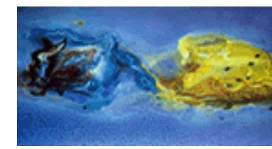
Competing Order in the Hexagonal Hubbard Model

**Pavel Buividovich, Dominik Smith,
Maksim Ulybyshev, Lorenz von Smekal**

XIIIth Quark Confinement &
Hadron Spectrum



Maynooth, 3 August 2018

CRC-TR 211
Strong-interaction matter under extreme conditions

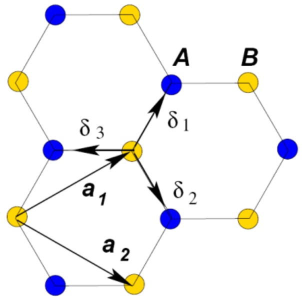
HIC for FAIR
Helmholtz International Center

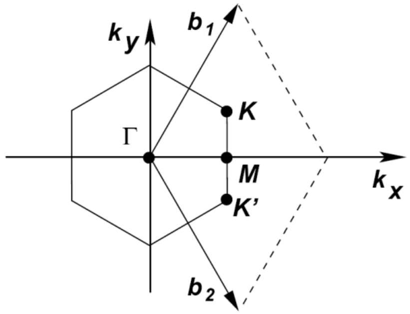
Outline

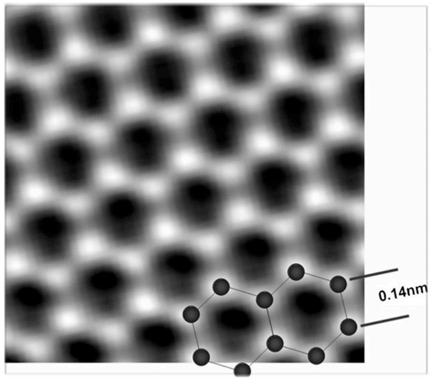
- Intro Honeycomb Lattice
- Hybrid Monte-Carlo of Extended Hubbard Model
- Improvements
- Phase Diagram
- Summary and Outlook

Honeycomb Lattice

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







graphene

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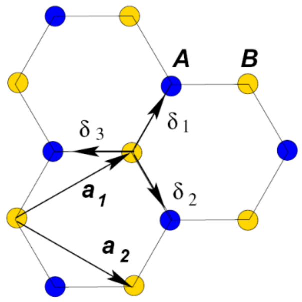
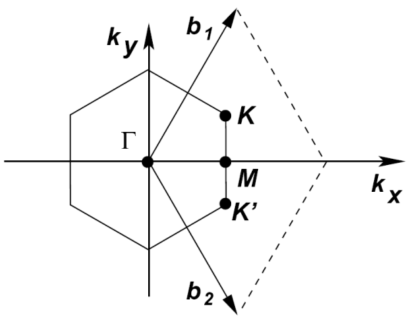
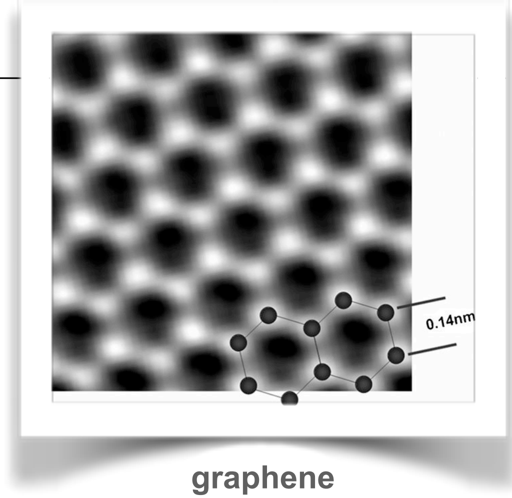
- **triangular lattice – hexagonal Brillouin zone (2 atoms per unit cell)**







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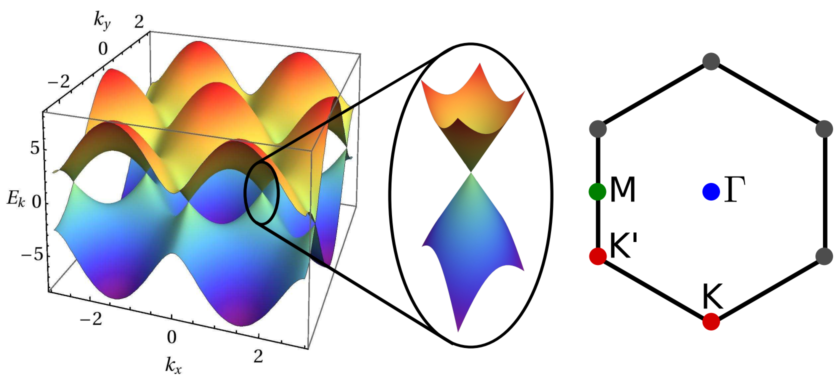
- **nearest-neighbor tight-binding Hamiltonian**

$$\mathcal{H}_{\rm tb} = -\kappa \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle,\sigma} \left(c^\dagger_{\boldsymbol{i},\sigma} c_{\boldsymbol{j},\sigma} + c^\dagger_{\boldsymbol{j},\sigma} c_{\boldsymbol{i},\sigma} \right)$$



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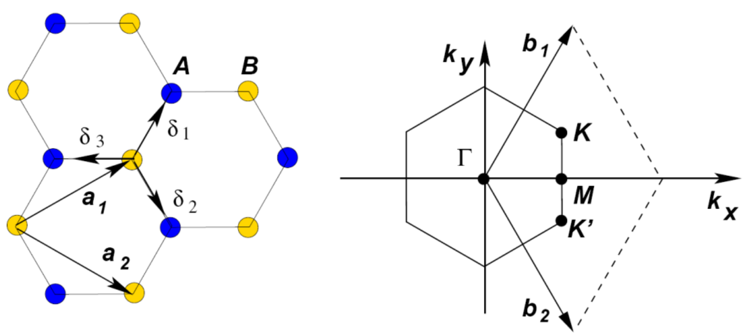

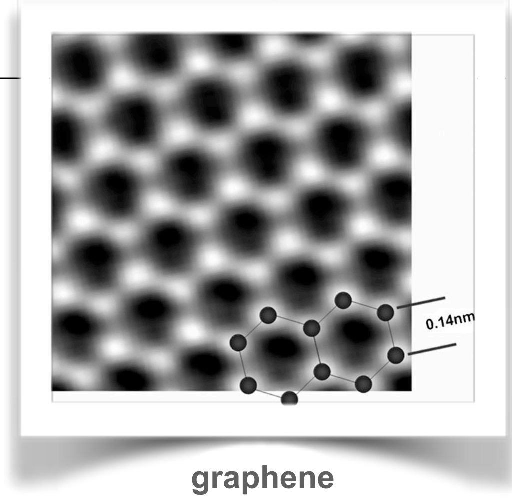

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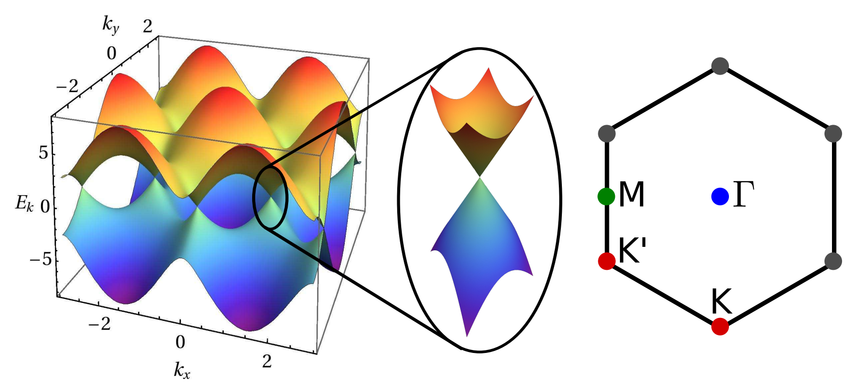

- **single-particle energy bands**

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

[Wallace, 1947]

structure factor:

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

Honeycomb Lattice

- mass terms (gaps)

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

$$\mathcal{H}_m = \sum_{\boldsymbol{i},\sigma} (-1)^s m_\sigma \, c^\dagger_{\boldsymbol{i},\sigma} c_{\boldsymbol{i},\sigma}$$

(pseudo-spin) staggered on-site potential

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- **spin (flavor) dependence**

with strong interactions:
Mott-insulator transition

$$m \to 0$$

$$m_{\mathrm{cdw}} = \frac{1}{2}(m_\uparrow + m_\downarrow) \longrightarrow$$ charge-density wave (CDW)

$$m_{\mathrm{sdw}} = \frac{1}{2}(m_\uparrow - m_\downarrow) \longrightarrow$$ AF spin-density wave (SDW)

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$$\mathcal{H}_{\text{int}} = \frac{1}{2} \sum_{\boldsymbol{i},\boldsymbol{j}} V_{\boldsymbol{i}\boldsymbol{j}} \; q_{\boldsymbol{i}} q_{\boldsymbol{j}}$$

$$q_{\boldsymbol{i}} = c^\dagger_{\boldsymbol{i},\sigma} c_{\boldsymbol{i},\sigma} - 1$$

charge at site

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on-site

$$V_{\boldsymbol{ij}} = U \delta_{\boldsymbol{ij}}$$

nearest neighbor

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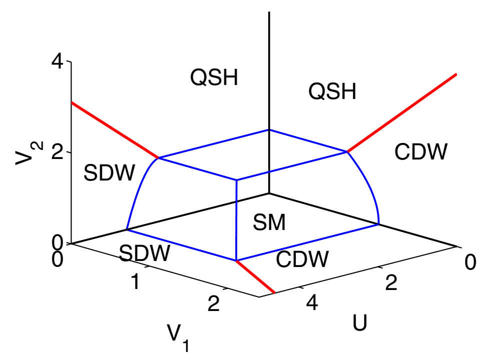
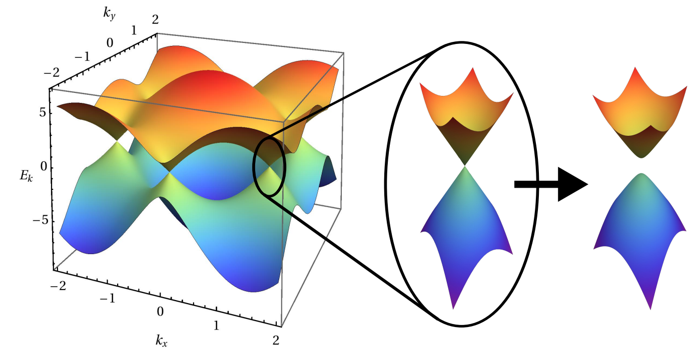


Raghu *et al.*, PRL 100 (2008) 156401

Previous Graphene Studies

- **semimetal insulator (SDW) transition:**



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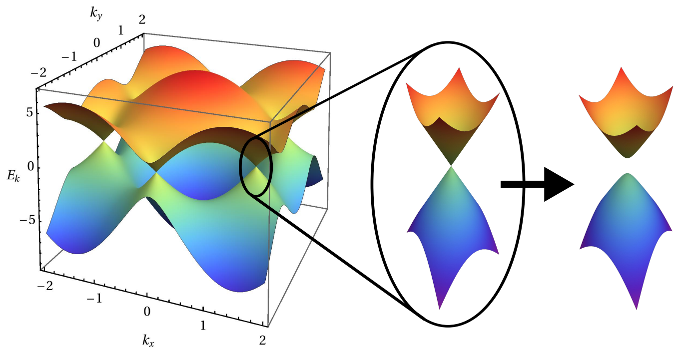

