Intro to auxiliary field Quantum Monte Carlo methods

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Outline

- Fermionic systems in nature
    - The Hubbard Hamiltonian
- Exact Diagonalization and why is limited
- Revision: Classical Monte Carlo Methods
- Quantum Monte Carlo:
    - The general problem
    - Hubbard-Stratonovich transformations
    - Observables and correlations
    - “Cake” recipe
    - Sign problem
    - Famous results in the literature
- Projector Quantum Monte Carlo
- Summary

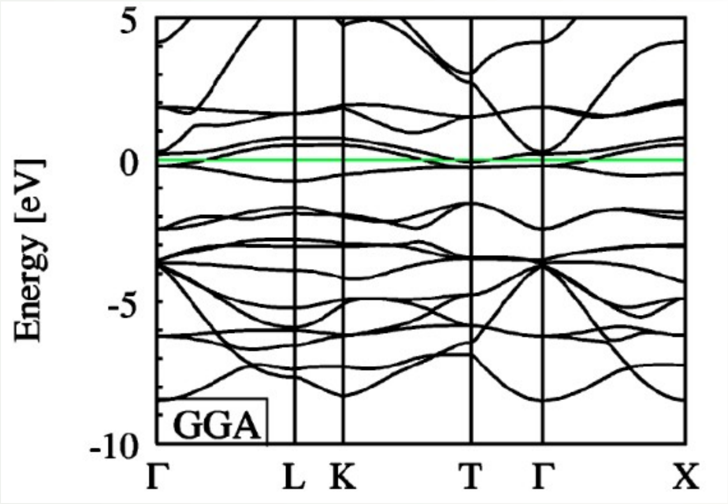
Fermionic systems in nature

- Interplay of charge and spin degrees of freedom explain several phenomena observed in real materials

Antiferromagnetism/ferromagnetism in Transition Metal oxides – MnO ; FeO; CoO

Band structure picture – DFT (GGA)

FeO



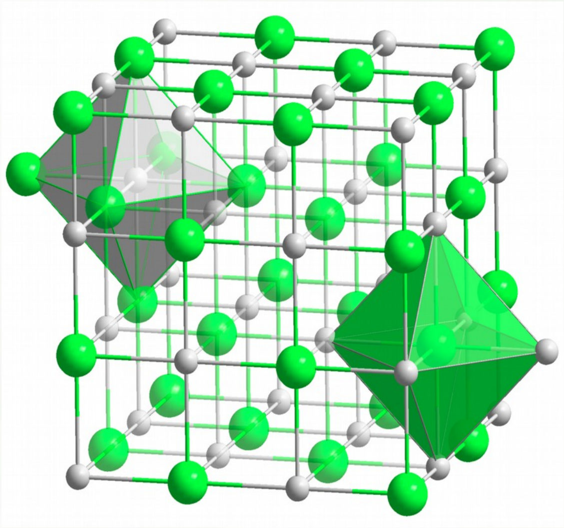
Metal!

$Fe^{3+} \rightarrow 3d^5$

Experimentally

Insulating and antiferromagnetic

$T_{Neél} = 200K$

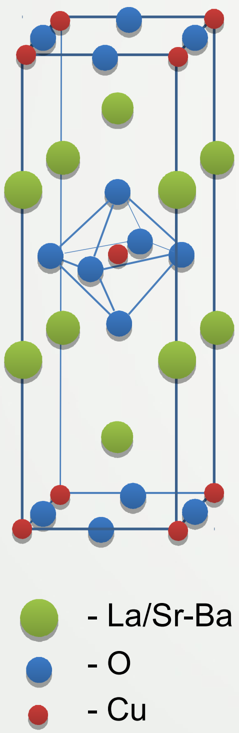


Fermionic systems in nature

- Interplay of charge and spin degrees of freedom explain several phenomena observed in real materials

