Monte Carlo Study of Competing Orders in a Nearly Antiferromagnetic Metal

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arXiv:1512.07257

Gießen

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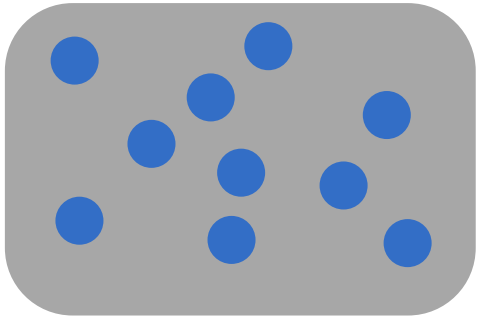
Overview

Condensed matter physics

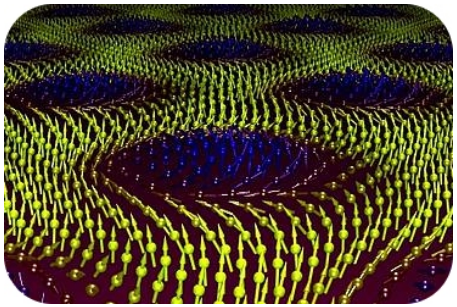
Collective phenomena



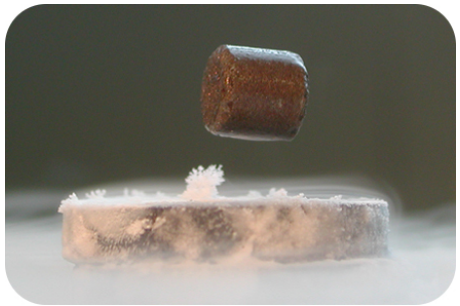
interacting quantum **many-particle** systems

$\Rightarrow$

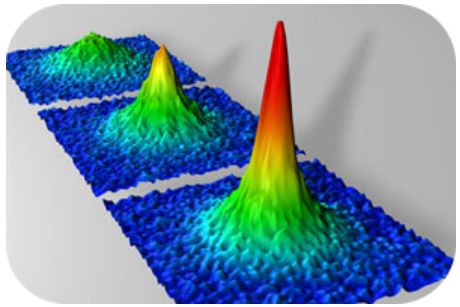
novel, distinctly **quantum phases** of matter



magnetic ordering

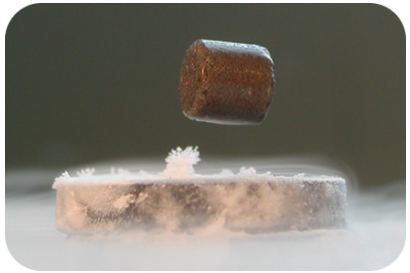


superconductivity



Bose-Einstein condensation

Superconductivity



Conventional superconductors

- $T_c \leq 39\,\mathrm{K}$
- e.g.: mercury, aluminum, . . .

Well understood by **BCS theory**

- electrons condense into **Cooper pairs**
- attractive interaction: quanta of **lattice vibrations**

High-temperature superconductors

- $T_c \leq 138\,\mathrm{K}$
- e.g.: cuprates, iron pnictides, . . .

BCS theory **fails**

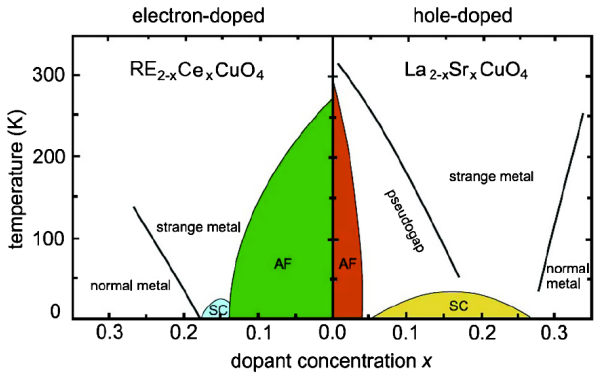
- **unknown** mechanism of pairing
- what is the **attractive interaction**?

Experimental phase diagrams

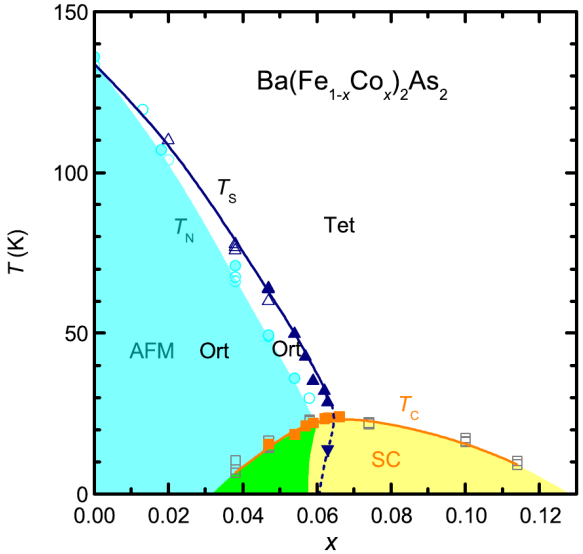
Strongly correlated metals show a plethora of phases with competing orders at low temperatures. Often in proximity:

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

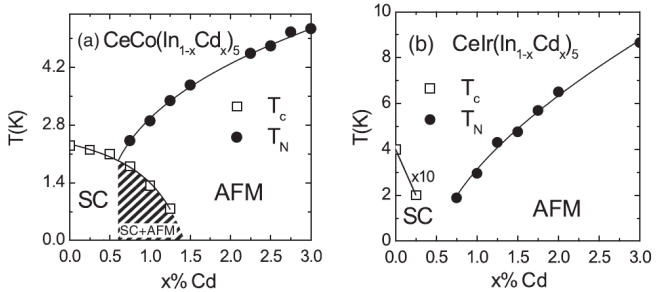
Cuprates



Fe-based superconductors



Heavy-fermion compounds



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

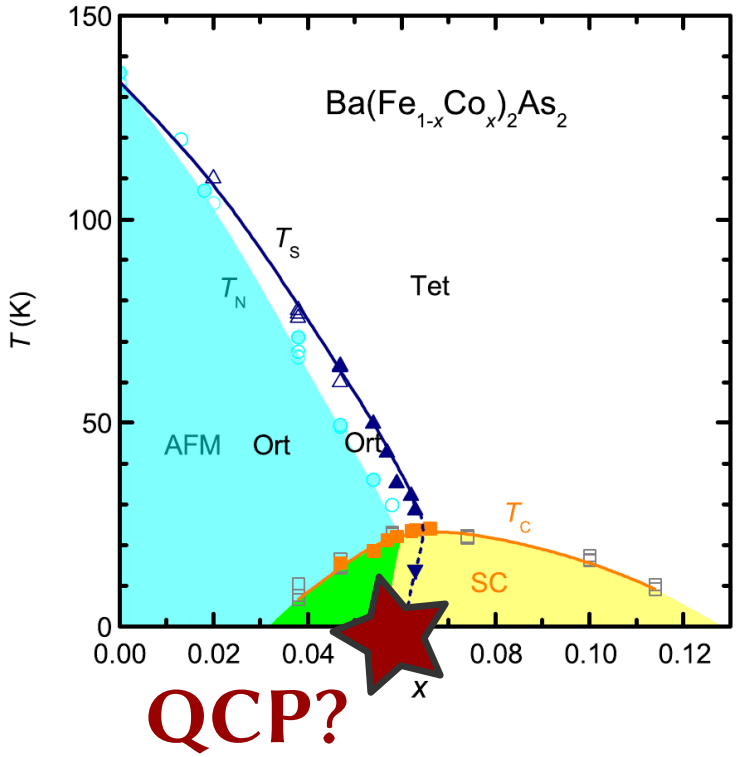
- **universal** mechanism?