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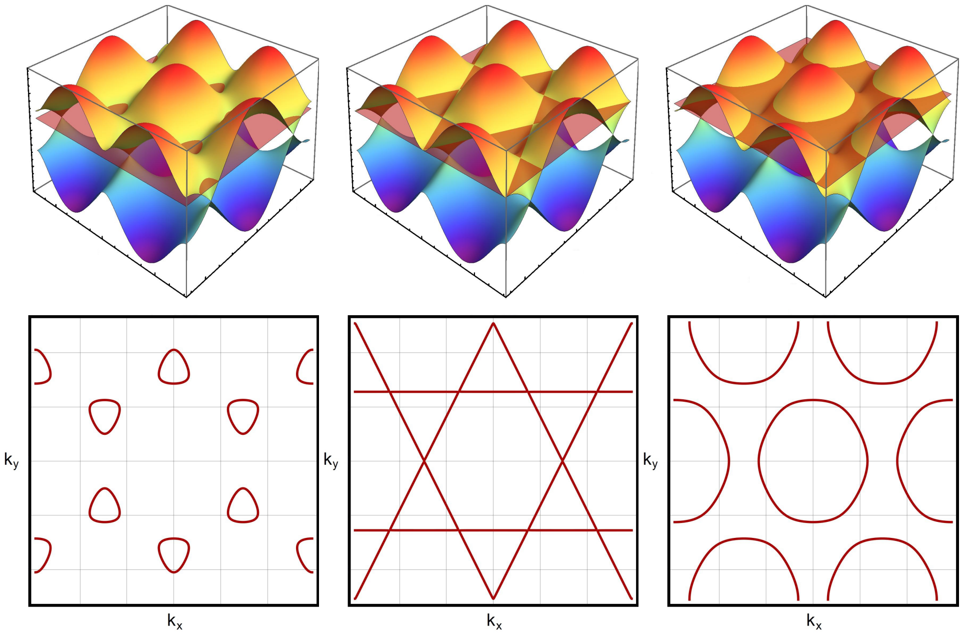

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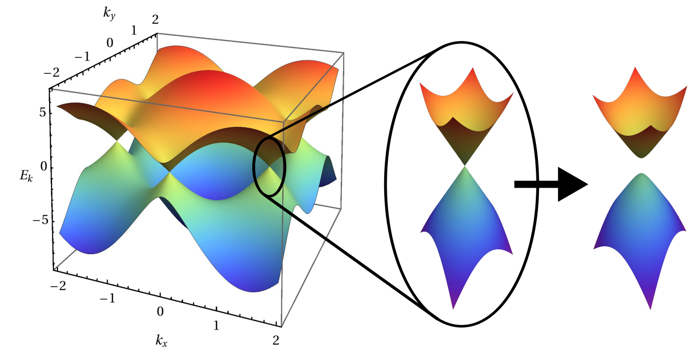

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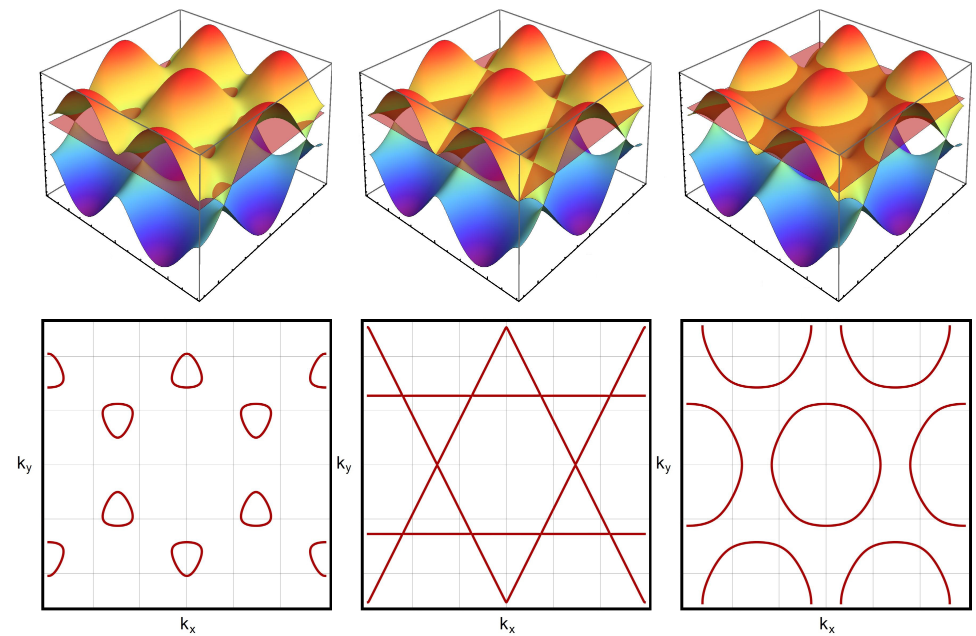
- **adatom (RKKY) interactions:**

  Buividovich, Smith, Ulybyshev, LvS, PRB 96 (2017) 165411

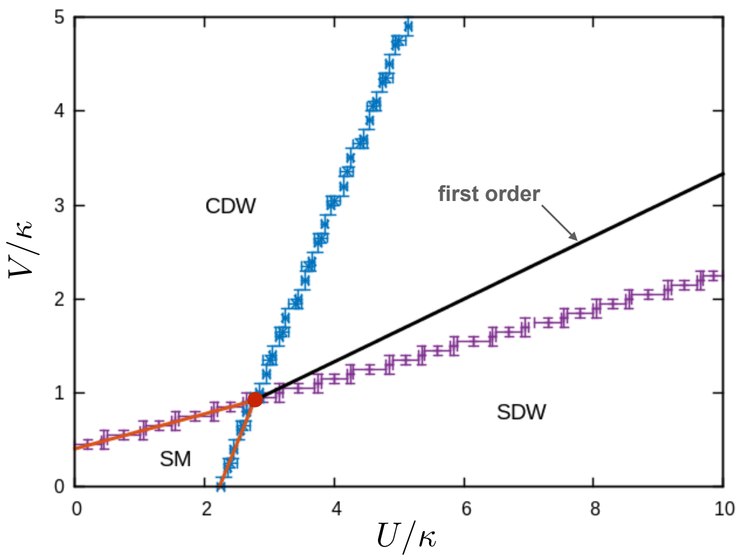


Extended Hubbard Model

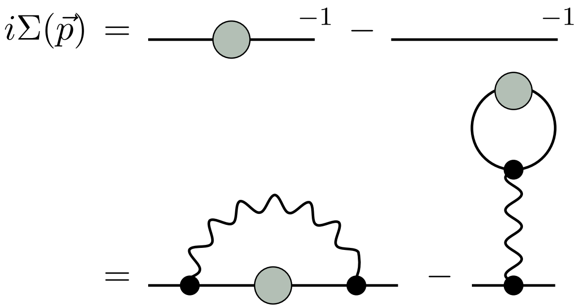
- **on-site + nearest neighbour interaction**

$$V_{ij} = U\delta_{ij} + V\delta_{ij\sim i}$$

- **Dyson-Schwinger eqns., Hartree-Fock**



fermion self-energy



from PoS (LATTICE 2016) 244, arXiv:1610.09855
Katja Kleeberg *et al.*, in preparation
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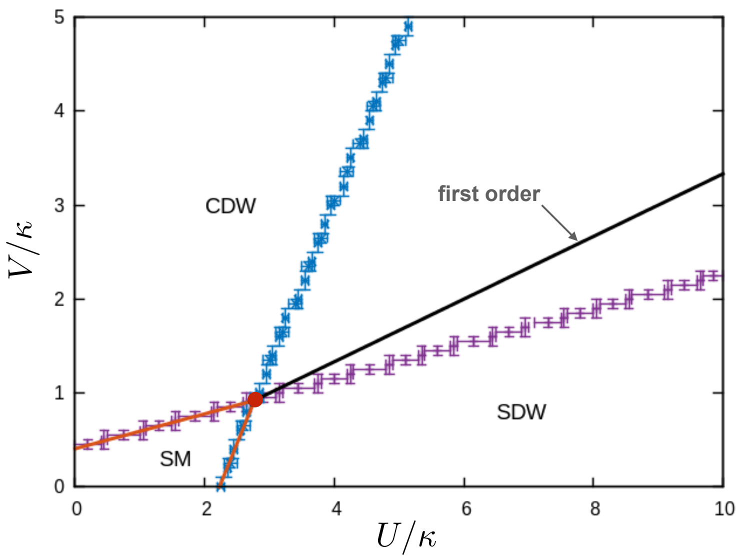

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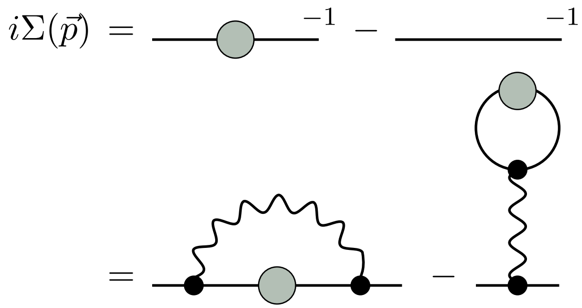
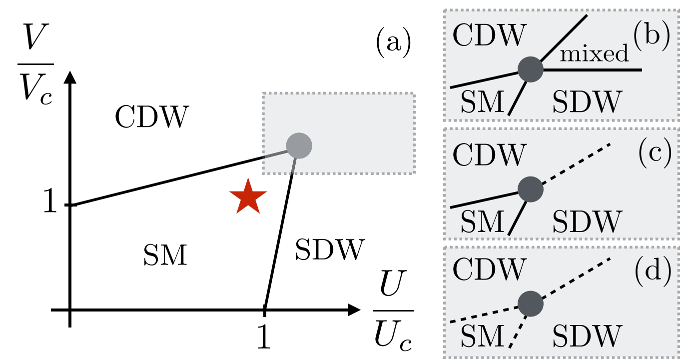


- ε-expansion, functional renormalization group



Classen, Herbut, Janssen, Scherer, PRB 92 (2015) 035429
Classen, Herbut, Janssen, Scherer, PRB 93 (2016) 125119