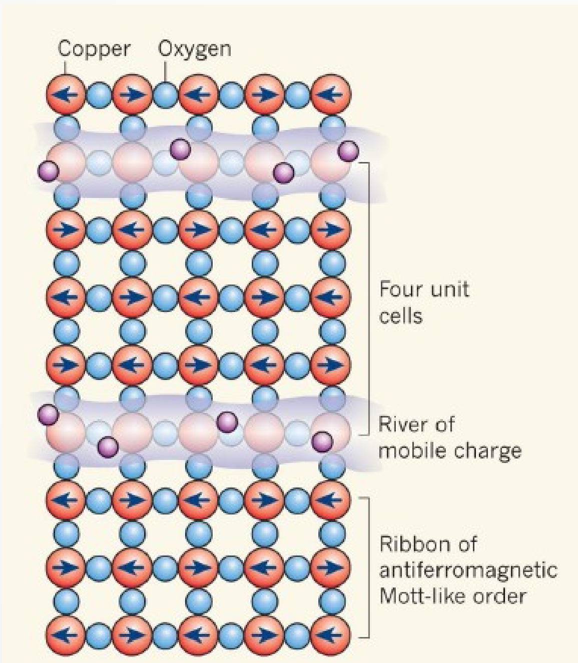
High-temperature superconductivity

- Crystalline structure:



perovskite

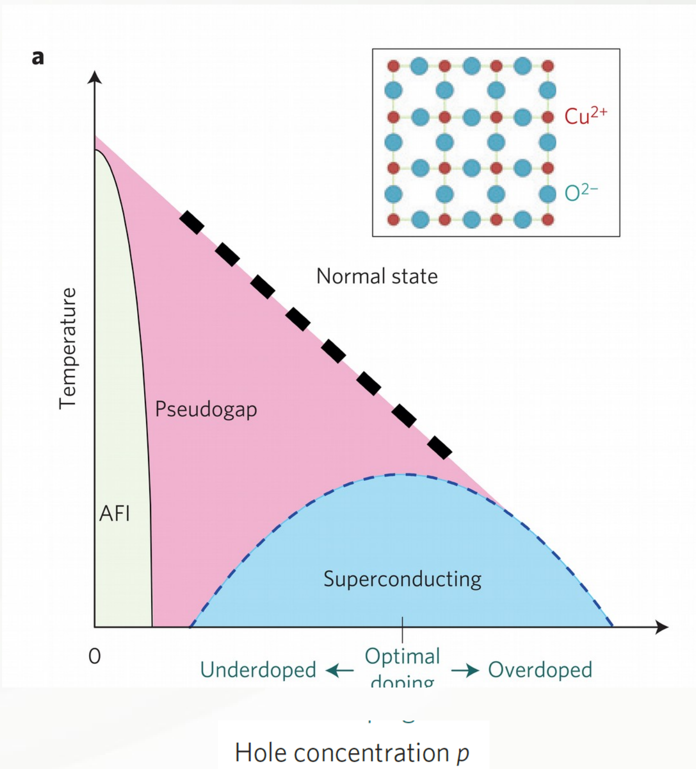
- Copper-Oxygen planes:



[K.A. Moler Nature **468**, 643–644 (2010)]

Stripes – hole rich quasi 1D region

- Proto phase diagram:



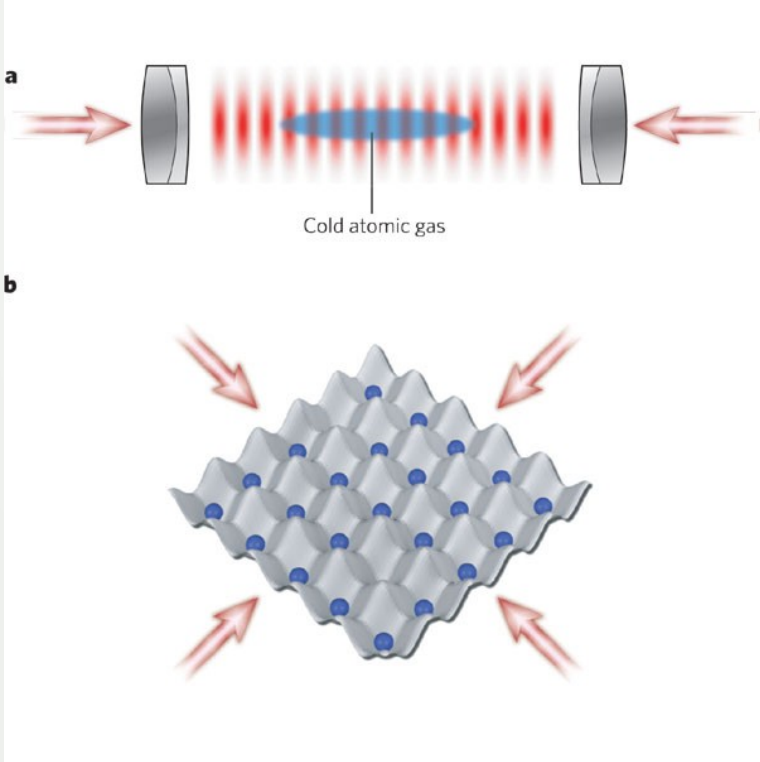
[M. Hashimoto *et al.*, Nature Physics 2014]