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

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



- Layered compounds: effectively **2D**

Challenge: Improve lacking understanding of **universal physics** in a metal close to an **AFM quantum phase transition**

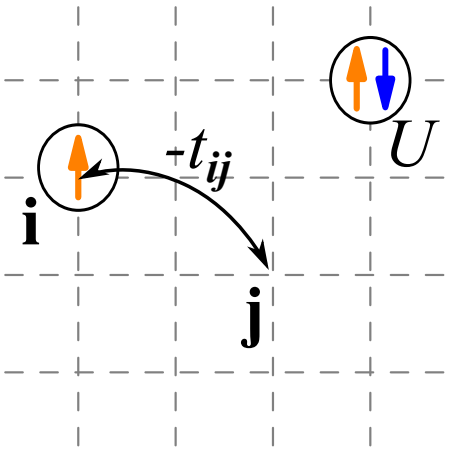
Setup of a generic model

Starting point: Hubbard model

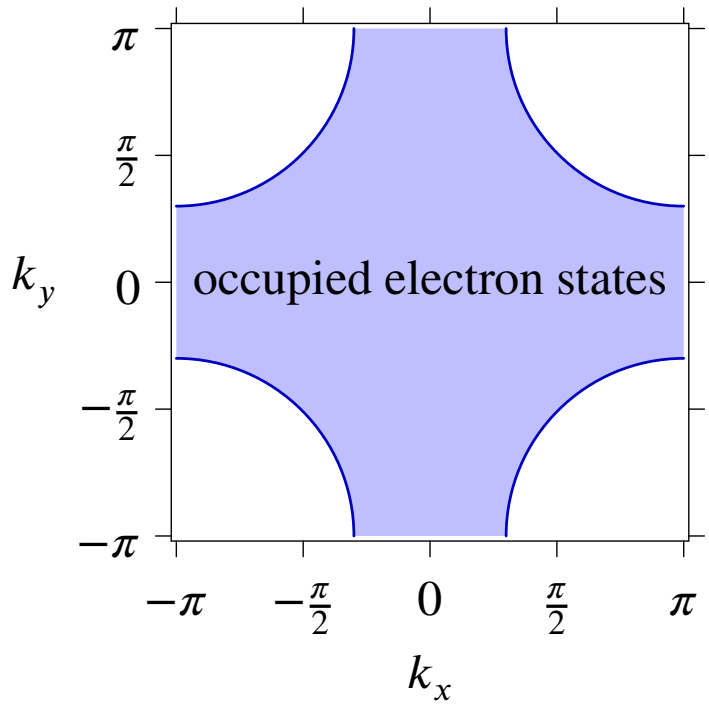
- one-band of $S = 1/2$ **itinerant fermions**, hopping on square lattice
- repulsive onsite **Hubbard** interaction $U > 0$

$$H = -\sum_{\mathbf{i},\mathbf{j},\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_{\mathbf{i}} c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} \qquad \text{or}$$

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{U}{N_s} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{\mathbf{k}',\downarrow} c_{\mathbf{k}'-\mathbf{q},\downarrow} c_{\mathbf{k}+\mathbf{q},\uparrow}$$



- typical **Fermi surface** given by $\varepsilon_{\mathbf{k}}$ for electron-doped cuprates:



Antiferromagnetic mean field

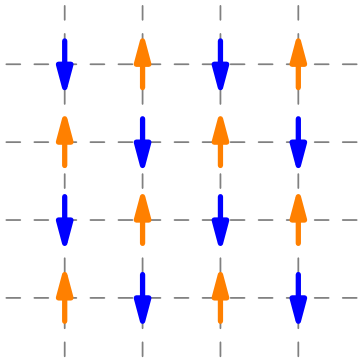
$$H = -\sum t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

- **rewrite** interaction using $S^\alpha_i = \frac{\hbar}{2} \sum_{\sigma,\tau} c^\dagger_{i\sigma} \left[\sigma^\alpha\right]_{\sigma\tau} c_{i\tau} \quad (\alpha = x, y, z)$

$$H = -\sum_{\mathbf{i},\mathbf{j},\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} - \frac{2U}{3\hbar^2} \sum_{\mathbf{i}} \vec{S}_i^{\,2} + \frac{1}{2} U N_e$$

- **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**:

$$\langle \vec{S}_{\mathbf{i}} \rangle = \vec{\varphi}_0 \cdot \cos(\mathbf{Q} \cdot \mathbf{i}), \qquad \mathbf{Q} = \begin{bmatrix} \pi \\ \pi \end{bmatrix}$$



- put together for **mean field Hamiltonian**:

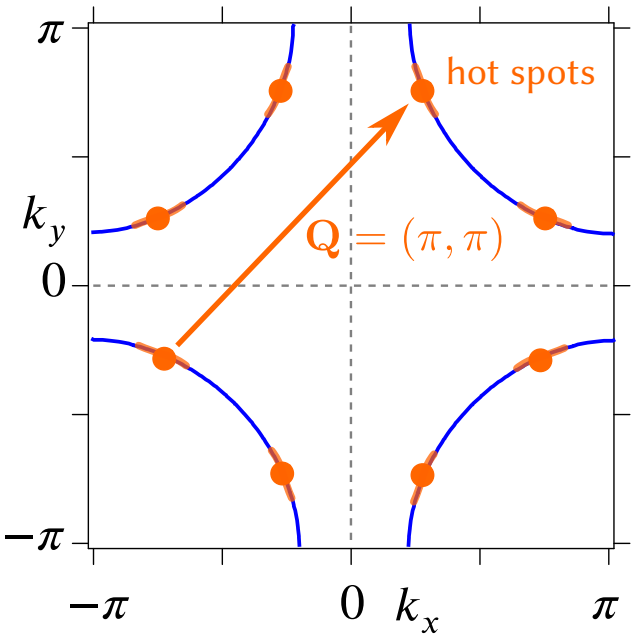
$$H_{\mathrm{MF}} = -\sum_{\mathbf{i},\mathbf{j},\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} - \frac{4U}{3\hbar} \sum_{\mathbf{i}} \vec{\varphi}_0 \cdot \vec{S}_i \cos(\mathbf{Q}\cdot\mathbf{i}) + \mathrm{const}$$

- retranslate $\vec{S}_i \to c^{(\dagger)}_{i,\sigma}$ and go to **Fourier representation**:

$$H_{\mathrm{MF}} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \frac{2U}{3} \sum_{\mathbf{k},\sigma,\tau} \left[c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k}+\mathbf{Q},\tau} \right] [\vec{\varphi}_0 \cdot \vec{\sigma}]_{\sigma\tau}, \qquad \mathbf{Q} = \begin{bmatrix} \pi \\ \pi \end{bmatrix}$$

Key insight: only electrons with momenta separated by $\mathbf{Q}$ scatter!

