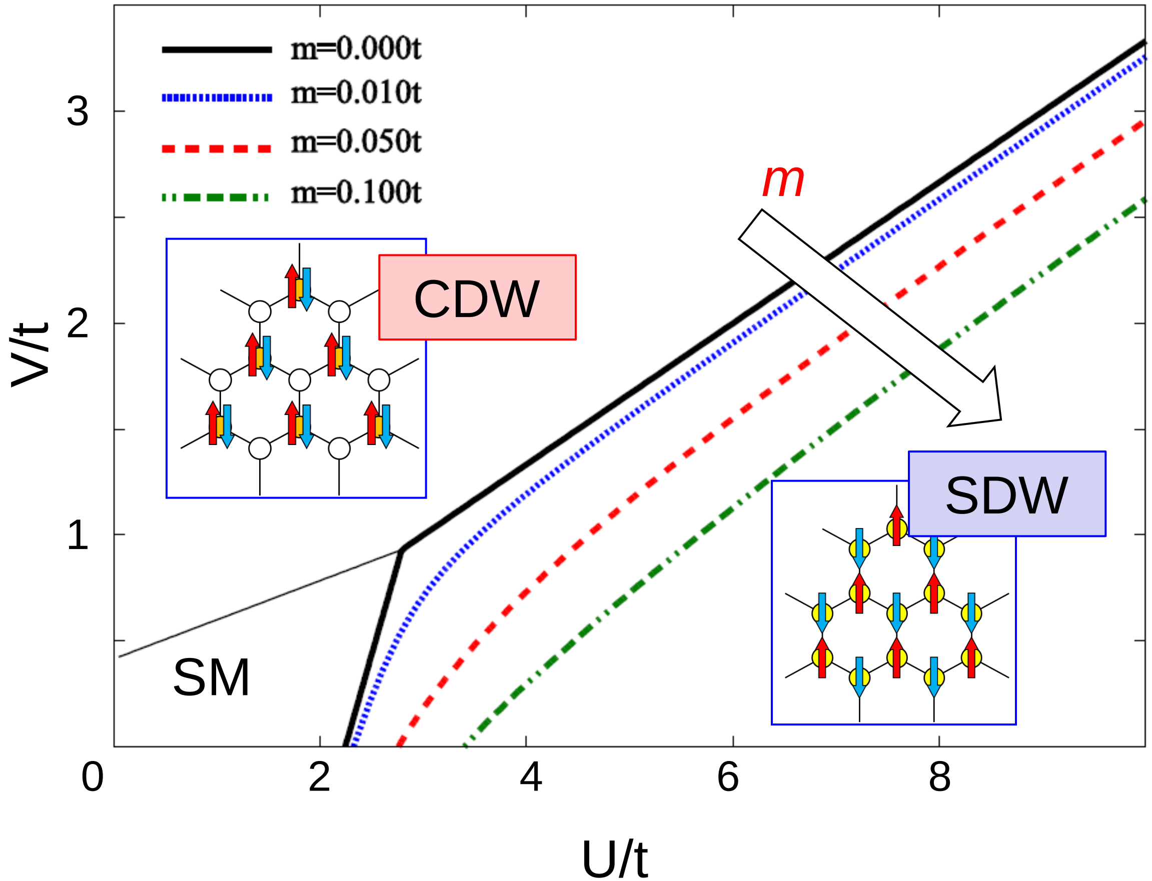
Input

U, V, m

variational gap eq.

Output

Δ_σ, Z_σ



$\Delta_\uparrow = \Delta_\downarrow = 0$:
Semimetallic (SM) phase
(only at m=0)

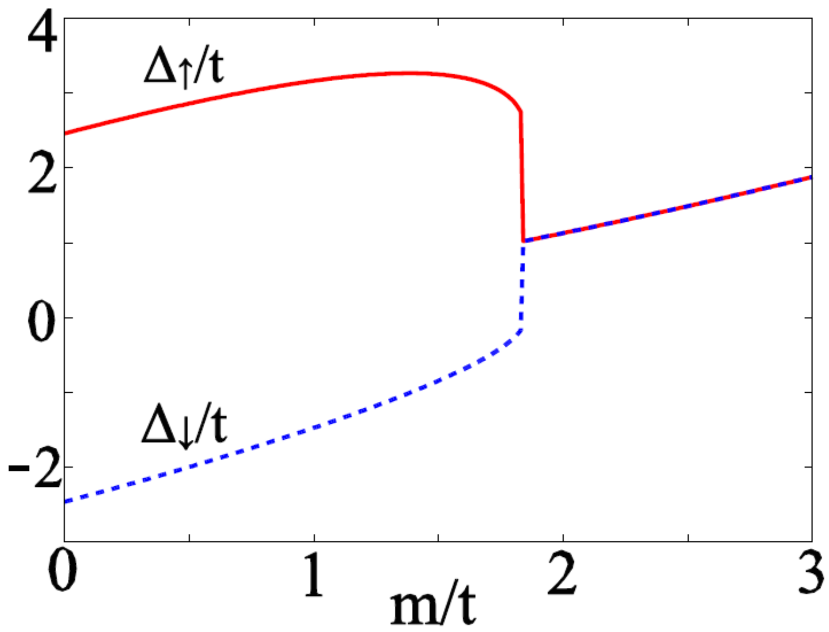
$\Delta_\uparrow = \Delta_\downarrow \neq 0$:
CDW phase