Fermionic systems in nature

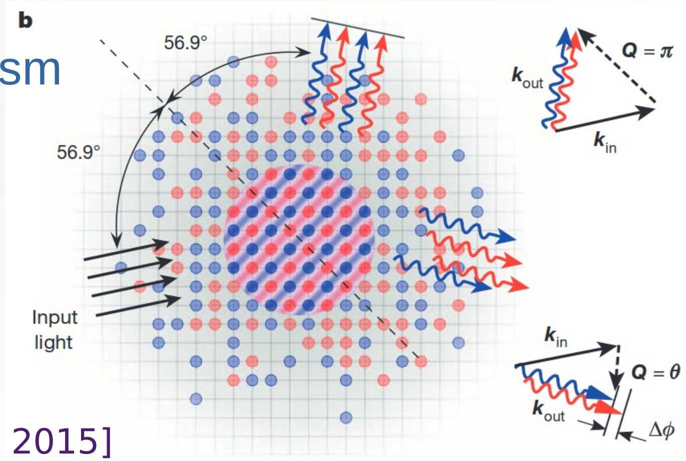
- Interplay of charge and spin degrees of freedom explain several phenomena observed in real materials

Emulation testbed to probe these effects: Optical lattices

- Counter propagating laser beams generate an optical trapping potential
- Trapping cold atoms
- Easily adjustable parameters (by tuning laser parameters) and external magnetic fields (Feschbach resonances)
- Proto magnetism



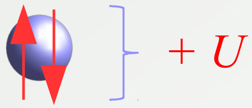
[I. Bloch *et al*., Nature 2008]



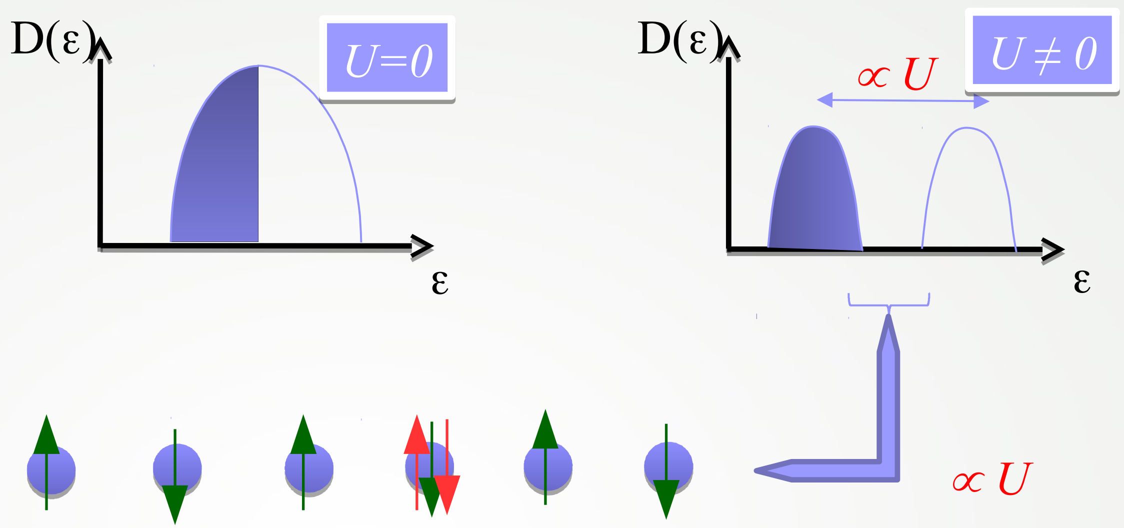
[R. Hart *et al*., Nature 2015]