- low-energy physics: states near Fermi surface most important
- discrete set of **"hot spots"** on the original Fermi surface
  $\varepsilon_{\mathbf{k}} = \varepsilon_{\mathbf{k}+\mathbf{Q}} = \varepsilon_{\mathrm{F}}$



Going beyond mean field

Full fluctuations: Spin-fermion model

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

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

$$Z = \mathrm{Tr}\, e^{-\beta H} \sim \int D(\{\vec{\varphi}_{\mathbf{q}}\}) e^{-S_\varphi}\, \mathrm{Tr}\, e^{-\beta H(\vec{\varphi}_{\mathbf{q}})}$$

$$H(\vec{\varphi}_{\mathbf{q}}) = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{k}} + \lambda \sum_{\mathbf{k},\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{Q}+\mathbf{q}} (\vec{\sigma}\cdot\vec{\varphi}_{\mathbf{q}}) c_{\mathbf{k}}, \qquad \mathbf{Q} = \begin{bmatrix} \pi \\ \pi \end{bmatrix}$$

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

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

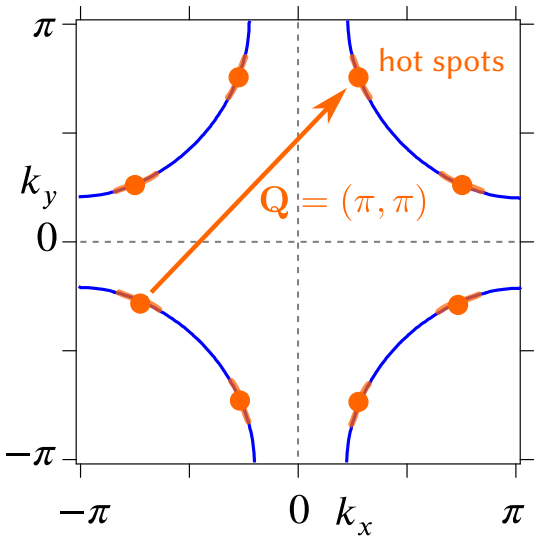
Analytical theory: **hard**

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

A. Abanov, A. V Chubukov, and J. Schmalian, Adv. Phys. **52**, 119 (2003)

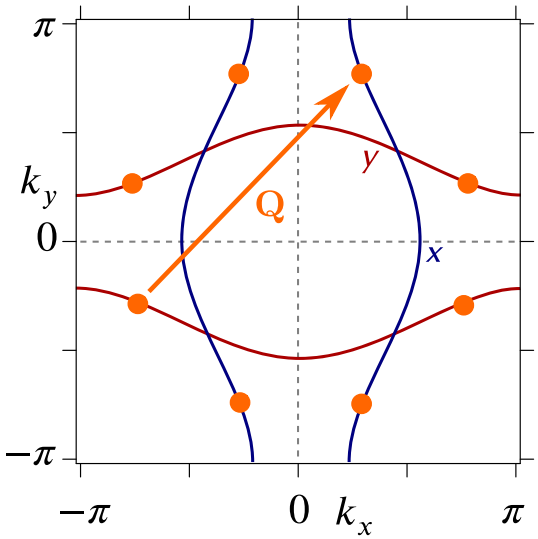
Enabling quantum Monte Carlo

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



- tendency towards **SDW order** at $\mathbf{Q} = (\pi, \pi)$
- 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** ψ_x, ψ_y
- split Fermi surfaces, **sustained hot spot structure**

- allows extra antiunitary symmetry $\mathcal{U} = i\sigma_3^{\text{band}}\sigma_2^{\text{spin}}\mathcal{C}$

$\Rightarrow$ **sign-problem-free** determinantal QMC

Want to learn more about this? Slides in the back

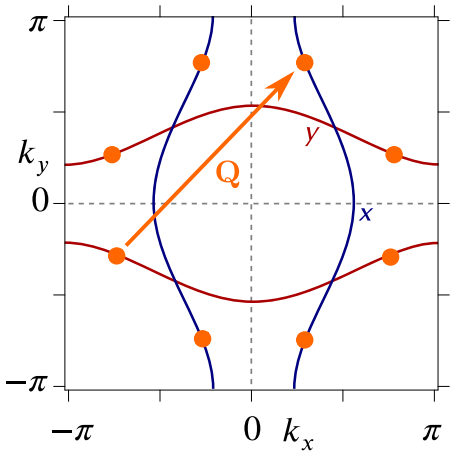
E. Berg, M. A. Metlitski, and S. Sachdev, Science **338**, 1606 (2012).

Model probed by QMC

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

- **two-flavor fermionic** action

$$L_F = \sum_{\substack{i,j,s \\ \alpha=x,y}} \psi^\dagger_{\alpha i s} \left[(\partial_\tau - \mu)\delta_{ij} - t_{\alpha ij} \right] \psi_{\alpha j s} + \lambda \sum_{i,s,s'} e^{i\mathbf{Q}\cdot\mathbf{r}_i} [\vec{s}\cdot\vec{\varphi}_i]_{ss'} \psi^\dagger_{xis} \psi_{yis'} + \mathrm{h.c.}$$



SDW coupling

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

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

r tunes across SDW transition

- **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

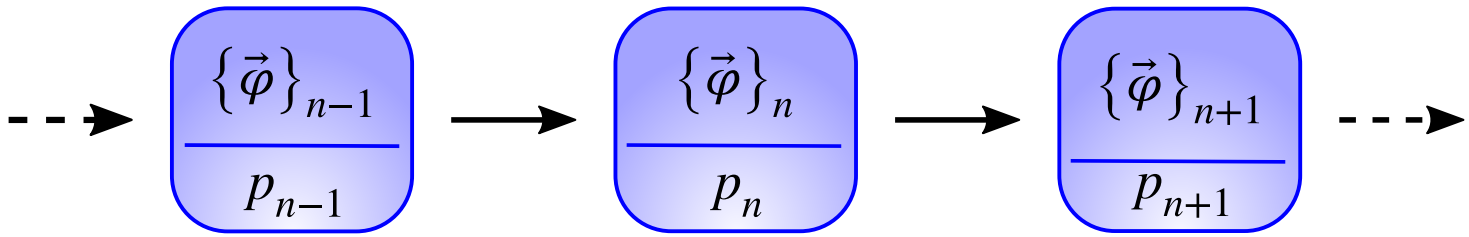
Quantum Monte Carlo (QMC)

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

$$\langle A \rangle = \frac{1}{Z} \int D(\vec{\varphi}, \psi) A \, e^{-S_F - S_\varphi}, \qquad Z = \int D(\vec{\varphi}, \psi) e^{-S_F - S_\varphi}$$

General idea of all quantum Monte Carlo approaches:

- map partition function to average over **configurations** $\{\vec{\varphi}\}_n$ 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

R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D **24**, 2278 (1981).

Recipe:

- Keep the bosonic field integral and write the fermionic integral as a **trace in Fock space**

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

- At each τ, H_F is evaluated for a different field configuration $\{\vec{\varphi}(\tau)\}$

- **Discretize imaginary time** into time slices $\ell = 1, \ldots, m$, $\beta = m\Delta\tau$:

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

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

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

$$H_K = -\sum_{\boldsymbol{i},\boldsymbol{j},\sigma} \sum_{\alpha=x,y} \psi^\dagger_{\alpha,\boldsymbol{i},\sigma} \left[\mu\delta_{ij} + t_{\alpha,ij}\right] \psi_{\alpha,\boldsymbol{j},\sigma} \qquad \text{kinetic energy}$$

$$H_V(\vec{\varphi}) = \lambda \sum_{\boldsymbol{i},\sigma,\tau} [\vec{\sigma} \cdot \vec{\varphi}_i]_{\sigma,\tau} \psi^\dagger_{x,\boldsymbol{i},\sigma} \psi_{y,\boldsymbol{i},\tau} + \mathrm{h.c.} \qquad \text{field-coupled interaction}$$

- 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**

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

$$U_{\varphi}(\ell) = e^{-\Delta\tau H_K/2} e^{-\Delta\tau H_V(\ell)} e^{-\Delta\tau H_K/2}$$

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

$$\operatorname{Tr}_{\psi} \left[\prod_{\ell=1}^{m} U_{\varphi}(\ell)\right] = \det \left[\mathbb{1} + \prod_{\ell=1}^{m} B_{\varphi}(\ell)\right],$$

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

- 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

DQMC – basic algorithm

Our formulation of the **partition function** contains statistic weights we can **directly compute**:

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

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

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

$$p = \min\left\{1, e^{-\left(S_\varphi^{\text{new}} - S_\varphi^{\text{old}}\right)} \times \frac{\det\left[\mathbb{1} + \prod_{\ell=1}^{m} B_\varphi^{\text{new}}(\ell)\right]}{\det\left[\mathbb{1} + \prod_{\ell=1}^{m} B_\varphi^{\text{old}}(\ell)\right]}\right\}$$