Hybrid Monte-Carlo

- **positivity of interaction matrix** requires $|V| < |U|/3$

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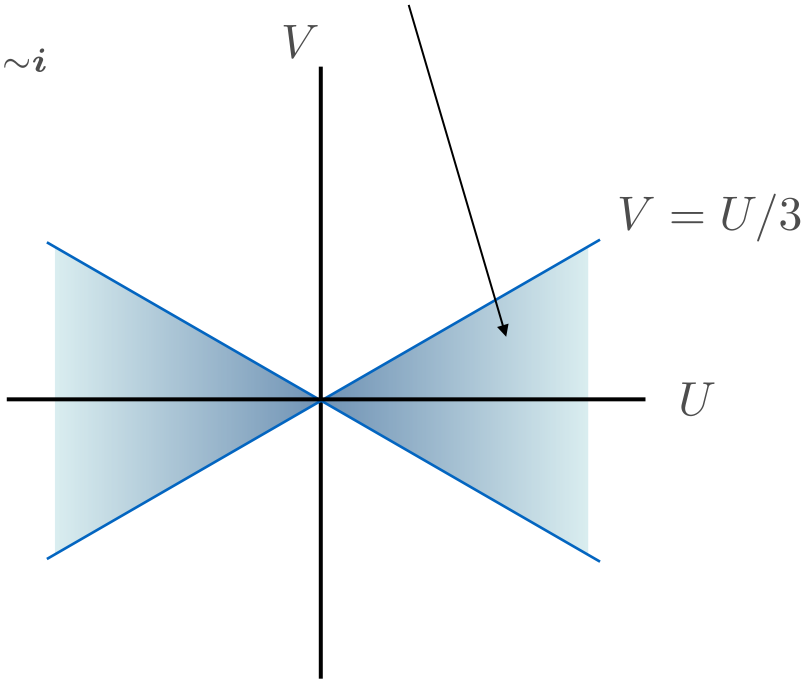

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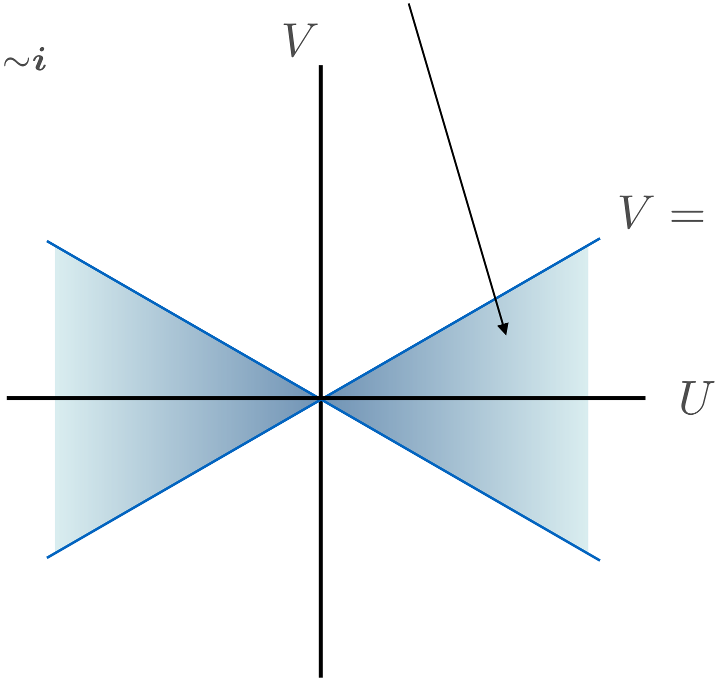

expect

SDW, chiral Heisenberg Gross-Neveu universality

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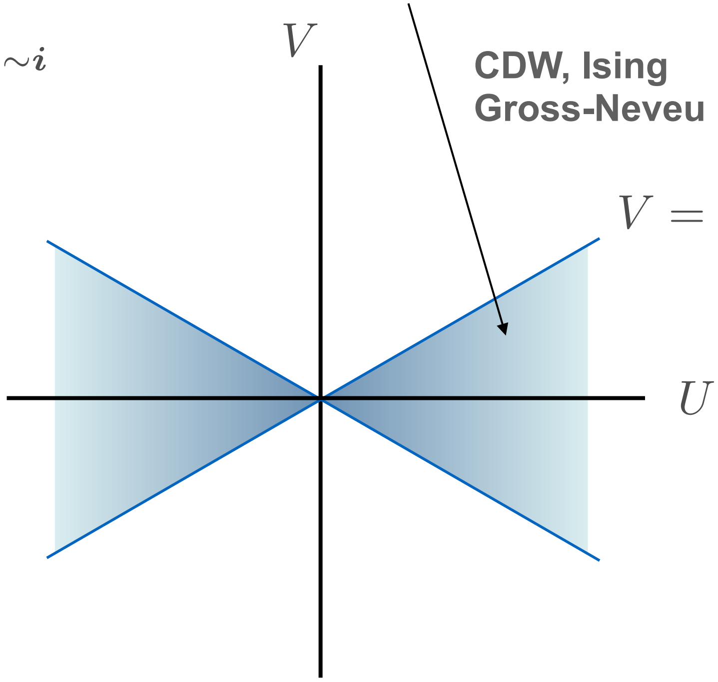

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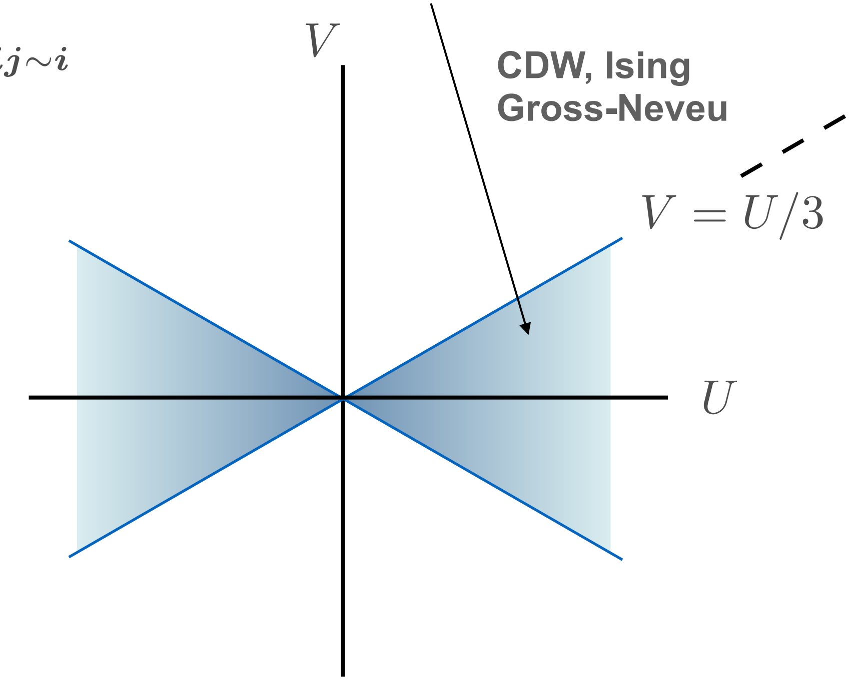
identical interaction energies at strong coupling

CDW, Ising Gross-Neveu



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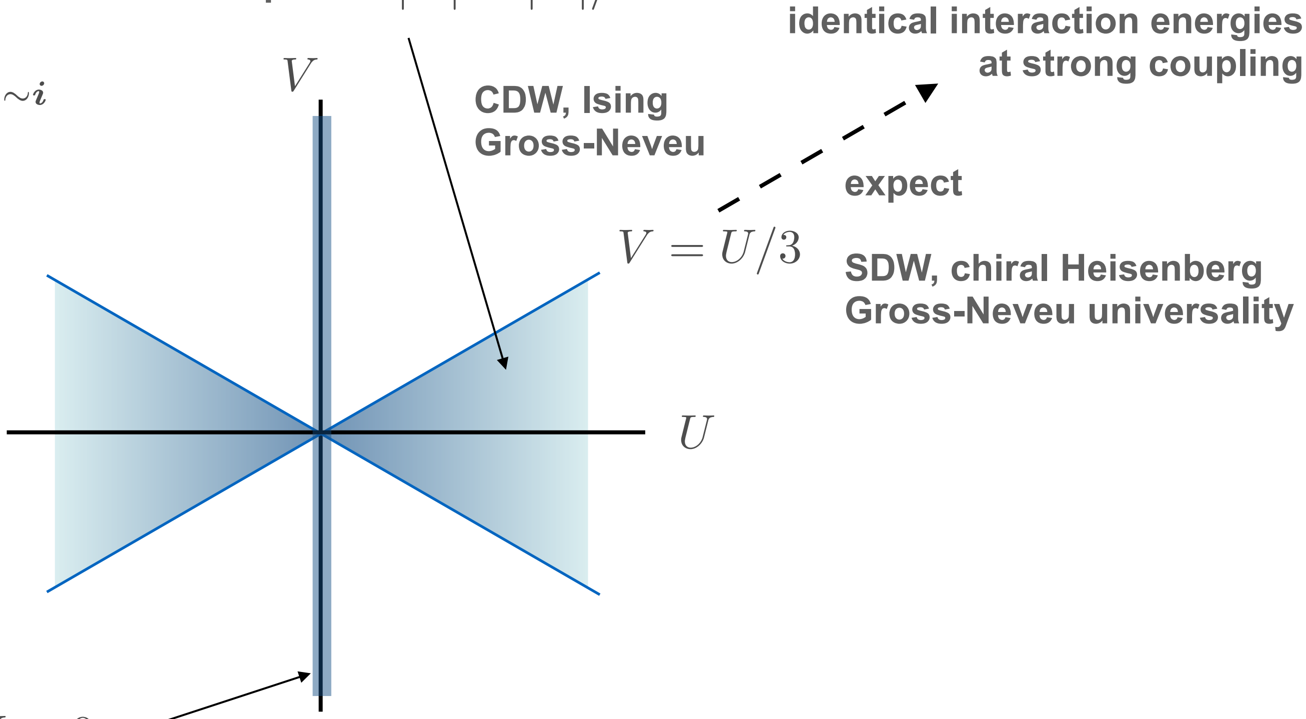

simulate without sign problem at $U = 0$

Chandrasekharan, Wiese, PRL 83 (1999) 3116

Huffman, Chandrasekharan, PRB 89 (2014) 111101(R)

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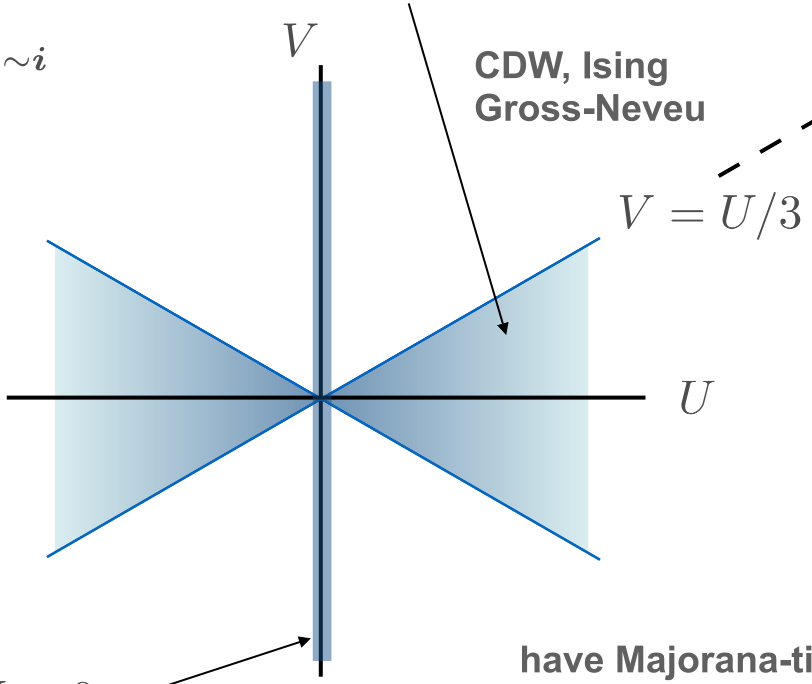

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Li, Jiang, Yao, PRB 91 (2015) 241117