The Hubbard Hamiltonian – qualitative aspects

- **Mott insulators**

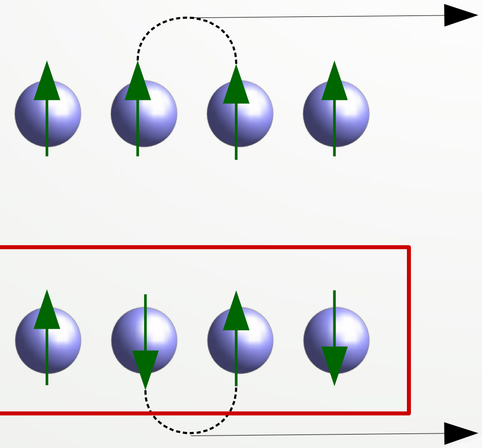


Ex: 1d lattice – s-band



- **Magnetic properties of the ground state**

Perturbation theory:
Virtual hopping processes



hopping not allowed
(Pauli exclusion principle)

hopping allowed

2nd order perturbation theory:

$$E_{FM} - E_{AF} \simeq \frac{|t|^2}{U}$$

AFM ground state is energetically favorable - **Magnetism**

- In the Hubbard model insulating behavior and antiferromagnetism go hand-in-hand

The Hubbard Hamiltonian

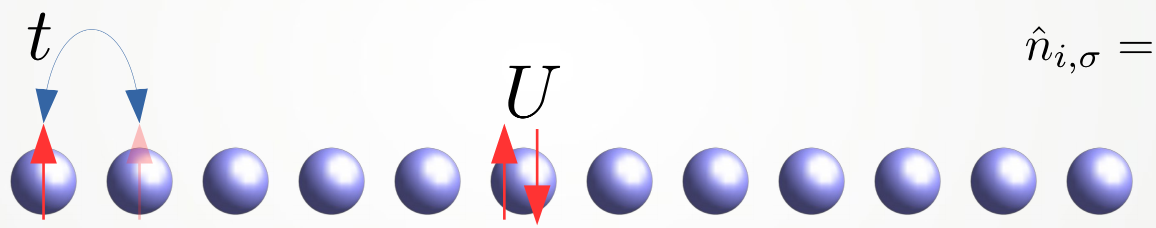
- Paradigmatic model for correlations in a tight-binding approximation

$$\hat{H} = \underbrace{-t \sum_{\langle i,j \rangle,\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + h.c. \right)}_{\text{Hopping term (Kinetic energy)}} + \underbrace{U \sum_{i} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}}_{\text{Local } e^- - e^- \text{ interactions}}$$

Hopping term (Kinetic energy)

Local *e^- - e^- interactions*

$\hat{n}_{i,\sigma} = \hat{c}^{\dagger}_{i,\sigma} \hat{c}_{i,\sigma}$: number operator



- Simplest case: s-band → maximum of 2 e^- per site

- Properties? Metal? Insulator? Magnetism?