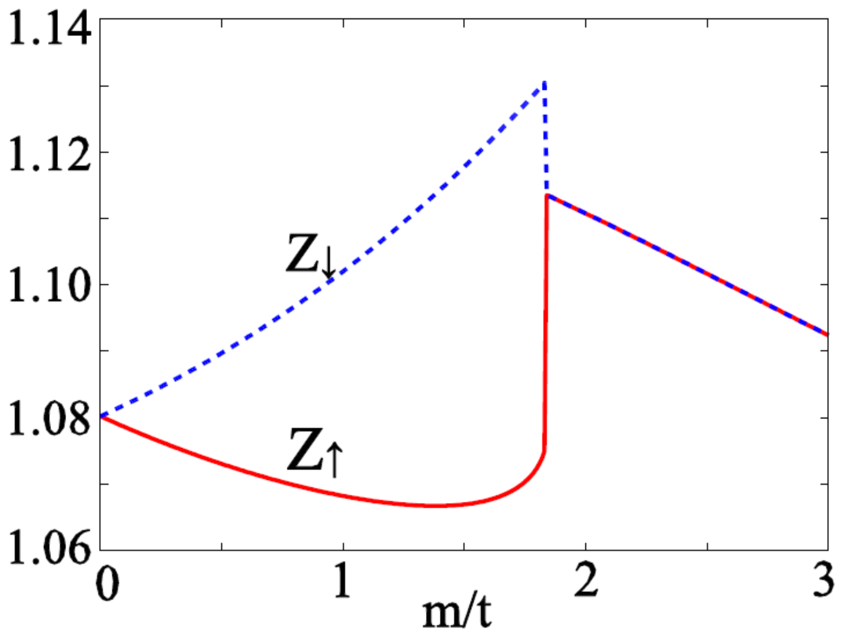
$\Delta_\uparrow \neq \Delta_\downarrow$:
SDW phase

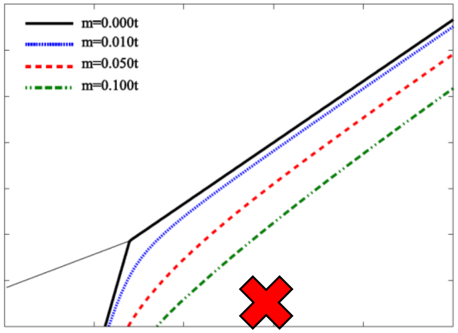
Introduction of *m*
⇨ SDW is suppressed over CDW.

Splitting of gap and velocity

- Fix U=6t, V=0.5t / Vary m:







$$|\Delta_\uparrow| \neq |\Delta_\downarrow| \quad \text{and} \quad Z_\uparrow \neq Z_\downarrow$$

in the SDW phase (if m,V≠0).

Summary

- Phase structure of extended Hubbard model with explicit staggered potential is investigated by the Hamiltonian variational method.
- There is an interplay between CDW and SDW.
- SDW is suppressed over CDW in the presence of staggered potential.
- Staggered potential (bare fermion “mass”) splits the degeneracy of quasiparticle gap and Fermi velocity between spin states.

- Extended Hubbard model ⇨ Coulomb interaction?

  Momentum-dependent Fermi velocity?

  cf. continuum limit: Sabio, Sols, Guinea(2010)

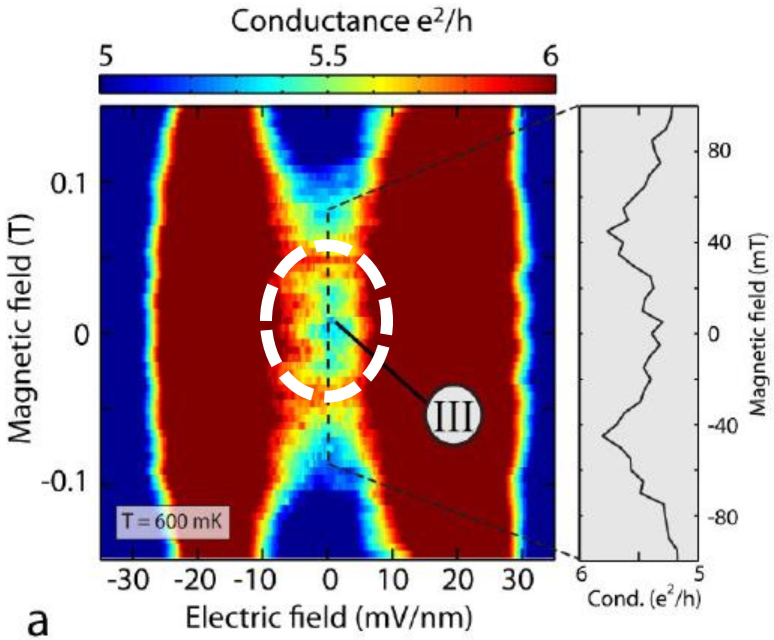
  Derivation from QED-related model...?

Recent topics

- Extension to bilayer graphene:

  Spontaneously gapped phase(?) is experimentally observed.

  Thomas Weitz *et al.*(2010)



<u>Bilayer:</u>

dispersion relation becomes quadratic.

What kind of symmetry is broken?

- sublattice (chiral)
- Dirac point (pseudospin)
- spin
- layer

- Effect of next-to-NN interaction (~NNLO): "Anomalous QH" state?
- Finite-size sample: edge states (zigzag edge) vs. bulk properties

Various phases are expected …