Li, Jiang, Yao, PRL 117 (2016) 267002

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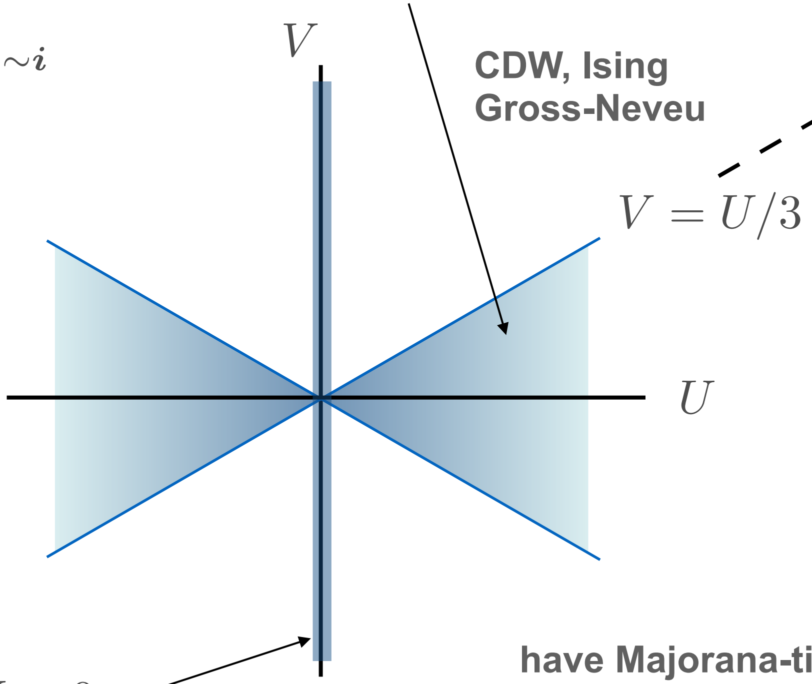

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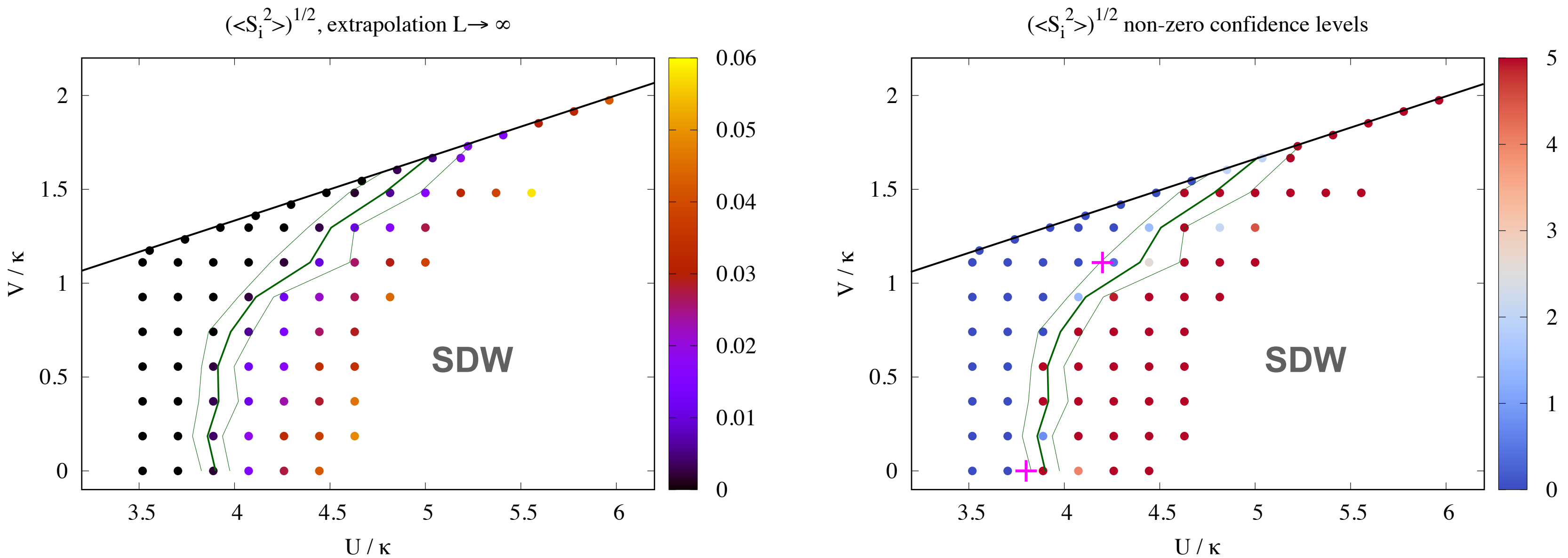
Buividovich, Smith, Ulybyshev, LvS, arXiv:1807.7025



$$N_\tau = 128,\ T = 0.046\kappa \approx 0.124\text{eV}$$

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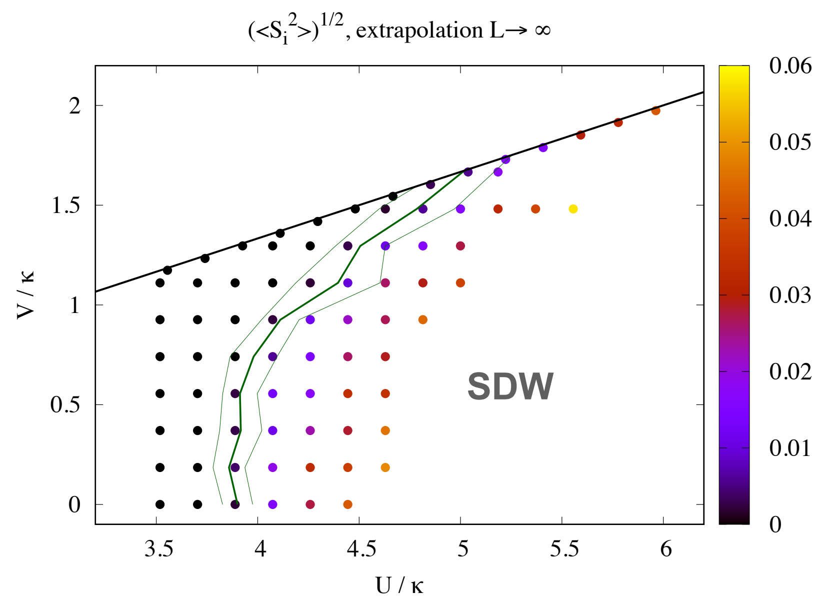

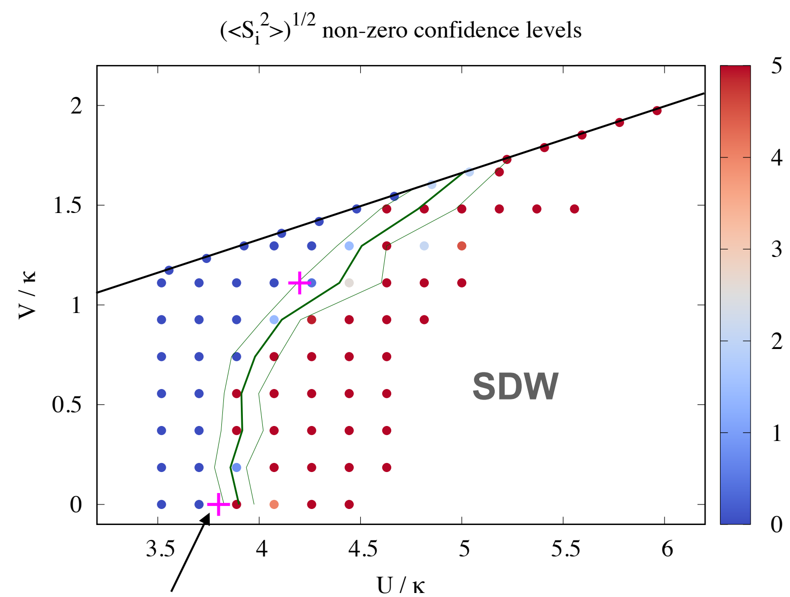

$$V = 0 : \quad U_c \approx 3.8$$

Assaad, Herbut, PRX 3 (2013) 031010

Parisen Toldin, Hohenadler, Assaad, Herbut, PRD 91 (2015) 165108

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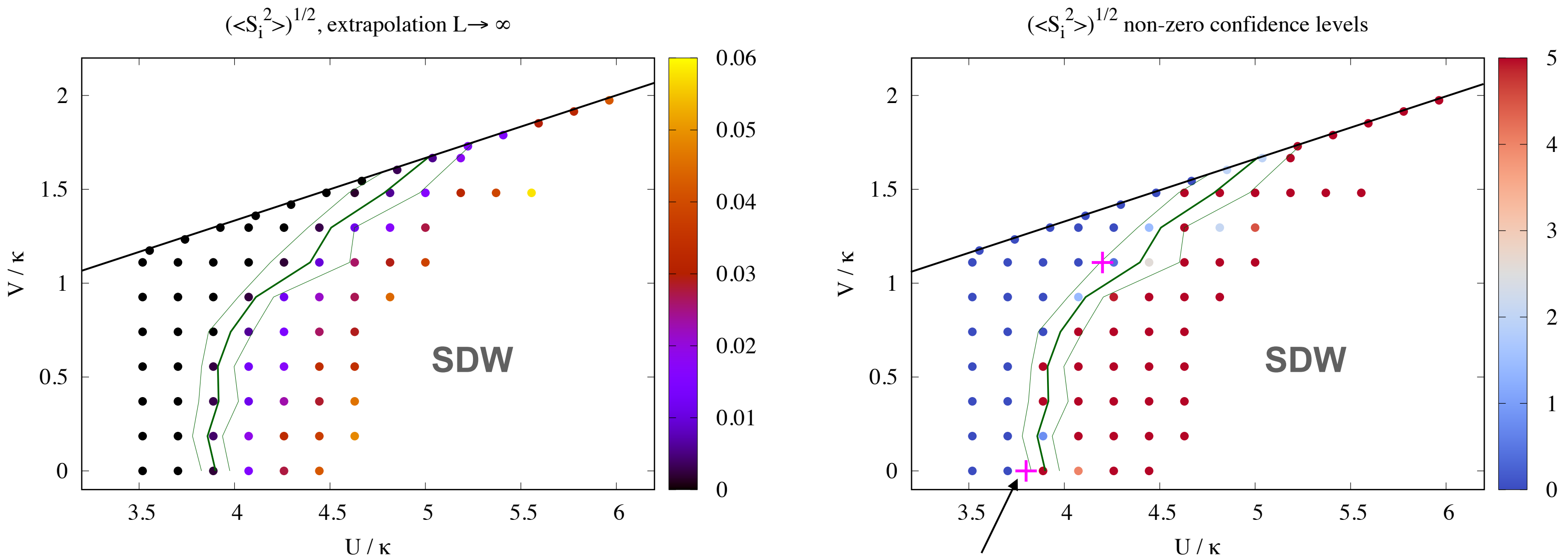

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no trace of multicritical (or triple) point there