- To measure **fermionic observables** we use the equal-time **Green's function** for a configuration of fields $\vec{\varphi}$ time slice ℓ

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

- A **Wick's theorem** holds, providing arbitrary correlation functions
- Imaginary time-displaced correlation functions:
  application of matrices B_φ, B_φ^{-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 $1/T = m\Delta\tau$

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

Problem: ill-conditioned matrices

- Numerical multiplication $B_1 \cdot B_2$ mixes very small and very large eigenvalues
- Scales are "washed out" $\Rightarrow$ **unstable** at low temperatures (long chains)

Solution:

- Separate scales by **singular value decomposition (SVD)**

$$B_1 = U_1 S_1 V_1^\dagger = \underbrace{\begin{pmatrix} x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{pmatrix}}_{\text{unitary}} \cdot \underbrace{\begin{pmatrix} x & & & \\ & x & & \\ & & X & \\ & & & X \end{pmatrix}}_{\text{diagonal}} \cdot \underbrace{\begin{pmatrix} x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{pmatrix}}_{\text{unitary}}$$

- To compute $B_1 \cdot B_2 = U_1 S_1 V_1^\dagger \cdot U_2 S_2 V_2^\dagger$, first take

$$\left(U_1 S_1 V_1^\dagger U_2\right) \cdot S_2 \qquad S_2 = \begin{pmatrix} x & & \\ & x & \\ & & \mathbf{x} \\ & & & \mathbf{x} \end{pmatrix}$$

- **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**

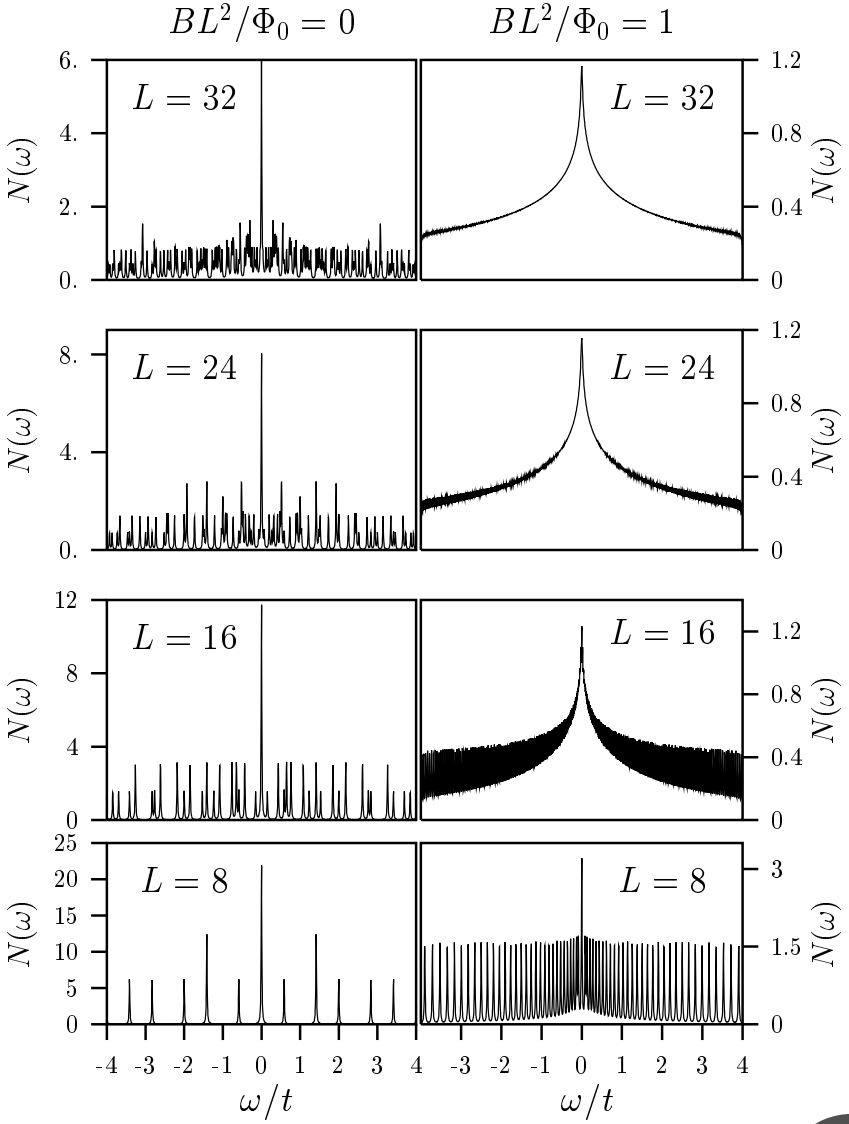
Effective remedy

Weak magnetic field, vanishing for $L \to \infty$

$$t_{\alpha sij}\psi^{\dagger}_{xis}\psi_{xjs} \to e^{iA^{\alpha s}_{ij}} t_{\alpha sij}\psi^{\dagger}_{\alpha is}\psi_{\alpha js}$$

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

density of states, tight-binding model



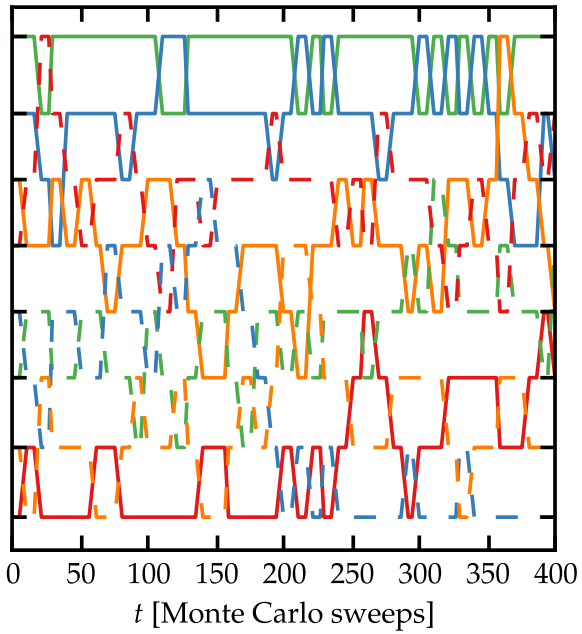
F. Assaad, Phys. Rev. B **65**, 115104 (2002).

