Monte Carlo Study of Competing Orders in a Nearly Antiferromagnetic Metal

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Overview

Motivation

A generic model
- Itinerant electrons
- Antiferromagnetic mean field
- Spin-fermion model
- Setting the stage for Monte Carlo

Numerical method
- Determinantal quantum Monte Carlo
- Stumbling blocks

Physical results
- Phase diagram
- Competing orders

Conclusions
Condensed matter physics

Collective phenomena

interacting quantum many-particle systems

⇒

novel, distinctly quantum phases of matter

magnetic ordering

superconductivity

Bose-Einstein condensation

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Competing orders in a nearly antiferromagnetic metal
Superconductivity

**Conventional superconductors**
- $T_c \leq 39 \text{ K}$
- e.g.: mercury, aluminum, …

Well understood by **BCS theory**
- electrons condense into **Cooper pairs**
- attractive interaction: quanta of **lattice vibrations**

**High-temperature superconductors**
- $T_c \leq 138 \text{ K}$
- e.g.: cuprates, iron pnictides, …

**BCS theory fails**
- **unknown** mechanism of pairing
  - what is the **attractive interaction**?
Experimental phase diagrams

Strongly correlated metals show a plethora of phases with competing orders at low temperatures. Often in proximity:

- antiferromagnetic (AFM) order
- unconventional superconductivity (SC) unusual symmetry

Cuprates

Fe-based superconductors

Heavy-fermion compounds

D. J. Scalapino, Rev. Mod. Phys. 84, 1383 (2012).

- universal mechanism?
Candidate for universal physics

Proposition: AFM fluctuations near quantum critical point (QCP) can mediate unconventional superconductivity

- **AFM exchange** may lead to formation of Cooper pairs
- enhancement of superconductivity close to quantum phase transition (QPT)
  - $T = 0$ transition driven by quantum fluctuations
  - continuous: quantum critical point (QCP)
- good understanding for insulators, **many open questions** for metals
- Layered compounds: effectively 2D

S. Sachdev, Quantum Phase Transitions, 2nd ed. (2011).

**Challenge:** Improve lacking understanding of universal physics in a metal close to an AFM quantum phase transition
Setup of a generic model
Starting point: Hubbard model

- one-band of $S = 1/2$ itinerant fermions, hopping on square lattice
- repulsive onsite Hubbard interaction $U > 0$

$$H = - \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} \quad \text{or} \quad$$

$$H = \sum_{k,\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \frac{U}{N_s} \sum_{k,k',q} c_{k,\uparrow}^\dagger c_{k',\downarrow}^\dagger c_{k'-q,\downarrow} c_{k+q,\uparrow}$$

- typical Fermi surface given by $\varepsilon_k$ for electron-doped cuprates:
Antiferromagnetic mean field

\[ H = - \sum t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} \]

- **rewrite** interaction using

\[ S_{i\alpha} = \frac{\hbar}{2} \sum_{\sigma,\tau} c_{i\sigma}^\dagger [\sigma^\alpha]_{\sigma\tau} c_{i\tau} \quad (\alpha = x, y, z) \]

\[ H = - \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - \frac{2U}{3\hbar^2} \sum_{i} \vec{S}_i^2 + \frac{1}{2} UN_e \]

- **mean field:**

\[ \vec{S}_i^2 = (\vec{S}_i - \langle \vec{S}_i \rangle)^2 + 2 \vec{S}_i \cdot \langle \vec{S}_i \rangle - \langle \vec{S}_i \rangle^2 \approx 2 \vec{S}_i \cdot \langle \vec{S}_i \rangle - \langle \vec{S}_i \rangle^2 \]

- solution with perfect **antiferromagnetic order:**

\[ \langle \vec{S}_i \rangle = \varphi_0 \cdot \cos(\mathbf{Q} \cdot \mathbf{i}), \quad \mathbf{Q} = \begin{bmatrix} \pi \\ \pi \end{bmatrix} \]
• put together for mean field Hamiltonian:

\[ H_{MF} = -\sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} - \frac{4U}{3\hbar} \sum_i \vec{\varphi}_0 \cdot \vec{S}_i \cos(Q \cdot i) + \text{const} \]

• retranslate \( \vec{S}_i \rightarrow c^\dagger_{i,\sigma} \) and go to Fourier representation:

\[ H_{MF} = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} - \frac{2U}{3} \sum_{k,\sigma,\tau} \left[ c^\dagger_{k,\sigma} c_{k+Q,\tau} \right] \left[ \vec{\varphi}_0 \cdot \vec{\sigma} \right]_{\sigma\tau}, \quad Q = \begin{bmatrix} \pi \\ \pi \end{bmatrix} \]

Key insight: only electrons with momenta separated by \( Q \) scatter!