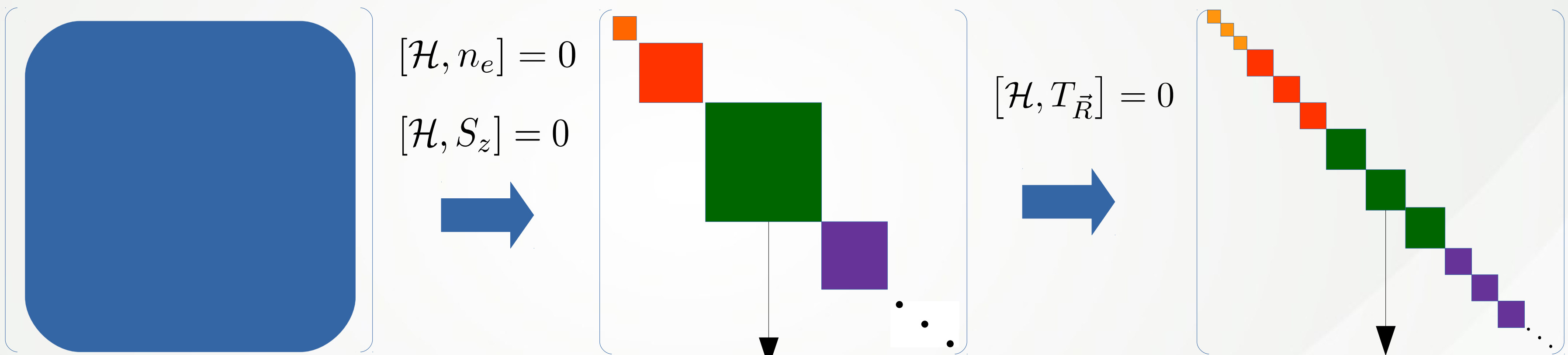
➡ Depends on a variety of factors…

Energy scales
Density
Lattice dimensionality
Lattice geometry
Temperature
…

Exact Diagonalization and why is limited

- Typical Fock state (occupation basis): $|\uparrow\ \uparrow\downarrow\ \downarrow\ \downarrow \dots\rangle$
- How are the thermodynamical properties of the Hubbard model? $\mathcal{Z} = \sum_\alpha e^{-\beta E_\alpha}$
- Physical observables: $\langle \hat{\mathcal{O}} \rangle = \dfrac{\mathrm{Tr}\hat{\mathcal{O}} e^{-\beta \hat{H}}}{\mathcal{Z}}$

$\left[\hat{\mathcal{H}}\right] \equiv$



$4^{N_{sites}} \times 4^{N_{sites}}$

$\left[\binom{N_{sites}}{N_\uparrow}\binom{N_{sites}}{N_\downarrow}\right]^2$

$\sim \left[\binom{N_{sites}}{N_\uparrow}\binom{N_{sites}}{N_\downarrow}\right]^2 \Big/ N_{sites}$

Ex.: $N_{sites} = 12 \rightarrow \sim 10^8$ states

$\sim 2.2\mathrm{Pb}$

Ex.: $N_{sites} = 12$

$N_\uparrow = N_\downarrow = \dfrac{N_{sites}}{2} \rightarrow \sim 10^6$ states

$\sim 5.8\mathrm{Tb}$

Ex.: $N_{sites} = 12$

$N_\uparrow = N_\downarrow = \dfrac{N_{sites}}{2} \rightarrow \sim 71148$ states

$\sim 40.1\mathrm{Gb}$

- Diag. complexity: $\sim O(N^3)$

Is there a way that we can still know $\langle \hat{O} \rangle$ without having to completely solve the quantum system?

- Even in a classical systems this is still a problem… Think of the classical Ising model:

$$\mathcal{H} \equiv -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z \quad ; \quad \sigma_i^z = \pm 1 \quad \Rightarrow \quad \mathcal{Z} = \sum_{\{\alpha\}} e^{-E_{\{\alpha\}}/k_b T}$$

Sum with 2^{N_s} terms!

- ***Motto*** of statistical physics: not all of those configurations are actually relevant

- Configuration α : ocurrence probability→ $p(\alpha) = \underbrace{e^{-E(\alpha)/k_b T}}_{\text{Can be } \ll 1}$: Boltzmann factor

- No need to generate all the configurations… ***Importance sampling***?