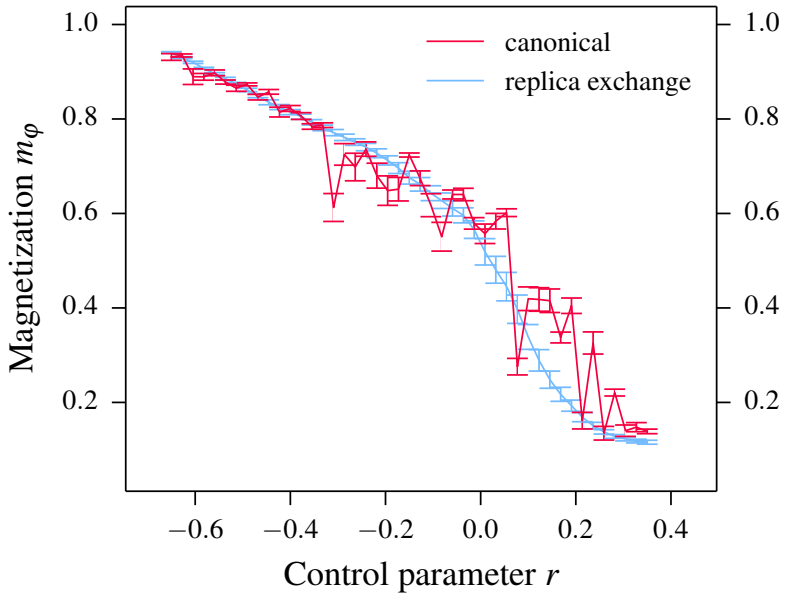
3: Efficient sampling

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



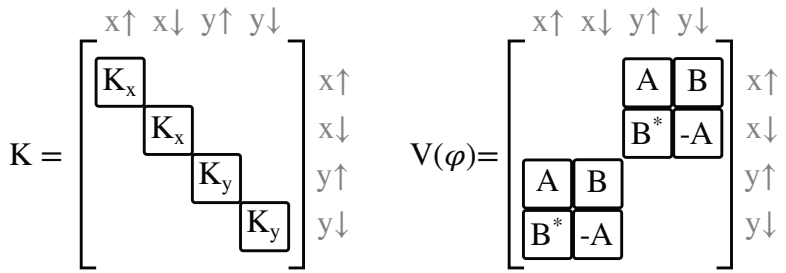


4: Computational cost of linear algebra

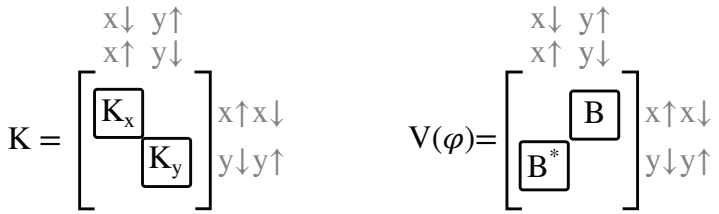
- exploit sparseness and low rank of matrices where possible
- still, computational effort scales like the **cubed** system size: $\sim O(\beta N^3)$

- 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



O(2) model: 2N×2N matrices
additional unitary symmetry $\boxed{A} = 0$



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

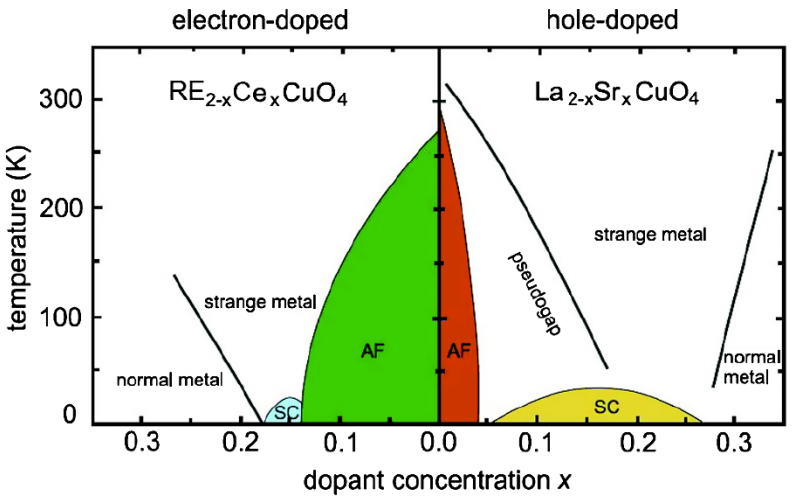
We would like to access larger systems: Can **Hybrid Monte Carlo** methods help?

Physical results

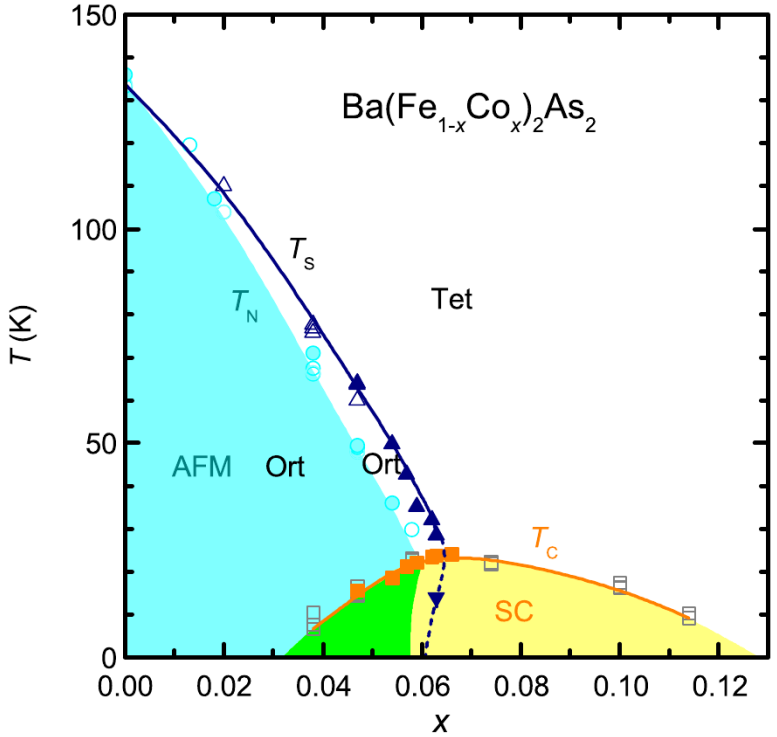
Reminder: Experimental phase diagrams

Strongly correlated metals

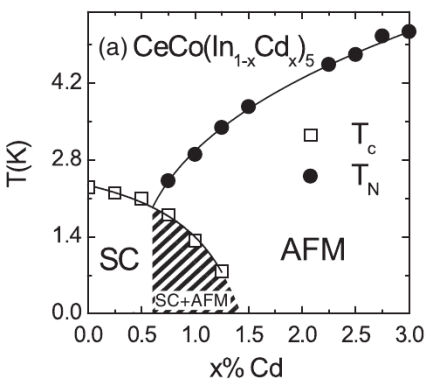
Cuprates

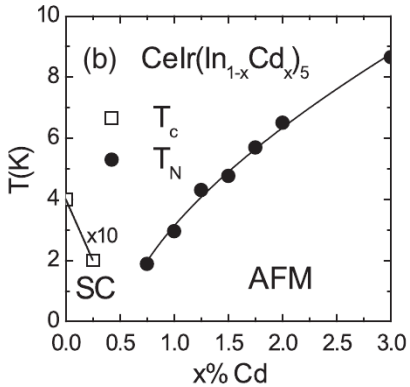


Fe-based superconductors

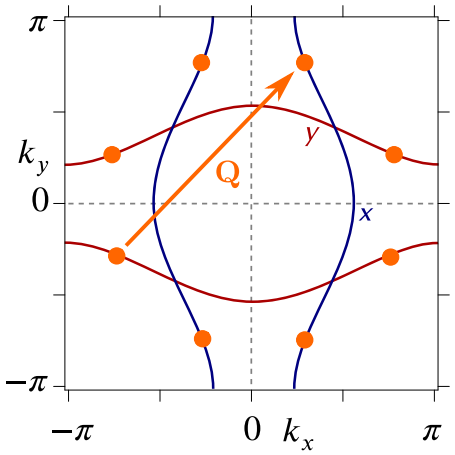


Heavy-fermion compounds





Reminder: Physical model



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

- **two-flavor fermionic** action

$$L_F = \sum_{\substack{i,j,s \\ \alpha=x,y}} \psi^\dagger_{\alpha i s} \left[(\partial_\tau - \mu)\delta_{ij} - t_{\alpha ij} \right] \psi_{\alpha j s} + \lambda \sum_{i,s,s'} e^{i\mathbf{Q}\cdot\mathbf{r}_i} [\vec{s}\cdot\vec{\varphi}_i]_{ss'} \psi^\dagger_{xis} \psi_{yis'} + \mathrm{h.c.}$$