• low-energy physics: states near Fermi surface most important
• discrete set of “hot spots” on the original Fermi surface
\( \varepsilon_k = \varepsilon_{k+Q} = \varepsilon_F \)
Going beyond mean field
Full fluctuations: Spin-fermion model

more general: Allow spin density wave (SDW) order fluctuations around $\bar{\varphi}_0$

- take full Hamiltonian, decouple interaction (Hubbard-Stratonovich field $\bar{\varphi}$)

$$Z = \text{Tr} e^{-\beta H} \sim \int D(\{\bar{\varphi}_q\}) e^{-S_{\varphi}} \text{Tr} e^{-\beta H(\bar{\varphi}_q)}$$

$$H(\bar{\varphi}_q) = \sum_k \varepsilon_k c_k^\dagger c_k + \lambda \sum_{k,q} c_{k+Q+q}^\dagger (\vec{\sigma} \cdot \bar{\varphi}_q) c_k^\dagger$$

- important fluctuations of $\bar{\varphi}_q$ at small $q \ll \pi$
- high-energy electrons integrated out: bare $\varphi^4$-theory for SDW order

$$S_{\varphi} = \int d\tau \int d^2x \left( \frac{1}{2c^2} (\partial_\tau \varphi)^2 + \frac{1}{2} (\nabla \varphi)^2 + \frac{r}{2} \varphi^2 + \frac{u}{4} (\varphi^2)^2 \right)$$

Analytical theory: hard

- flow to strong coupling, no controlled solutions available
- conflicting predictions

Enabling quantum Monte Carlo

Unbiased, numerically exact method: Quantum Monte Carlo (QMC)

- tendency towards **SDW order** at \( Q = (\pi, \pi) \)
- structure of **hot spots** and Fermi surface curvature in vicinity important for universal physics
  - generically: fermion **sign-problem**
  - simulations prohibitively expensive

- small modification: **two fermion flavors** \( \psi_x, \psi_y \)
- split Fermi surfaces, **sustained hot spot structure**
  - allows extra antiunitary symmetry
    \[ \mathcal{U} = i \sigma_3^{\text{band}} \sigma_2^{\text{spin}} C \]
    \( \Rightarrow \) **sign-problem-free** determinantal QMC

Want to learn more about this? Slides in the back
Model probed by QMC

Lattice field theory \( S = \int_0^\beta d\tau (L_F + L_\varphi) \) with

- **two-flavor fermionic** action

\[
L_F = \sum_{i,j,s} \psi_{\alpha is}^\dagger \left[(\partial_\tau - \mu)\delta_{ij} - t_{\alpha ij}\right] \psi_{\alpha js} \\
+ \lambda \sum_{i,s,s'} e^{i \mathbf{Q} \cdot \mathbf{r}_i} [\mathbf{g} \cdot \mathbf{\varphi}_i]_{ss'} \psi_{xis}^\dagger \psi_{yis'} + \text{h.c.}
\]

- **bosonic** action for \( \text{O}(2) \) order parameter \( \mathbf{\varphi} \):

\[
L_\varphi = \frac{1}{2} \sum_i \frac{1}{c^2} \left( \frac{d\mathbf{\varphi}_i}{d\tau} \right)^2 + \frac{1}{2} \sum_{\langle i,j \rangle} (\mathbf{\varphi}_i - \mathbf{\varphi}_j)^2 \\
+ \sum_i \left[ \frac{r}{2} \varphi_i^2 + \frac{u}{4}(\varphi_i^2)^2 \right]
\]

- **\( \text{O}(2) \) symmetry**: allows us to track **finite-temperature** phase transitions

Mermin-Wagner theorem: no continuous symmetry broken at \( T > 0 \) in 2D
Determinantal quantum Monte Carlo
**Quantum Monte Carlo (QMC)**