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Basics of Formulation

- **particle-hole transformation**

$$c_\uparrow \to a \qquad c_\downarrow \to (-1)^s\, b^\dagger$$

$$c_\uparrow^\dagger \to a^\dagger \qquad c_\downarrow^\dagger \to (-1)^s\, b$$

(nearest-neighbor) tight-binding Hamiltonian unchanged

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- **charge**

$$q = n_\uparrow + n_\downarrow - 1 = n_a - n_b \ = (a^\dagger, b^\dagger)\sigma_3 \begin{pmatrix} a \\ b \end{pmatrix}$$

part of SO(3) vector

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$$q^2 = (c_\uparrow^\dagger c_\uparrow + c_\downarrow^\dagger c_\downarrow - 1)^2 = -\frac{1}{3}(c^\dagger \vec{\sigma} c) \cdot (c^\dagger \vec{\sigma} c)$$

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$$\frac{U}{2} q^2 = \alpha \frac{U}{6}\Big((a^\dagger, b^\dagger)\vec{\sigma} \begin{pmatrix} a \\ b \end{pmatrix} \Big)^2 - (1-\alpha)\frac{U}{2}\big(a^\dagger a + b^\dagger b - 1\big)^2$$

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repulsive model: $U > 0$

linearize with: imaginary Hubbard field ↑ (first term) — real Hubbard field ↑ (second term)

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- **charge**

$$q = n_\uparrow + n_\downarrow - 1 = n_a - n_b \;= (a^\dagger, b^\dagger)\sigma_3 \begin{pmatrix} a \\ b \end{pmatrix}$$

part of SO(3) vector

- **Fierz identity**

$$q^2 = (c_\uparrow^\dagger c_\uparrow + c_\downarrow^\dagger c_\downarrow - 1)^2 = -\frac{1}{3}(c^\dagger \vec{\sigma} c) \cdot (c^\dagger \vec{\sigma} c)$$

- **on-site interaction**

$$\frac{U}{2} q^2 = \alpha \frac{U}{6} \left((a^\dagger, b^\dagger)\vec{\sigma} \begin{pmatrix} a \\ b \end{pmatrix} \right)^2 - (1-\alpha)\frac{U}{2}\left(a^\dagger a + b^\dagger b - 1\right)^2$$

repulsive model:
$U > 0$

linearize with: imaginary Hubbard field ↑ (first term) — real Hubbard field ↑ (second term)

- **need both to avoid ergodicity problems**

Beyl, Goth, Assaad, PRB 97 (2017) 085144
Ulybyshev, Valgushev, 1712.02188

Lagrangian

- continuous (Euclidean) time

$$\psi = \begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix}$$

$$\mathcal{L}_i = \psi_i^\dagger \big(\partial_t + (\rho_i + i\vec{\sigma}\vec{\varphi}_i)\big)\psi_i - \kappa \sum_{j\sim i} \psi_j^\dagger \psi_i$$

tight-binding and Hubbard-field couplings

$$+(-1)^s \big(m_{\rm sdw}\, \psi_i^\dagger \psi_i + m_{\rm cdw}\, \psi_i^\dagger \sigma_3 \psi_i\,\big)$$

mass terms (gaps)

$$-\big(\mu_Q\, \psi_i^\dagger \sigma_3 \psi_i + \big(\mu_S - \frac{U}{2}\big)\, \psi_i^\dagger \psi_i\,\big)$$

chemical potentials (charge Q and spin S)

$$+\,\frac{3}{2\alpha U}\,\vec{\varphi}_i^{\,2} \,+\, \frac{1}{2(1-\alpha)U}\,\rho_i^2$$

Hubbard-fields (on-site repulsion)

Lagrangian

- continuous (Euclidean) time

$$\psi = \begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix}$$

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Hubbard-fields (on-site repulsion)

- identical to attractive Hubbard model with

$$\psi = \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix}$$

and map

$$U \to -U \qquad \alpha \to 1-\alpha$$

$$m_{\mathrm{sdw}} \leftrightarrow m_{\mathrm{cdw}} \qquad \mu_Q \leftrightarrow \mu_S$$

without particle-whole transformation

i.e. SDW $\leftrightarrow$ CDW

Time Discretization

- **symmetric Suzuki-Trotter**

$$e^{-\delta(\mathcal{H}_{\rm tb}+\mathcal{H}_{\rm int})} = e^{-\frac{\delta}{2}\mathcal{H}_{\rm tb}} e^{-\delta\mathcal{H}_{\rm int}} e^{-\frac{\delta}{2}\mathcal{H}_{\rm tb}} + \mathcal{O}(\delta^3)$$

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- **fermionic coherent states**

$$\langle\bar{\xi}|e^{-\delta h_{ij} c_i^\dagger c_j}|\xi\rangle = e^{\bar{\xi}_i (e^{-\delta h})_{ij} \xi_j}$$

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- fermion matrices

$$M(\pm\phi) = \begin{pmatrix} 1 & -e^{-\delta h} & 0 & 0 & 0 & \dots \\ 0 & 1 & -e^{\pm i\phi_1} & 0 & 0 & \dots \\ 0 & 0 & 1 & -e^{-\delta h} & 0 & \dots \\ 0 & 0 & 0 & 1 & -e^{\pm i\phi_2} & \dots \\ \vdots & & & & \ddots & \\ e^{\pm i\phi_{N_\tau}} & 0 & 0 & & \dots & 1 \end{pmatrix}$$

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- **partition function**

$$Z = \int D\phi \, |\det M(\phi)|^2 \, e^{-S_\phi}$$

Particle-Hole and Spin Symmetry

- **linear action**

time discretisation breaks particle-hole hence spin symmetry

$\Sigma : \ (-1)^s$

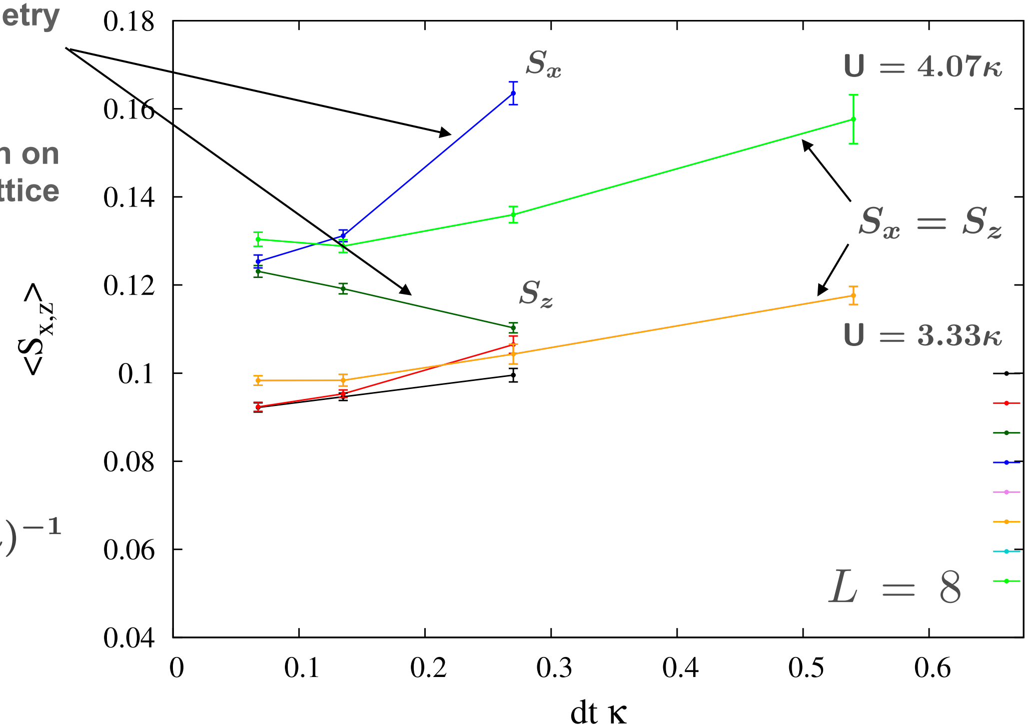
swap sign on one sublattice

$\Sigma h \Sigma = -h$

but

$\Sigma(1-\delta h)\Sigma$

$\neq (1-\delta h)^{-1}$



N_t: 320 160 80 40

- **exponential (chiral) action**

exact sublattice-particle-hole & spin symmetry

$$\Sigma e^{-\delta h}\Sigma = e^{\delta h}$$

$$= e^{-\delta h}$$

from PoS (LATTICE 2016) 244, arXiv:1610.09855

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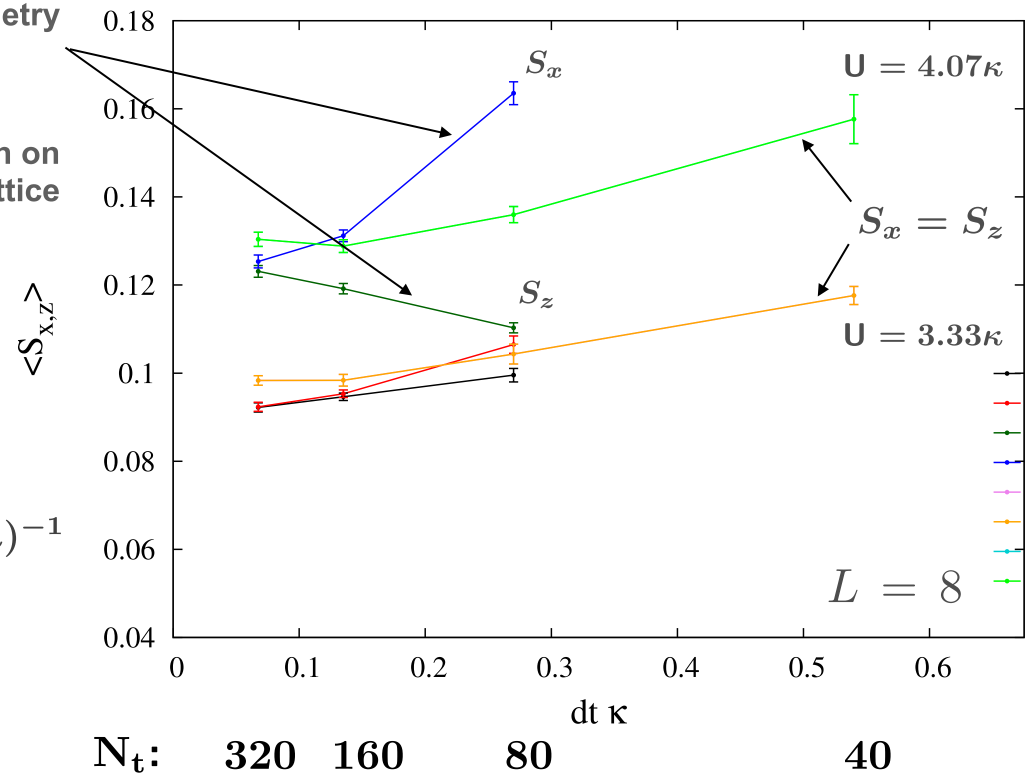