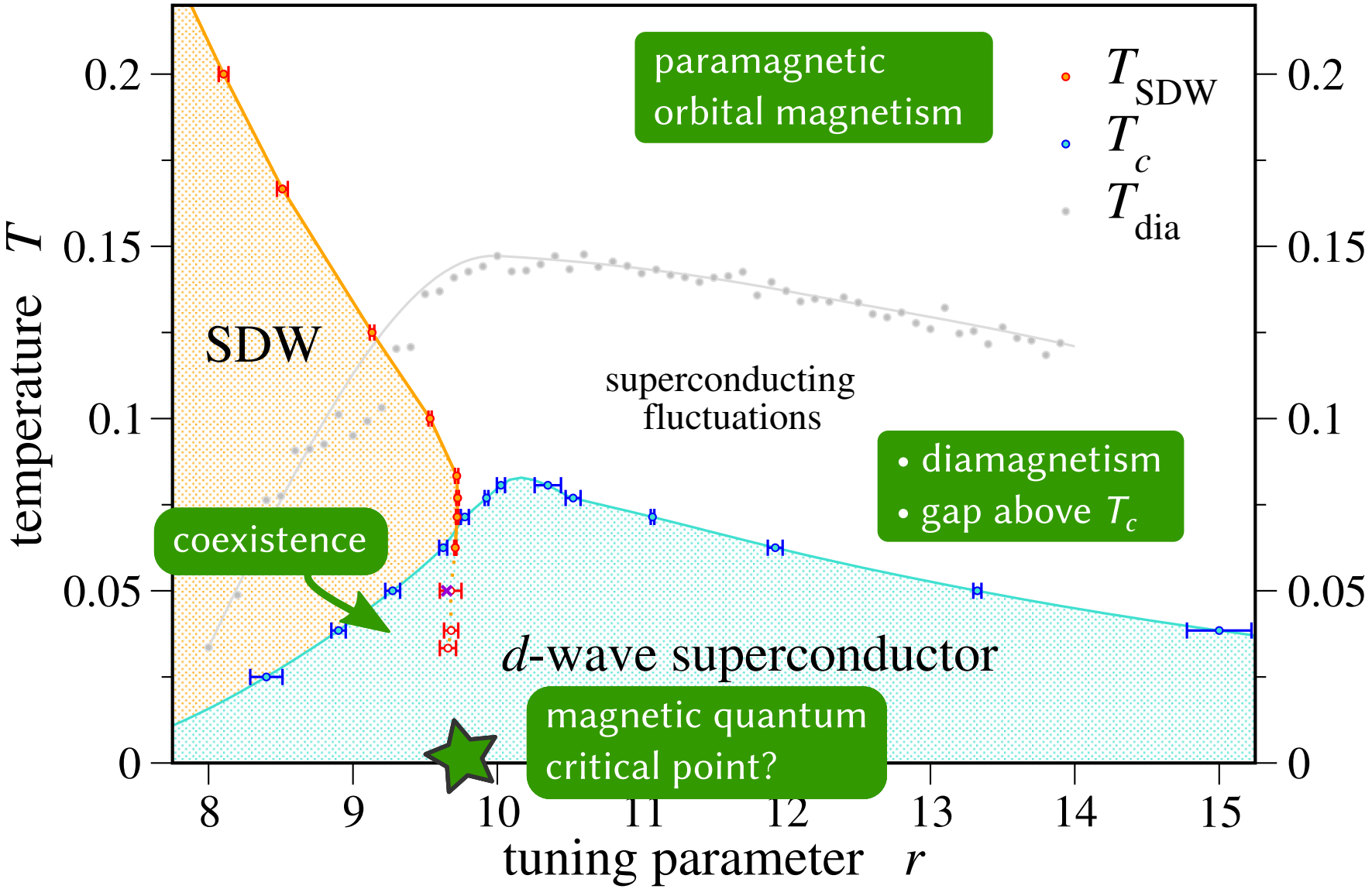
SDW coupling

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

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

r tunes across SDW transition

Numerically obtained phase diagram



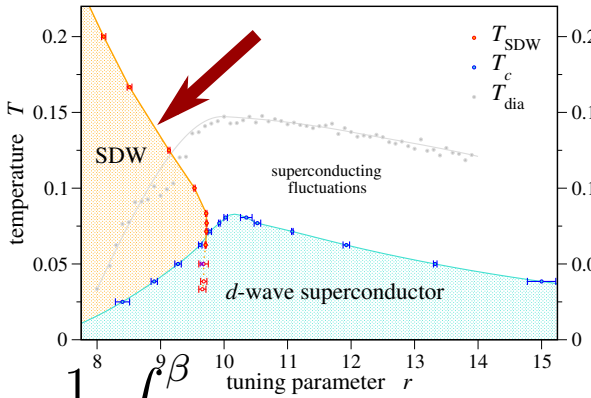
energy scale $E_F \approx 2.5$

$\lambda = 3, c = 2$

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:

$$\langle \vec{m}_i \cdot \vec{m}_{i+\mathbf{x}} \rangle \sim \begin{cases} e^{-|\mathbf{x}|/\xi}, & T > T_{\mathrm{SDW}}, \\ |\mathbf{x}|^{-\eta(T)}, & T \leq T_{\mathrm{SDW}} \end{cases} \qquad \vec{m}_i = \frac{1}{\beta} \int_0^\beta \mathrm{d}\tau \vec{\varphi}_i(\tau)$$

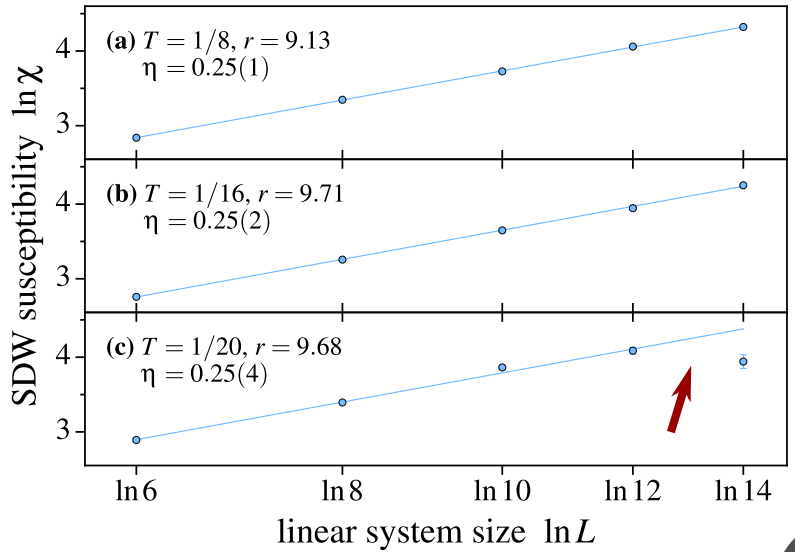
- **universal** exponent $\eta = 1/4$ for $T = T_{\mathrm{SDW}}$
- Finite-size scaling of SDW susceptibility to locate $r(T = T_{\mathrm{SDW}})$
  $\chi = \int_0^\beta \mathrm{d}\tau \sum_i \langle \vec{\varphi}_i(\tau) \vec{\varphi}_0(0) \rangle \sim L^{2-\eta(T)}$ for $T \leq T_{\mathrm{SDW}}$

High temperatures

- Consistent scaling

Below superconducting dome

- $T < T_c$: Scaling breaks down
- weakly first-order?