**Goal:** From the action \( S = \int_0^\beta d\tau [L_F + L_\phi] = S_F + S_\phi \) compute expectation values of a physical quantity \( A \) at some finite inverse temperature \( \beta = 1/T \)

\[
\langle A \rangle = \frac{1}{Z} \int D(\vec{\phi},\psi) A e^{-S_F - S_\phi}, \quad Z = \int D(\vec{\phi},\psi) e^{-S_F - S_\phi}
\]

**General** idea of all quantum Monte Carlo approaches:

- map partition function to average over **configurations** \( \{ \vec{\phi} \}_n \) with **statistical weights** \( p_n > 0 \)
- generate **Markov chain** of samples and measure weighted averages of observables
- different procedures for the mapping
Determinantal quantum Monte Carlo (DQMC)

Standard algorithm in condensed matter physics for strongly correlated fermions coupled to bosonic degrees of freedom

Recipe:
• Keep the bosonic field integral and write the fermionic integral as a trace in Fock space

\[
Z = \int D(\vec{\phi}, \psi) e^{-S_\phi - S_F} = \int D(\vec{\phi}) e^{-S_\phi} \text{Tr}_\psi \left[ e^{-\int_0^\beta d\tau H_F(\vec{\phi}(\tau))} \right]
\]

• At each \( \tau \), \( H_F \) is evaluated for a different field configuration \( \{\vec{\phi}(\tau)\} \)
• Discretize imaginary time into time slices $\ell = 1, \ldots, m$, $\beta = m \Delta \tau$:

\[
S_\varphi = \int_0^\beta d\tau L_\varphi(\tau) \approx \Delta \tau \sum_{\ell=1}^m L_\varphi(\ell \Delta \tau)
\]

\[
\text{Tr}_\psi \left[ e^{-\int_0^\beta d\tau H_F(\bar{\varphi}(\tau))} \right] \approx \text{Tr}_\psi \left[ e^{-\Delta \tau \sum_{\ell=1}^m H_F(\bar{\varphi}(\ell \Delta \tau))} \right]
\]

• Split up Hamiltonian $H_F = H_K + H_V(\bar{\varphi})$, $[H_K, H_V(\bar{\varphi})] \neq 0$:

\[
H_K = - \sum_{i,j,\sigma} \sum_{\alpha=x,y} \psi_\alpha,\bar{i},\sigma \left[ \mu \delta_{ij} + t_{\alpha,ij} \right] \psi_{\alpha,j,\sigma}
\]

kinetic energy

\[
H_V(\bar{\varphi}) = \lambda \sum_{i,\sigma,\tau} [\bar{\sigma} \cdot \bar{\varphi}_i]_{\sigma,\tau} \psi_\alpha,\bar{i},\sigma \psi_{\alpha,\tau,\sigma} + \text{h.c.}
\]

field-coupled interaction

• Apply a symmetric Trotter decomposition

\[
e^{-\Delta \tau \sum_{\ell=1}^m H_F(\ell)} = e^{-\Delta \tau \sum_{\ell=1}^m (H_K + H_V(\ell))}
\]

\[
\approx \prod_{\ell=1}^m e^{-\Delta \tau H_K/2} e^{-\Delta \tau H_V(\ell)} e^{-\Delta \tau H_K/2}
\]
• Put together: **partition function** with **systematic error**

\[
Z = \int D(\vec{\phi}) e^{-\Delta \tau \sum_{\ell=1}^{m} L_{\phi}(\ell)} \text{Tr}_\psi \left[ \prod_{\ell=1}^{m} U_{\phi}(\ell) \right] + O(\Delta \tau^2),
\]

\[
U_{\phi}(\ell) = e^{-\Delta \tau V(\ell)} e^{-\Delta \tau \frac{K}{2}} e^{-\Delta \tau H_V(\ell)} e^{-\Delta \tau \frac{H_K}{2}}
\]

• Integrating out the fermions, we can express the Fock trace as a regular **matrix determinant**

\[
\text{Tr}_\psi \left[ \prod_{\ell=1}^{m} U_{\phi}(\ell) \right] = \det \left[ 1 + \prod_{\ell=1}^{m} B_{\phi}(\ell) \right],
\]

with \( B_{\phi}(\ell) = e^{-\Delta \tau K/2} e^{-\Delta \tau V(\ell)} e^{-\Delta \tau K/2} \)