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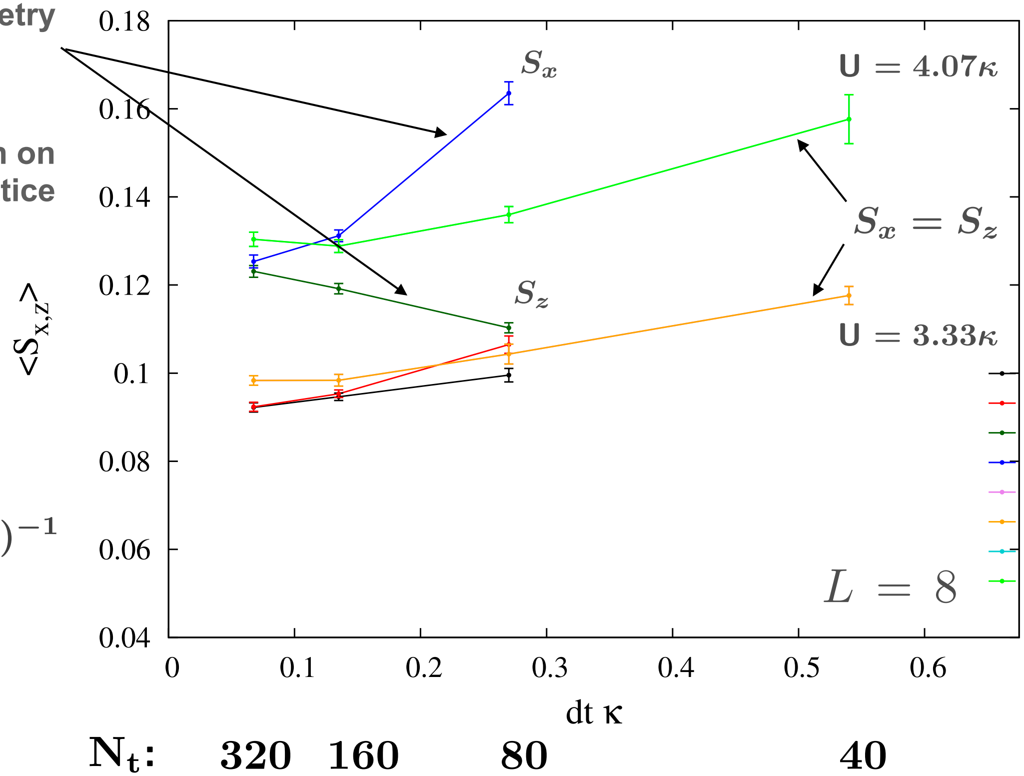

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exact sublattice-particle-hole & spin symmetry

$$\Sigma e^{-\delta h}\Sigma = e^{\delta h}$$

$$= e^{-\delta h}$$

$\mathcal{O}(\delta)$ improved

⇝ no-longer sparse

Schur complement solver

Ulybyshev, Kintscher, Kahl, Buividovich, arXiv:1803.05478

from PoS (LATTICE 2016) 244, arXiv:1610.09855

Spin and Charge per Sublattice

- **for competing order (zero-mass) simulations**

  use

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

  for

- **spin-density wave:**

  with

$$\mathcal{O}_i \;\to\; \vec{S}_i = \frac{1}{2}\,(c^\dagger_{i,\uparrow}, c^\dagger_{i,\downarrow})\,\vec{\sigma}\begin{pmatrix} c_{i,\uparrow} \\ c_{i,\downarrow}\end{pmatrix}$$

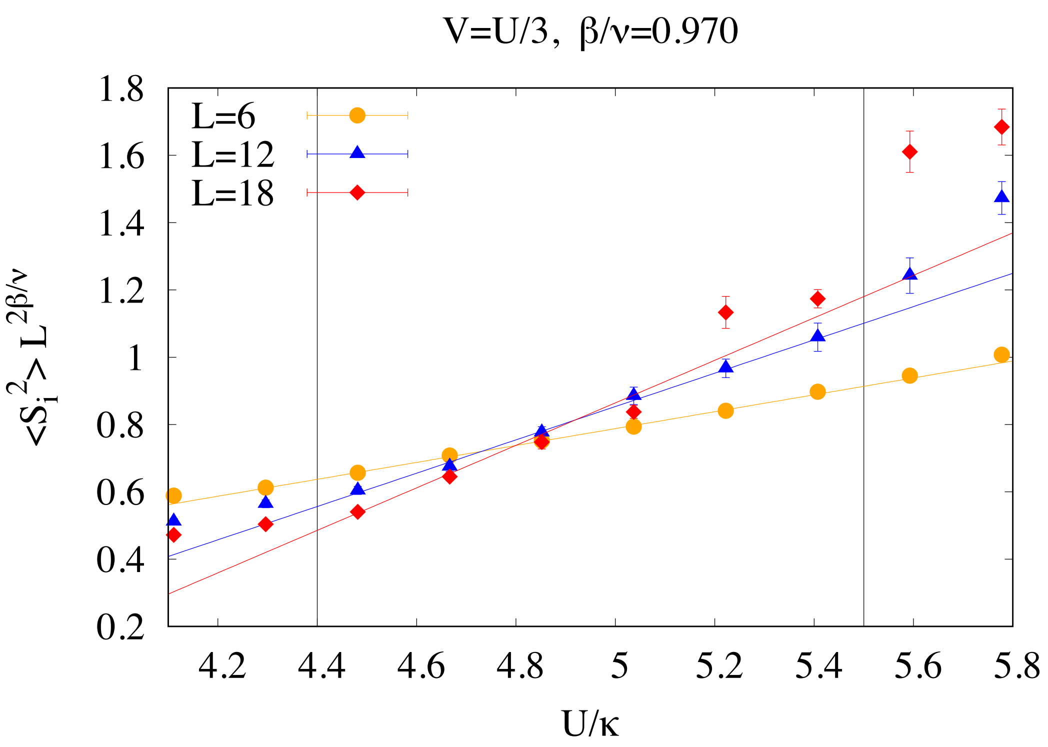
- **charge-density wave:**

  with

$$\mathcal{O}_i \;\to\; q_i = c^\dagger_{i,\uparrow}c_{i,\uparrow} + c^\dagger_{i,\downarrow}c_{i,\downarrow} - 1 = a^\dagger_i a_i - b^\dagger_i b_i$$

Finite-Size Scaling

- **extract critical coupling and exponents**



$$\langle S_i^2 \rangle \big|_{U_c} \propto L^{-2\beta/\nu}$$

Finite-Size Scaling

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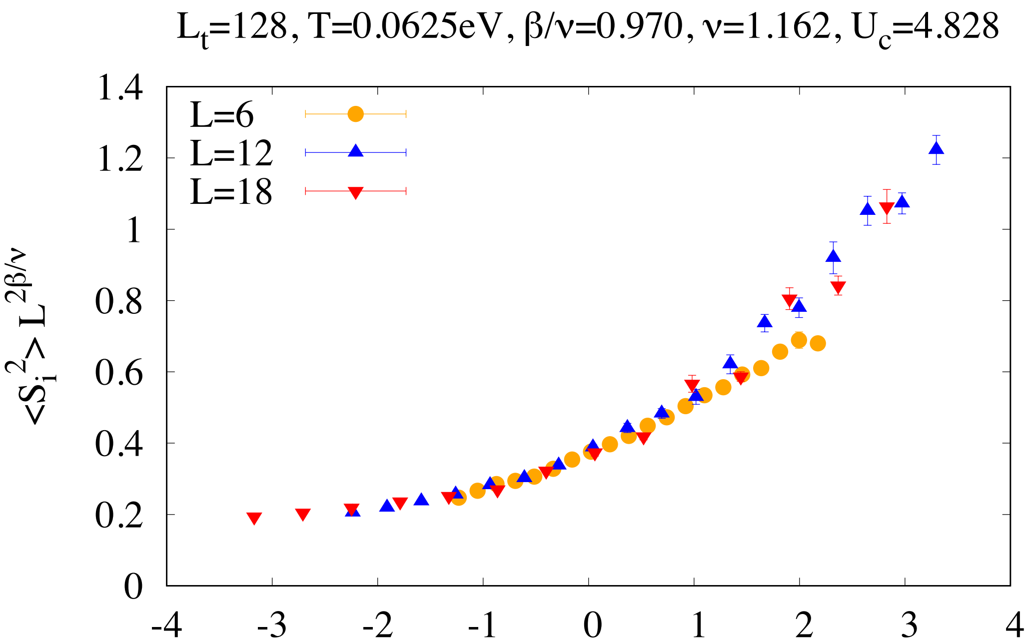


$$x = L^{1/\nu}(U - U_c)/U_c$$

consistent with chiral Heisenberg Gross-Neveu

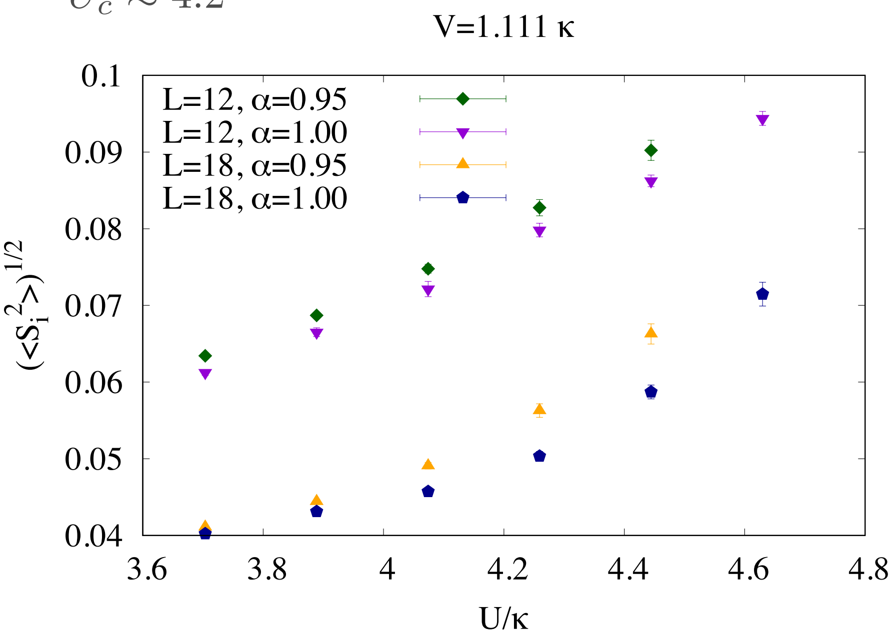
$$\langle S_i^2 \rangle = L^{-2\beta/\nu} f(x)$$

Ergodicity

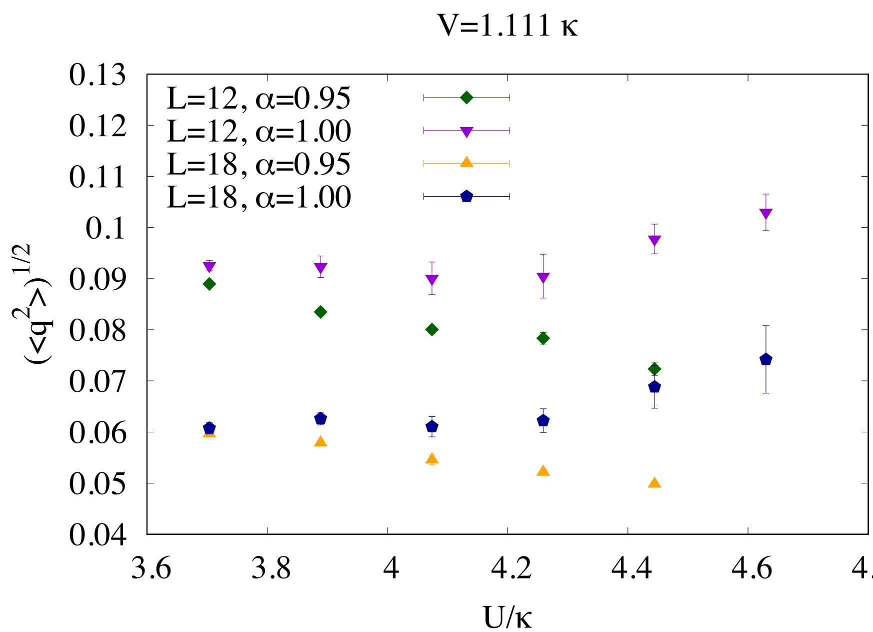
- **two Hubbard fields (real and imaginary)**

$$\frac{U}{2}q^2 = \alpha\frac{U}{6}\Big((a^\dagger,b^\dagger)\vec{\sigma}\begin{pmatrix}a\\ b\end{pmatrix}\Big)^2 - (1-\alpha)\frac{U}{2}\big(a^\dagger a + b^\dagger b - 1\big)^2$$