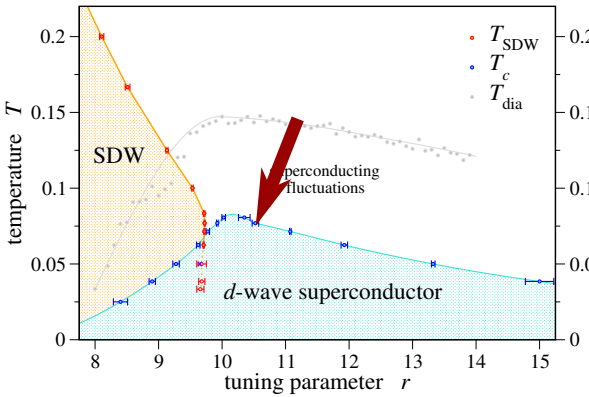
Superconducting transition

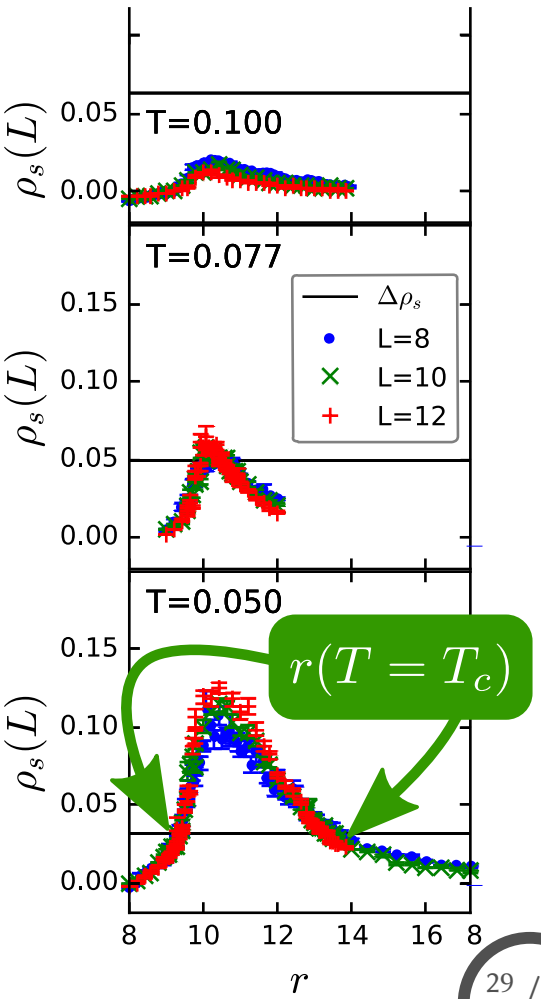
Linear response theory:

- current-current correlator:
  $\Lambda_{xx}(\mathbf{q}) = \sum_i \int_0^\beta d\tau e^{-i\mathbf{q}\cdot\mathbf{r}_i} \langle j_x(\mathbf{r}_i,\tau) j_x(0,0)\rangle$
- 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**: $\rho_s = \frac{1}{4}\left[\Lambda^{\parallel} - \Lambda^{\perp}\right]$

BKT transition at T_c:

- ρ_s jumps by **universal amount** $\Delta\rho_s = \frac{2T_c}{\pi}$
- $\rho_s > \Delta\rho$: superconducting phase

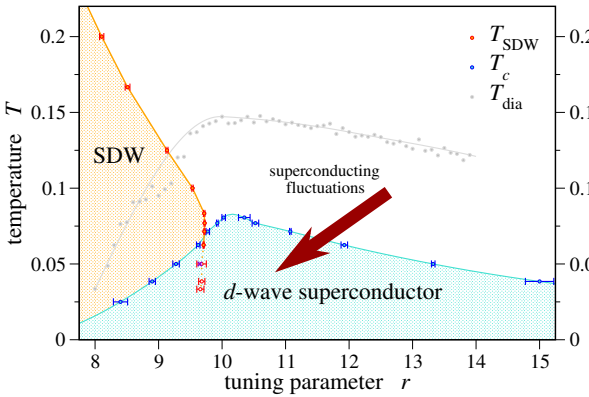




d-wave superconductivity

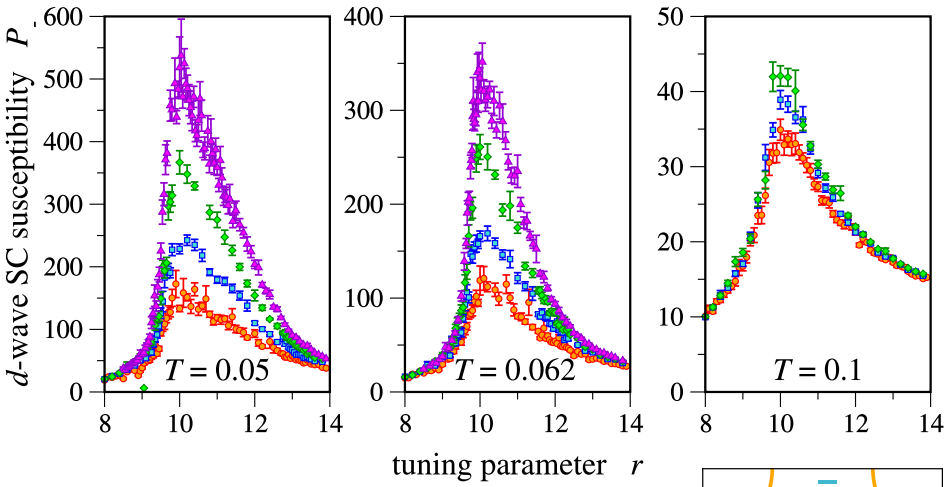
Pairing susceptibilities

$$\Delta_{\pm}(\mathbf{r}_i) = 2\left(\psi^{\dagger}_{xi\uparrow}\psi^{\dagger}_{xi\downarrow} \pm \psi^{\dagger}_{yi\uparrow}\psi^{\dagger}_{yi\downarrow}\right)$$



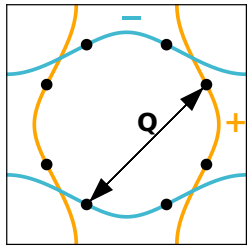
- d-wave:

$$P_{-} = \int d\tau \sum_i \langle \Delta^{\dagger}_{-}(\mathbf{r}_i,\tau)\Delta_{-}(\mathbf{0},0)\rangle$$



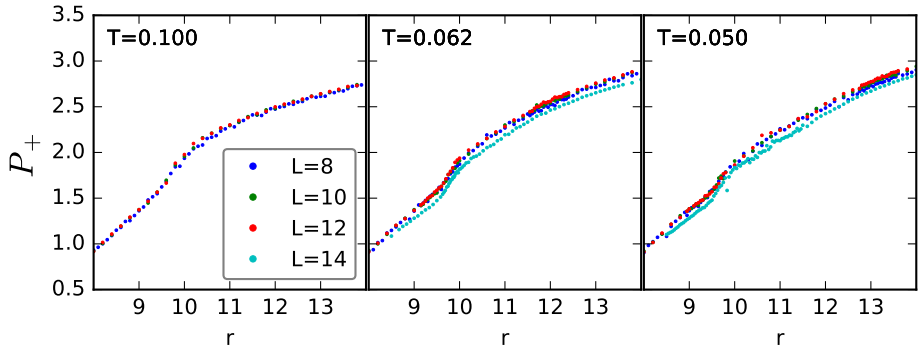
$L = 14$ $L = 10$

$L = 12$ $L = 8$



- s-wave:

$$P_{+} = \int d\tau \sum_i \langle \Delta^{\dagger}_{+}(\mathbf{r}_i,\tau)\Delta_{+}(\mathbf{0},0)\rangle$$



Finite-size scaling

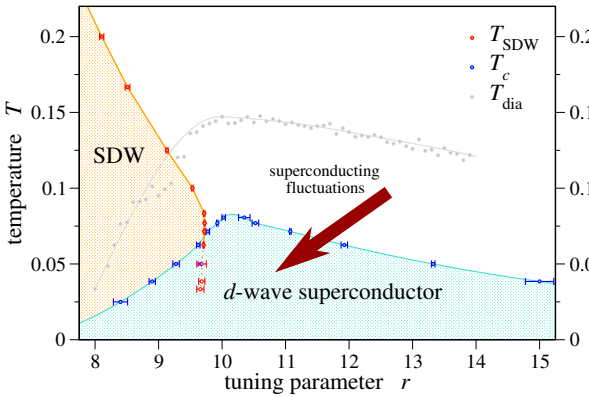
P_- diverges with system size ⇒ superconducting phase has ***d*-wave symmetry**