• \( K \) and \( V(\ell) \) are **complex** \( 4N \times 4N \)-**matrices**, indexed by **flavor** \( \alpha = x, y \), **spin** \( \sigma = \uparrow, \downarrow \) and **site** \( i = 1, \ldots, N \)

Their entries are just the **matrix elements** of \( H_K \) and \( H_V \)
Our formulation of the partition function contains statistic weights we can directly compute:

\[
Z = \int D(\vec{\phi}) e^{-S_{\phi}} \cdot \det [1 + \prod_{\ell=1}^{m} B_{\phi}(\ell)]
\]

We have all the basic ingredients to setup a Monte Carlo simulation:

- Start with a random configuration of fields $\vec{\phi}_i(\ell)$ for each site $i$ and time slice $\ell$
- Repeat the following Monte Carlo sweep many times:
  - For each time slice $\ell$ and site $i$ propose a new field vector $\vec{\phi}_i(\ell)^{\text{new}}$
  - Accept the new field vector with Metropolis transition probability

\[
p = \min \left\{ 1, e^{-(S_{\phi}^{\text{new}} - S_{\phi}^{\text{old}})} \times \frac{\det [1 + \prod_{\ell=1}^{m} B_{\phi}^{\text{new}}(\ell)]}{\det [1 + \prod_{\ell=1}^{m} B_{\phi}^{\text{old}}(\ell)]} \right\}
\]
To measure **fermionic observables** we use the equal-time **Green’s function** for a configuration of fields $\vec{\varphi}$ time slice $\ell$

$$\langle \psi_a \psi_b^\dagger \rangle_{\varphi} = [\mathbb{1} + B_{\varphi}(\ell) \cdot \ldots \cdot B_{\varphi}(1) \cdot B_{\varphi}(m) \cdot \ldots \cdot B_{\varphi}(\ell + 1)]_{a,b}^{-1}$$

- A **Wick’s theorem** holds, providing arbitrary correlation functions
- Imaginary time-displaced correlation functions: application of matrices $B_{\varphi}, B_{\varphi}^{-1}$
- Average over all sites and time slices, for many field configurations
Four stumbling blocks
1: Numerical stability

Core of the algorithm: Computation of long chains of matrix products, their
determinants and inverses

\[ 1/T = m \Delta \tau \]

\[ G_\varphi = [1 + B_1 B_2 \ldots B_m]^{-1}, \quad B_\ell = e^{-\Delta \tau K/2} e^{-\Delta \tau V_\ell} e^{-\Delta \tau K/2} \]

Problem: ill-conditioned matrices

- Numerical multiplication \( B_1 \cdot B_2 \) mixes very small and very large eigenvalues
- Scales are “washed out” \( \Rightarrow \text{unstable} \) at low temperatures (long chains)

Solution:

- Separate scales by singular value decomposition (SVD)

\[ B_1 = U_1 S_1 V_1^\dagger = \begin{pmatrix} x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{pmatrix} \cdot \begin{pmatrix} x \\ x \\ x \\ x \end{pmatrix} \cdot \begin{pmatrix} x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{pmatrix} \]

\[ \text{unitary} \quad \text{diagonal} \quad \text{unitary} \]
• To compute $B_1 \cdot B_2 = U_1 S_1 V_1^\dagger \cdot U_2 S_2 V_2^\dagger$, first take
\[
\left(U_1 S_1 V_1^\dagger U_2\right) \cdot S_2
\]
\[
S_2 = \begin{pmatrix}
\times & \times \\
\times & x & x
\end{pmatrix}
\]

• **OK:** entries of $S_2$ rescale distinct rows, scales of $S_2$ are never mixed
• **Safe** to compute SVD:
\[
(U_1 S_1 V_1^\dagger U_2) \cdot S_2 \overset{\text{SVD}}{=} U_x S_x V_x^\dagger
\]

• Finally
\[
B_1 \cdot B_2 = (U_x S_x)(V_x^\dagger V_2^\dagger)
\]

With this procedure:
Algorithm stable at **low temperatures** and **strong interactions**
2: Finite-size effects