$U_c \approx 4.2$

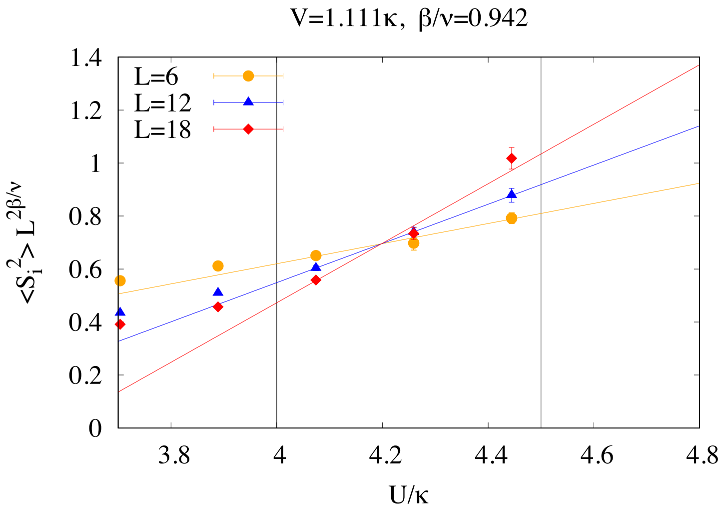


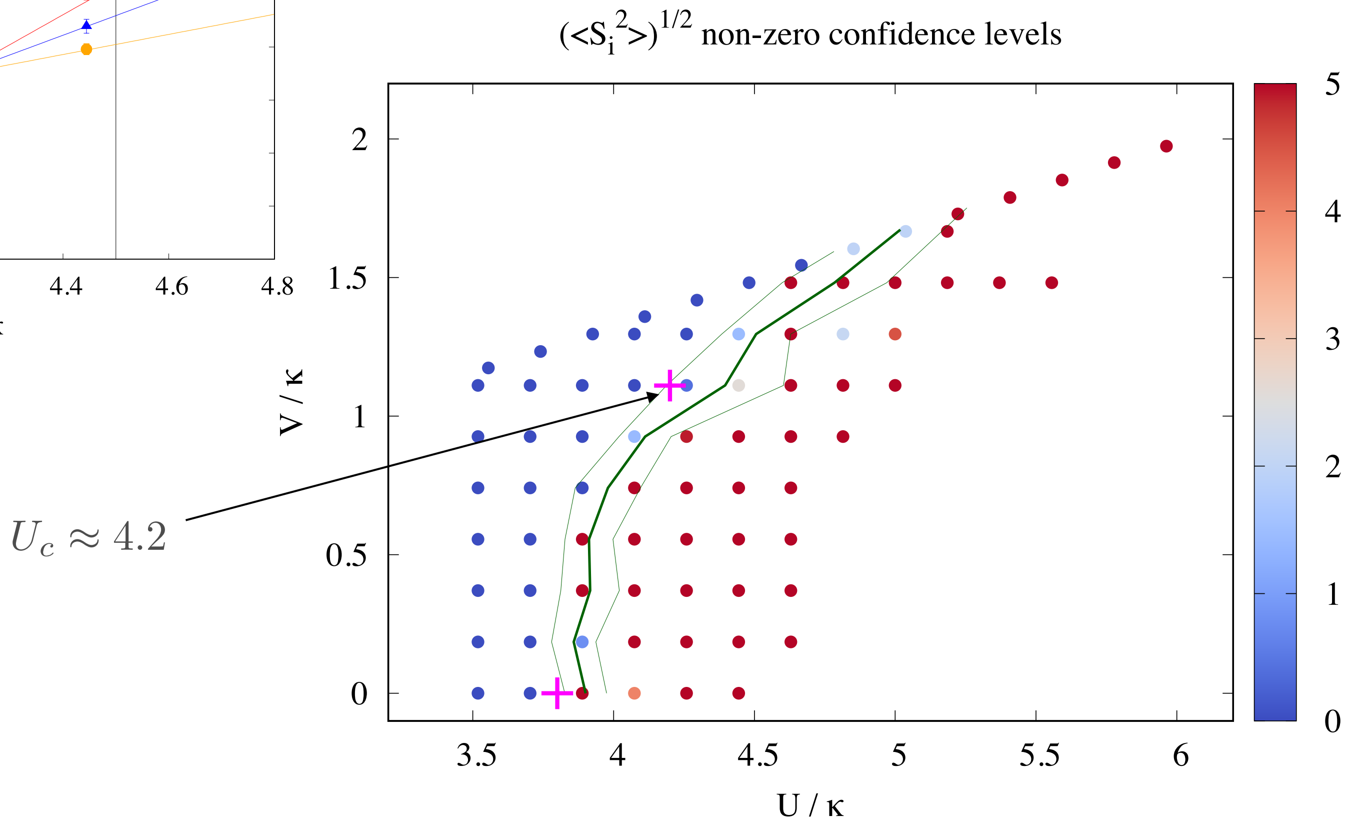
staggered spin



staggered charge

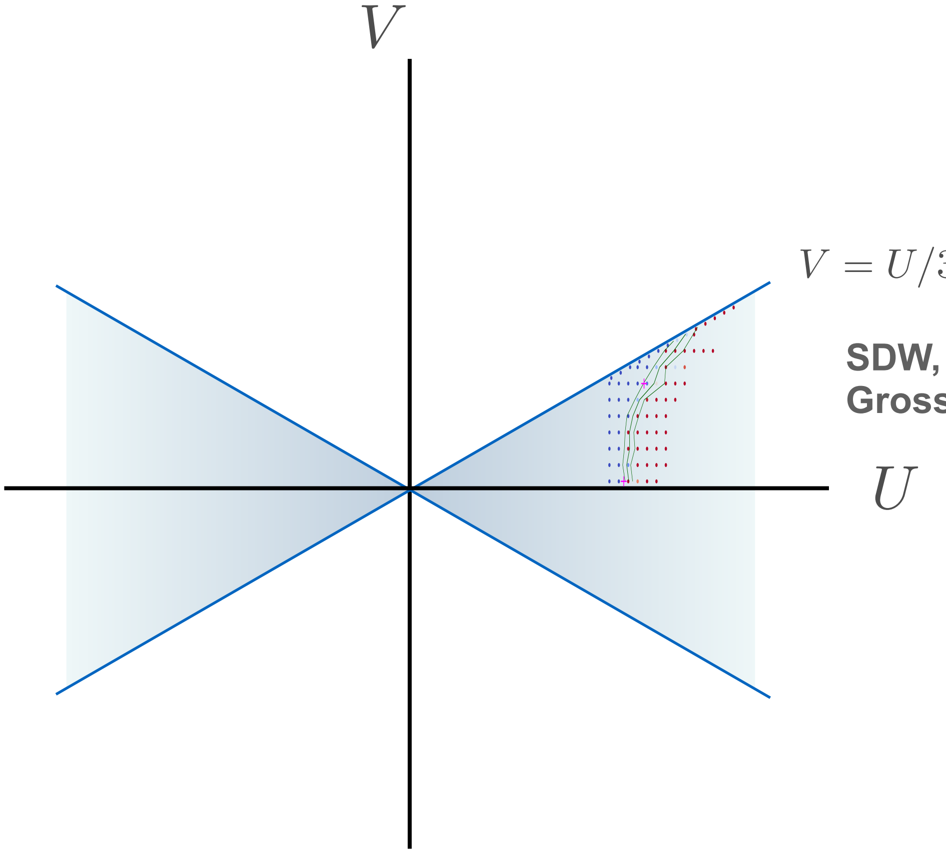
Phase Diagram





Summary and Outlook

- **Extended Hubbard Model on Hexagonal Lattice**



no trace of multicritical (or triple) point

SDW, chiral Heisenberg Gross-Neveu universality

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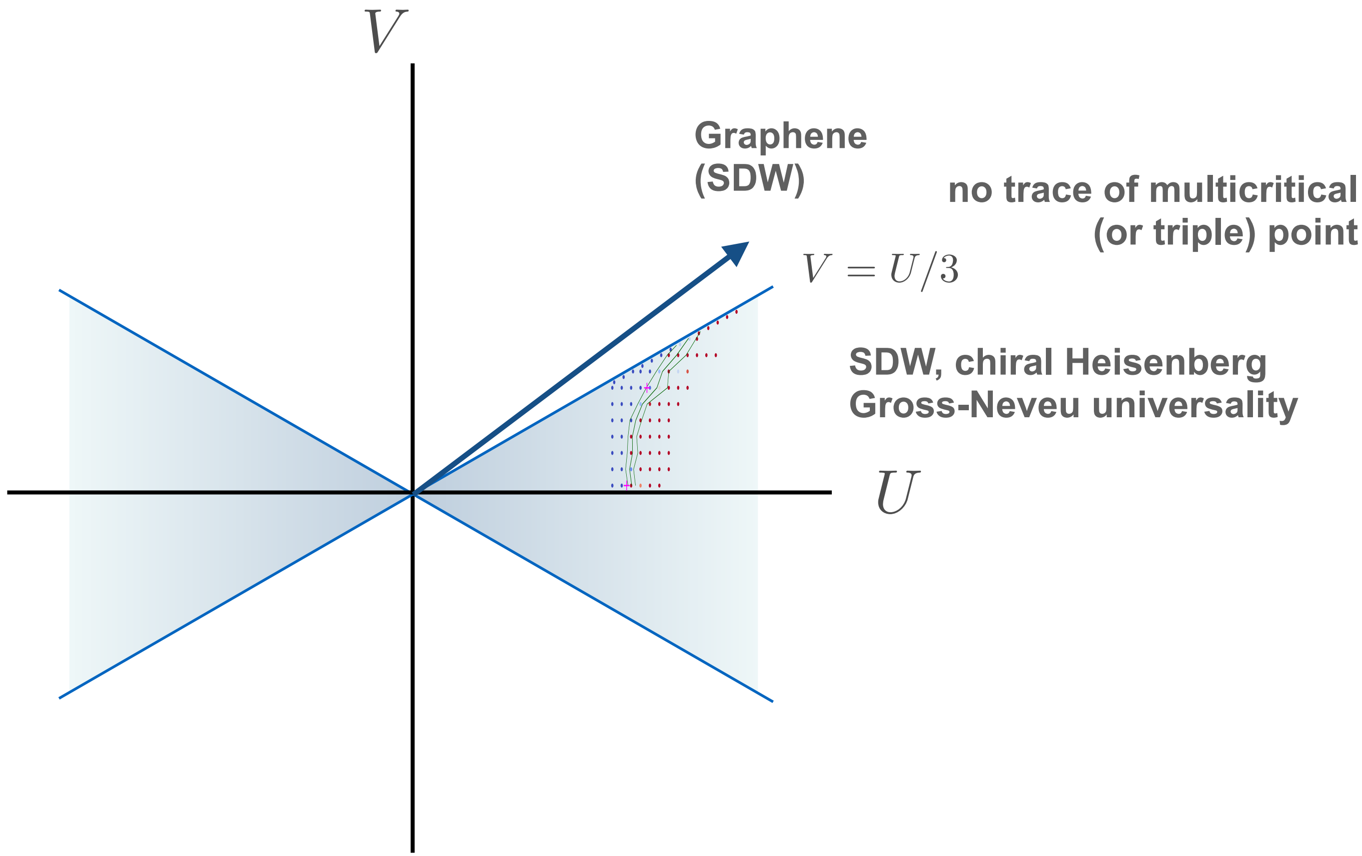