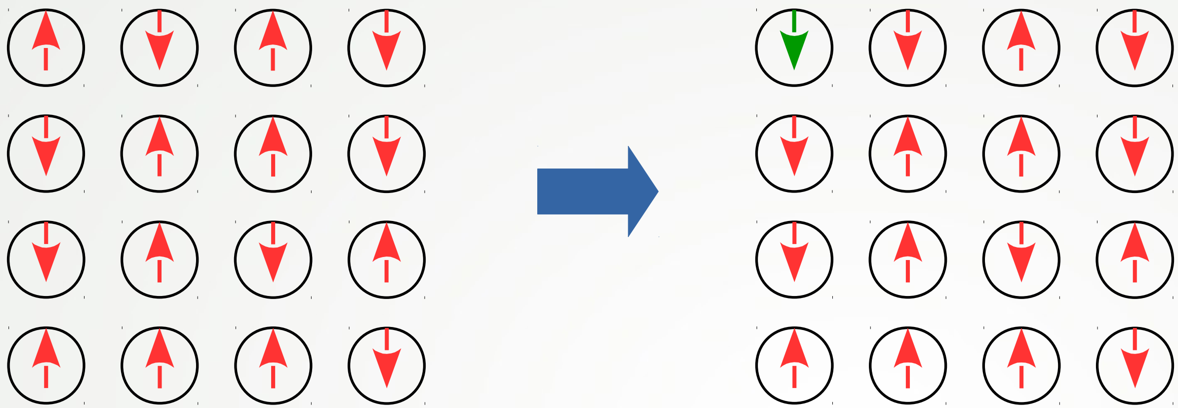
- Start from a random spin configuration $\alpha = |\sigma_1^z \sigma_2^z \ldots \sigma_{N_s}^z\rangle$

- Generate a chain of the most likely configurations (plus fluctuations) by visiting each site of the lattice and attempting a flip

Classical Monte Carlo: Ising model

- Attempting local spin flips

α : α' :



Energy difference between configurations:

$$\Delta E = E(\alpha') - E(\alpha)$$
$$= 2J\sigma_i \sum_{j \in \mathrm{NN\ of}\ i} \sigma_j$$

- Ratio between the correspondent Boltzmann factors: $r \equiv \dfrac{p(\alpha')}{p(\alpha)} = e^{-\Delta E/k_b T}$

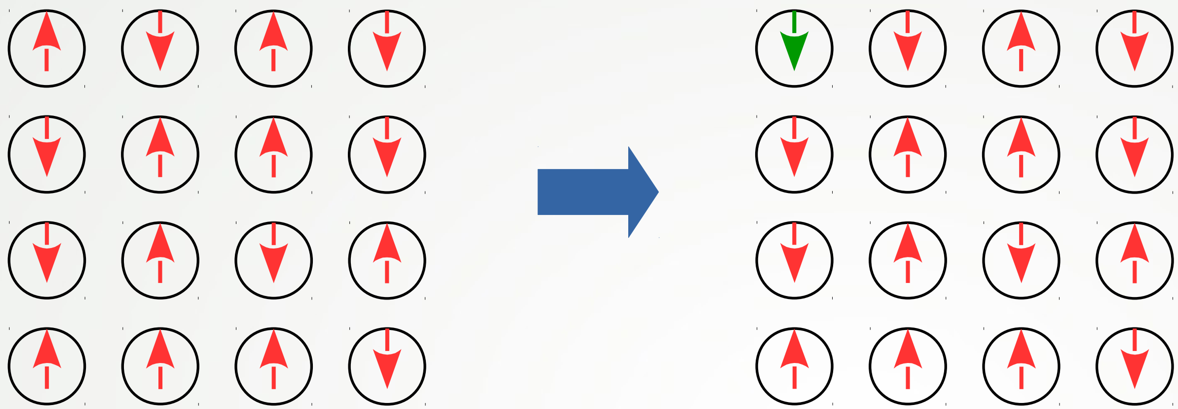
- **Metropolis algorithm:**
  - If $\Delta E < 0$ accept the move
  - If $\Delta E > 0$ accept it with probability $r = e^{-\Delta E/k_b T}$: accounts for fluctuations

- **Heat-bath algorithm:**
  - If $\Delta E < 0$ accept the move
  - If $\Delta E > 0$ accept it with probability $r' = \dfrac{r}{1+r}$