- Main limitation: moderate system sizes
- **Metallic systems**: Non-localized wave function, sensitive to boundary conditions
  \[ \Rightarrow \] Particularly **severe finite-size effects**

**Effective remedy**

Weak magnetic field, vanishing for \( L \to \infty \)

\[
t_{\alpha sij} \psi_{xis} \psi_{xjs} \xrightarrow{=} e^{iA_{ij}} t_{\alpha sij} \psi_{\alpha is} \psi_{\alpha js}
\]

- lifts energy degeneracy (\( \Rightarrow \) Landau levels), single particle states forced to cover energy bandwidth

3: Efficient sampling

QMC is numerically exact, provided simulations **equilibrate** and **statistical autocorrelations are under control** (fight critical slowing down)

Accurate Monte Carlo sampling:

- **local** $\vec{\varphi}_i(\tau)$ moves
- additional **global** moves: overall shift + Wolff single cluster update
- extended ensemble with **replica exchange** ("parallel tempering")
  - parallel simulations at various $r$ (degrees of order)
  - configurations: random walk in $r$-space

![Graph showing magnetization $m_\varphi$ vs control parameter $r$](image)
4: Computational cost of linear algebra

• exploit sparseness and low rank of matrices where possible
• still, computational effort scales like the cubed system size: \( \sim O(\beta N^3) \)

• in our case: magnetic order parameter choice of \( O(3) \) vs. \( O(2) \) saves factor of \( 2^3 = 16 \)

O(3) model: 4N×4N matrices

\[
K = \begin{bmatrix} K_x & & & \\ & K_x & & \\ & & K_y & \\ & & & K_y \end{bmatrix}
\quad \text{V}(\varphi) = \begin{bmatrix} A & B \\ B^* & -A \end{bmatrix}
\]

O(2) model: 2N×2N matrices

additional unitary symmetry

\[
K = \begin{bmatrix} K_x \\ & K_y \end{bmatrix}
\quad \text{V}(\varphi) = \begin{bmatrix} A \\ B^* \end{bmatrix}
\quad \text{A} = 0
\]
Stumbling blocks

Technical troublemakers:

- **Numerical stability at low** $T$
  - ✓ matrix factorization

- **Slow equilibration**
  - ✓ global updates, replica exchange

- **Finite-size effects**
  - ✓ artificial magnetic flux

- **Computational cost**
  - ✗ $O(\beta N^3)$ scaling

We would like to access larger systems: Can **Hybrid Monte Carlo** methods help?
Physical results
Reminder: Experimental phase diagrams

Strongly correlated metals

Cuprates

Fe-based superconductors

Heavy-fermion compounds
Reminder: Physical model

Lattice field theory $S = \int_0^\beta d\tau (L_F + L_\varphi)$ with

- **two-flavor fermionic** action

\[
L_F = \sum_{i,j,s,\alpha=x,y} \psi^{\dagger}_{\alpha is} \left[ (\partial_\tau - \mu)\delta_{ij} - t_{\alpha ij} \right] \psi_{\alpha js} \\
+ \lambda \sum_{i,s,s'} e^{iQ \cdot r_i} [\bar{s} \cdot \varphi_i]_{ss'} \psi^{\dagger}_{xis} \psi_{yis'} + \text{h.c.}
\]

- **bosonic** action for $O(2)$ order parameter $\varphi$:

\[
L_\varphi = \frac{1}{2} \sum_i \frac{1}{c^2} \left( \frac{d\varphi_i}{d\tau} \right)^2 + \frac{1}{2} \sum_{\langle i,j \rangle} (\varphi_i - \varphi_j)^2 \\
+ \sum_i \left[ \frac{r}{2} \varphi_i^2 + \frac{u}{4} (\varphi_i^2)^2 \right]
\]
Numerically obtained phase diagram

-SDW
- superconducting fluctuations
- paramagnetic orbital magnetism
- diamagnetism
- gap above $T_c$

energy scale $E_F \approx 2.5$

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Competing orders in a nearly antiferromagnetic metal
Competing orders
Spin density wave order