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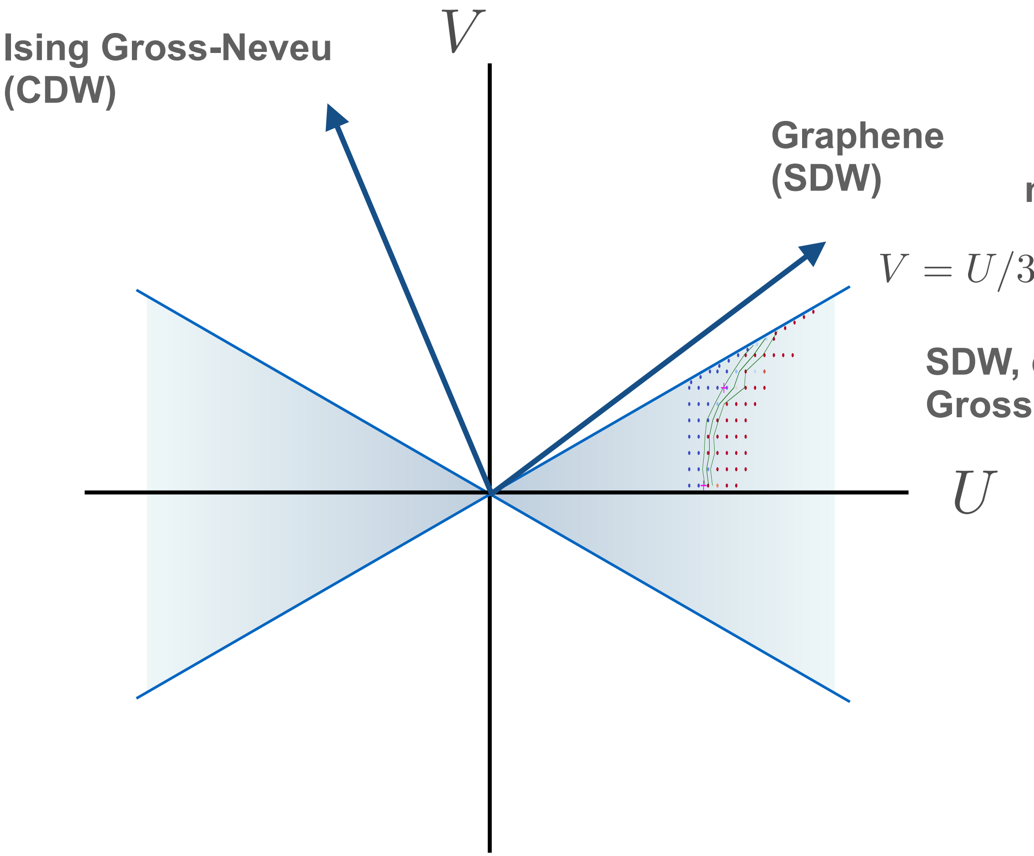

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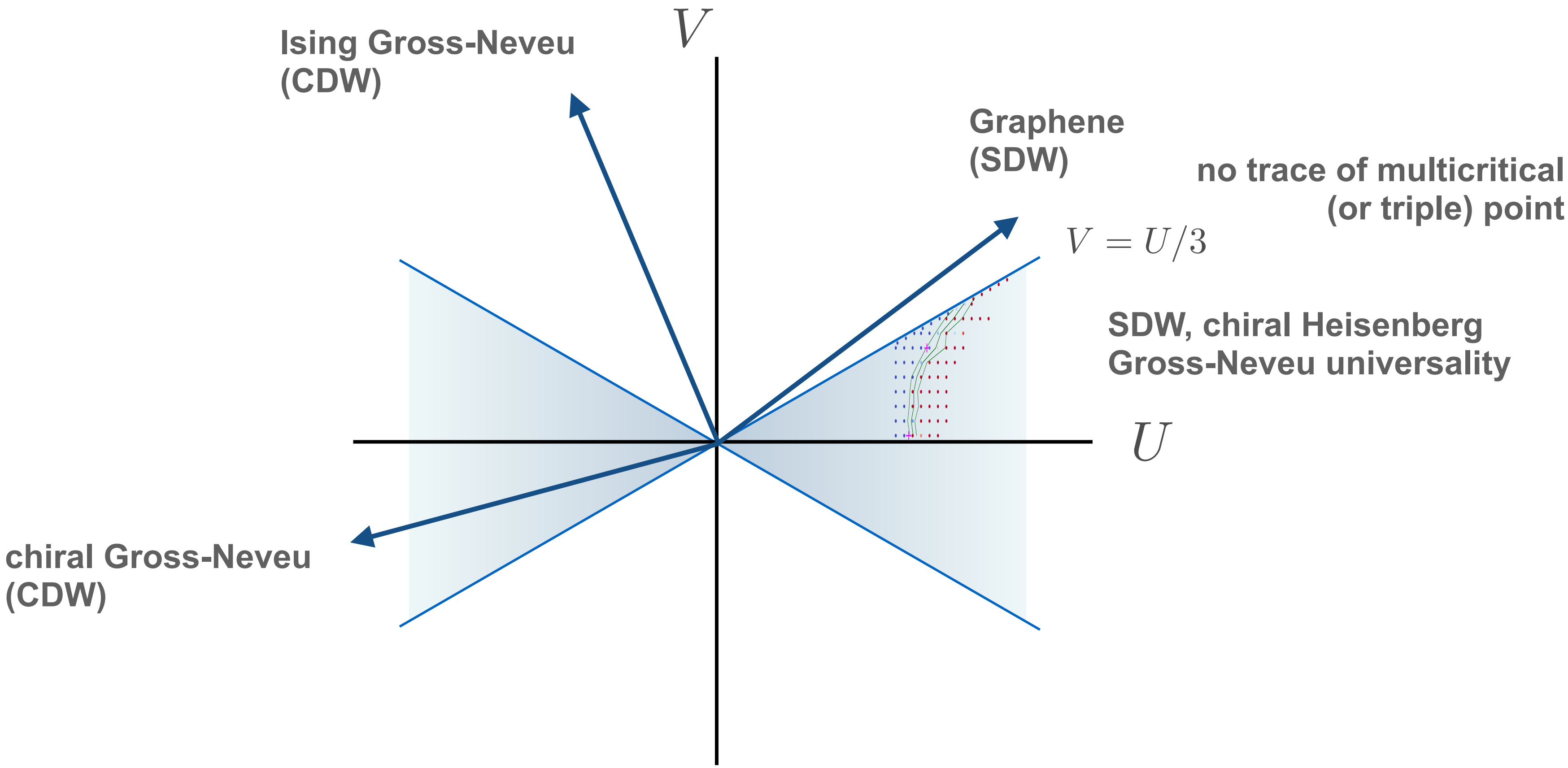
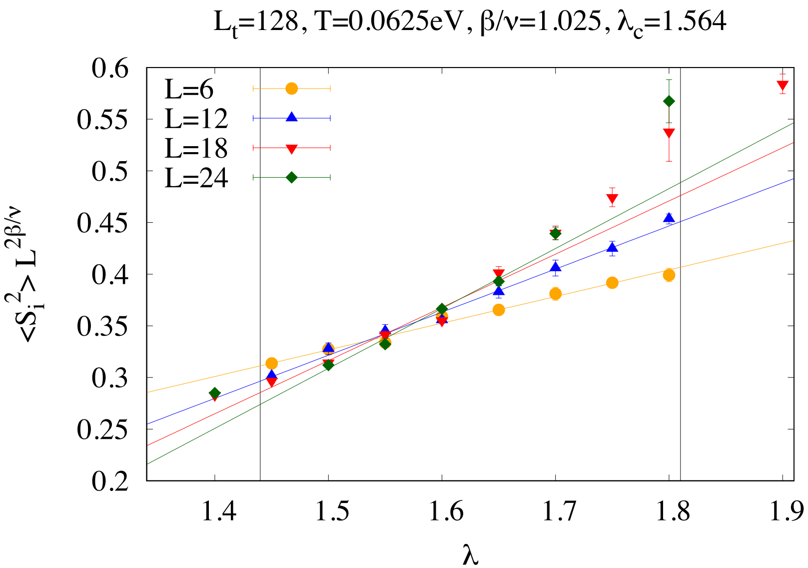
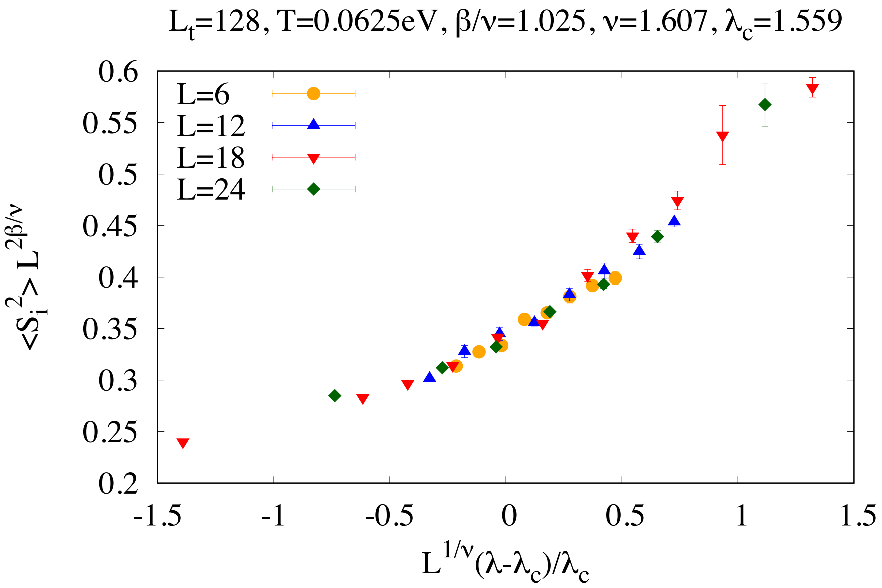


Graphene Update

- partially screened, long-range Coulomb





staggered spin (SDW),
chiral GN or Miranksy?

Summary and Outlook

- **Extended Hubbard Model on Hexagonal Lattice**

  chiral fermion action, complex Hubbard fields, non-iterative Schur complement solver

- **Update on Graphene with realistically screened long-range Coulomb interactions**

  no sign problem, in progress

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  finite charge carrier density away form half filling, with Kurt Langfeld, in progress

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  staggered lattice regularisation without doubling, study inhomogeneous phases

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Thank you for your attention!