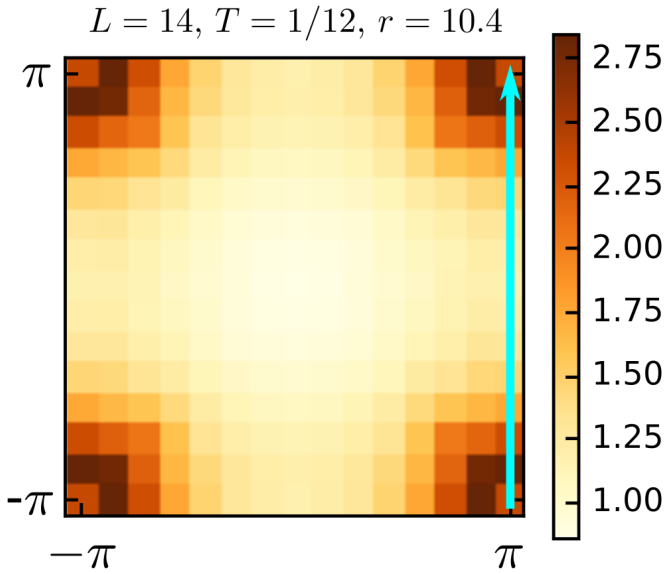
Charge density wave (CDW) fluctuations

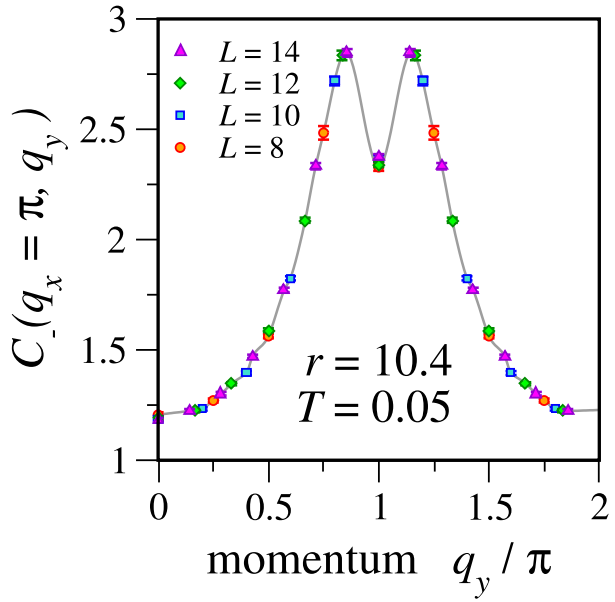
d-wave CDW susceptibility

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

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







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

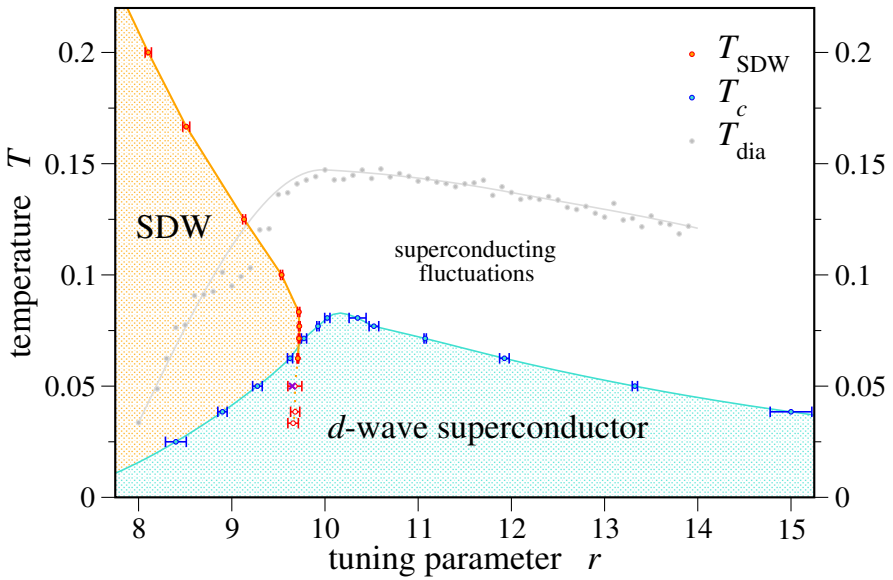
Conclusions

Numerically exact, unbiased results:

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

Read more:

- full discussion: arXiv:1512.07257
- recent related papers:
  - Li *et. al*, arXiv:1512.04541 running on Tianhe-2!
  - Xu *et. al*, arXiv:1602.07150
  - ...
- commentary: JCCMP Jan 2016



Coming up:

- a closer look on quantum criticality
- algorithmic advances?

Thank you!

Appendix

DQMC – What about the sign problem?

We just tacitly assumed the **weights**

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

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

- If some p_φ are **negative**, they cannot be interpreted as statistical weights for the evaluation of observable estimates:

$$\langle A \rangle_{\text{estim}} = \frac{\sum_{\vec{\varphi}} p_\varphi \langle A \rangle_\varphi}{\sum_{\vec{\varphi}} p_\varphi}$$

sums over all
field configurations $\vec{\varphi}$
sampled during a simulation

would **not** hold

- One can instead use the **absolute value** $|p_\varphi|$ for the statistical weight:

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

- Additionally measure **the sign** $s_\varphi = p_\varphi / |p_\varphi|$, then recover

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

- For $\langle \text{sign} \rangle \not\approx 1$: divide by average of **strongly fluctuating** ± 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

$$p_\varphi = e^{-S_\varphi} \cdot \det\left[\mathbb{1} + \prod_{\ell=1}^{m} B_\varphi(\ell)\right],$$
$$\text{with } B_\varphi(\ell) = e^{-\Delta\tau K/2} e^{-\Delta\tau V(\ell)} e^{-\Delta\tau K/2}.$$

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

$$K_{\alpha\alpha',ij,\sigma\sigma'} = \delta_{\sigma\sigma'}\delta_{\alpha\alpha'}(-t_{\alpha,ij} - \mu\delta_{ij}),$$
$$V(\ell)_{\alpha\alpha',ij,\sigma\sigma'} = \lambda \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}_{\alpha\alpha'} \delta_{ij} \left[\vec{\sigma} \cdot \vec{\varphi}_i(\ell\Delta\tau)\right]_{\sigma\sigma'}$$

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 $\mathcal{U}$ also commutes with $M = [\mathbb{1} + \prod_{\ell=1}^{m} B_\varphi(\ell)]$.
Also remember: $\mathcal{U}^2 = -\mathbb{1}$

- Assume an **eigenvector** v:

$$Mv = \lambda v$$

- Use **anti-unitarity**: $\mathcal{U}^\dagger M \mathcal{U} = M$

$$\mathcal{U}^\dagger M \mathcal{U} v = \lambda v$$

- Use $\mathcal{U}^\dagger \mathcal{U} = \mathbb{1}$ and **anti-linearity** $\mathcal{U}\lambda v = \lambda^* \mathcal{U} v$

$$M\mathcal{U}v = \lambda^* \mathcal{U} v$$

So to every eigenvector v with eigenvalue λ, also $\mathcal{U}v$ is an eigenvector with eigenvalue λ^*.
v and $\mathcal{U}v$ are linearly independent:

$$\mathcal{U}v = \alpha v \implies \mathcal{U}^2 v = \alpha^* \mathcal{U} v \implies -v = |\alpha|^2 v$$

- All eigenvalues of $M = [\mathbb{1} + \prod_{\ell=1}^{m} B_\varphi(\ell)]$ occur in **complex-conjugate pairs**
- So $\det M = \prod_k |\lambda_k|^2 \geq 0$

All weights are **positive**:

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

There is no sign-problem