2D system, continuous $O(2)$ symmetry

$\Rightarrow$ expect Berezinsky-Kosterlitz-Thouless (BKT) transition at $T > 0$

• critical low-temperature phase:

$$\langle \vec{m}_i \cdot \vec{m}_{i+x} \rangle \sim \begin{cases} e^{-|x|/\xi}, & T > T_{SDW}, \\ |x|^{-\eta(T)}, & T \leq T_{SDW} \end{cases}$$

• universal exponent $\eta = 1/4$ for $T = T_{SDW}$

• Finite-size scaling of SDW susceptibility to locate $r(T = T_{SDW})$

$$\chi = \int_0^\beta d\tau \sum_i \langle \phi_i(\tau) \phi_0(0) \rangle \sim L^{2-\eta(T)} \text{ for } T \leq T_{SDW}$$

High temperatures

• Consistent scaling

Below superconducting dome

• $T < T_c$: Scaling breaks down

• weakly first-order?
Superconducting transition

Linear response theory:

- current-current correlator:
  \[ \Lambda_{xx}(q) = \sum_i \int_0^\beta d\tau e^{-i q \cdot r_i} \langle j_x(r_i, \tau) j_x(0, 0) \rangle \]

- longitudinal response: \[ \Lambda^\parallel = \lim_{q_x \to 0} \Lambda_{xx}(q_x, q_y = 0) \]
  transversal response: \[ \Lambda^\perp = \lim_{q_y \to 0} \Lambda_{xx}(q_x = 0, q_y) \]

- superfluid density: \[ \rho_s = \frac{1}{4} [\Lambda^\parallel - \Lambda^\perp] \]

BKT transition at \( T_c \):

- \( \rho_s \) jumps by **universal amount** \( \Delta \rho_s = \frac{2 T_c}{\pi} \)
- \( \rho_s > \Delta \rho \): superconducting phase
**d-wave superconductivity**

**Pairing susceptibilities**

\[ \Delta_{\pm}(r_i) = 2 \left( \psi_{xi}^{\uparrow} \psi_{xi}^{\downarrow} \pm \psi_{yi}^{\uparrow} \psi_{yi}^{\downarrow} \right) \]

- **d-wave:**
  \[ P_- = \int d\tau \sum_i \langle \Delta_+^\dagger(\mathbf{r}_i, \tau) \Delta_- (\mathbf{0}, 0) \rangle \]

- **s-wave:**
  \[ P_+ = \int d\tau \sum_i \langle \Delta_-^\dagger(\mathbf{r}_i, \tau) \Delta_+ (\mathbf{0}, 0) \rangle \]

Finite-size scaling

\( P_- \) diverges with system size \( \Rightarrow \) superconducting phase has **d-wave symmetry**

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**Competing orders in a nearly antiferromagnetic metal**
Charge density wave (CDW) fluctuations

d-wave CDW susceptibility

\[ \tilde{\Delta}_-(\mathbf{r}_i) = \sum_{s=\uparrow,\downarrow} \left( \psi^\dagger_{xis} \psi_{xis} - \psi^\dagger_{yis} \psi_{yis} \right) \]

\[ C_-(\mathbf{q}) = \int d\tau \langle \tilde{\Delta}^\dagger_-(\mathbf{q},\tau) \tilde{\Delta}_-(\mathbf{q},0) \rangle \]

- enhanced CDW fluctuations, but short correlation length ⇒ no CDW phase
- peak at \( \mathbf{q} \approx (\pi, 0.83\pi) \) effect of band structure
Conclusions

Numerically exact, unbiased results:

- **d-wave superconducting phase** from spin density wave fluctuations
- phase diagram similar to various unconventional superconductors
- charge or pair density wave phases would require additional interactions

Read more:

- recent related papers:
  - running on Tianhe-2!
  - ...
- commentary: JCCMP Jan 2016

Coming up:

- a closer look on quantum criticality
- algorithmic advances?

Thank you!
Appendix
We just tacitly assumed the weights

\[ p_\varphi = e^{-S_\varphi} \cdot \det \left[ 1 + \prod_{\ell=1}^{m} B_\varphi(\ell) \right] \]

to be real and positive. Generally this is not necessarily true.

- If some \( p_\varphi \) are negative, they cannot be interpreted as statistical weights for the evaluation of observable estimates:

\[ \langle A \rangle_{\text{estim}} = \frac{\sum_\varphi p_\varphi \langle A \rangle_\varphi}{\sum_\varphi p_\varphi} \]

sums over all field configurations \( \varphi \) sampled during a simulation

would not hold
• One can instead use the **absolute value** $|p_{\phi}|$ for the statistical weight:

$$\langle A \rangle_{\text{estim}}^{p} = \frac{\sum_{\phi} p_{\phi} |\langle A \rangle_{\phi}|}{\sum_{\phi} p_{\phi}}$$

• Additionally measure **the sign** $s_{\phi} = p_{\phi}/|p_{\phi}|$, then recover

$$\langle A \rangle_{\text{estim}} = \frac{\sum_{\phi} p_{\phi} \langle A \rangle_{\phi}}{\sum_{\phi} p_{\phi}} = \frac{\sum_{\phi} s_{\phi} p_{\phi} |\langle A \rangle_{\phi}|}{\sum_{\phi} s_{\phi} p_{\phi} |p_{\phi}|} = \frac{\langle sA \rangle_{\text{estim}}^{p}}{\langle s \rangle_{\text{estim}}^{p}}$$

• For $\langle\text{sign}\rangle \not\approx 1$: divide by average of **strongly fluctuating** $\pm 1$
  ○ Need about a factor of $\langle\text{sign}\rangle^{-2}$ more samples compared to $\langle\text{sign}\rangle = 1$

• **E.g. Hubbard model:** $\langle\text{sign}\rangle \sim e^{-\beta N \gamma}$
  ○ in special cases $\gamma = 0$, else: only **small** systems at **high** temperatures are feasible
No sign-problem in the SDW model

Prove that these issues do not apply to the two-band model

Recall

\[ p_\phi = e^{-S_\phi} \cdot \det \left[ 1 + \prod_{\ell=1}^m B_\phi(\ell) \right], \]

with \( B_\phi(\ell) = e^{-\Delta \tau K/2} e^{-\Delta \tau V(\ell)} e^{-\Delta \tau K/2} \).

The matrices \( K, V(\ell) \) are given by (Indexes: band, site, spin)

\[
K_{\alpha \alpha', i j, \sigma \sigma'} = \delta_{\sigma \sigma'} \delta_{\alpha \alpha'} \left( -t_{\alpha, i j} - \mu \delta_{i j} \right),
\]

\[
V(\ell)_{\alpha \alpha', i j, \sigma \sigma'} = \lambda \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}_{\alpha \alpha'} \delta_{i j} \left[ \vec{\sigma} \cdot \vec{\varphi}_i(\ell \Delta \tau) \right]_{\sigma \sigma'}
\]

Now introduce an anti-unitary operator

\[
\mathcal{U} = i \sigma_3^{\text{band}} \sigma_2^{\text{spin}} \mathcal{C}
\]

with Pauli matrices acting on band or spin index and complex conjugation \( \mathcal{C} \)

Easy to check: \( \mathcal{U} \) commutes with both \( K \) and \( V(\ell) \), also: \( \mathcal{U}^2 = -\mathbb{1} \)
Hence, the anti-unitary $U$ also commutes with $M = [1 + \prod_{\ell=1}^{m} B_{\varphi}(\ell)]$. Also remember: $U^2 = -1$

- Assume an eigenvector $v$:

\[ Mv = \lambda v \]

- Use anti-unitarity: $U^\dagger MU = M$

\[ U^\dagger MUv = \lambda v \]

- Use $U^\dagger U = 1$ and anti-linearity $U\lambda v = \lambda^* Uv$

\[ MUv = \lambda^* Uv \]

So to every eigenvector $v$ with eigenvalue $\lambda$, also $Uv$ is an eigenvector with eigenvalue $\lambda^*$.

$v$ and $Uv$ are linearly independent:

$Uv = \alpha v \implies U^2v = \alpha^* Uv \implies -v = |\alpha|^2 v$
• All eigenvalues of $M = [1 + \prod_{\ell=1}^{m} B_{\phi}(\ell)]$ occur in **complex-conjugate pairs**

• So $\det M = \prod_{k} |\lambda_{k}|^2 \geq 0$

All weights are **positive**:

$$e^{-S_{\phi}} \cdot \det [1 + \prod_{\ell=1}^{m} B_{\phi}(\ell)] \geq 0$$

There is no sign-problem