Classical Monte Carlo: Ising model

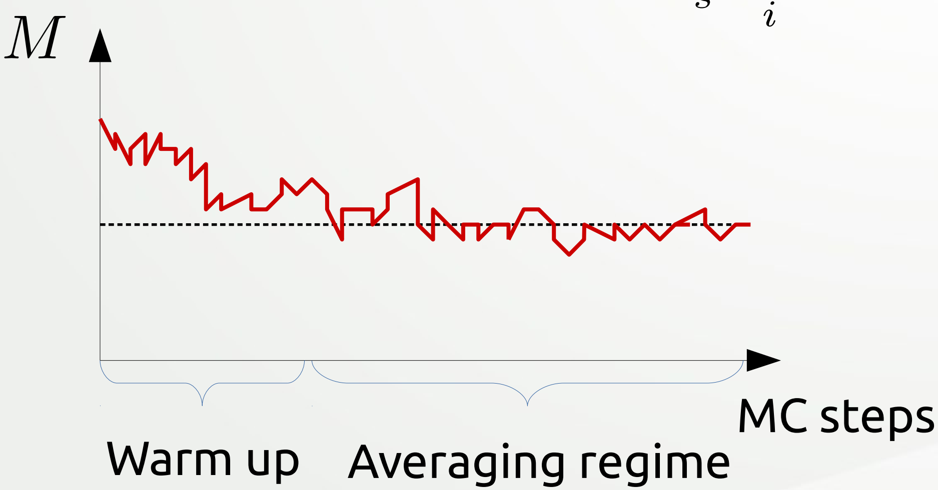
- Attempting local spin flips

α : $\qquad\qquad\qquad$ α' :



- Traversing the whole lattice constitutes a ***sweep*** or one MC step

Observables: $\quad M = \frac{1}{N_s}\sum_i \sigma_i^z$: Magnetization



$$\langle M \rangle = \frac{1}{N_{\text{meas.}}} \sum_{\alpha=1}^{N_{\text{meas.}}} M_\alpha$$

$$\delta M = \sqrt{\frac{\frac{1}{N_{\text{meas.}}}\sum_\alpha^{N_{\text{meas.}}} M_\alpha^2 - \langle M \rangle^2}{N_{\text{meas.}} - 1}}$$

Good… but how about **QUANTUM** Monte Carlo?

- As before, is it possible to devise an ***importance sampling*** mechanism that will prevent us to average over all possible configurations? In this case ***all possible states*** ?

	Classical system:	Quantum system:
Boltzmann factor:	$e^{-\beta E_\alpha}$: number	$e^{-\beta\hat{\mathcal{H}}}$: operator
Partition function:	$\mathcal{Z} = \sum_\alpha e^{-\beta E_\alpha}$	$\mathcal{Z} = \mathrm{Tr}_{\{\vert\alpha\rangle\}} e^{-\beta\hat{\mathcal{H}}} = \sum_{\vert\alpha\rangle} \langle\alpha\vert e^{-\beta\hat{\mathcal{H}}}\vert\alpha\rangle$

- The quantum partition function can be interpreted as a sum of closed path integrals in Hilbert space:
- One term:

$$\langle\alpha|e^{-\beta\hat{\mathcal{H}}}|\alpha\rangle = \sum_{|i_1\rangle,|i_2\rangle,\ldots,|i_{N_t}\rangle} \langle\alpha|e^{-\Delta\tau\hat{\mathcal{H}}}|i_1\rangle\langle i_1|e^{-\Delta\tau\hat{\mathcal{H}}}|i_2\rangle\ldots\langle i_{N_t-1}|e^{-\Delta\tau\hat{\mathcal{H}}}|\alpha\rangle$$

- "Imaginary time": $\beta = it/\hbar$
- Discretized path integral→ small "time" steps: $\Delta\tau = \beta/N_t$
- Discretizing the inverse temperature $\beta = 1/T$

The Suzuki-Trotter aproximation

- Breaking up one body and two body terms in the Hamiltonian… It will be clear why later

- Recall that:

$$e^{\Delta\tau(A+B)} = e^{\Delta\tau A}e^{\Delta\tau B} + \mathcal{O}[(\Delta\tau)^2][A,B]$$

- For the (grand-canonical and particle-hole symmetric) Hubbard Hamiltonian:

$$\hat{\mathcal{H}} = \hat{\mathcal{K}} + \hat{\mathcal{V}}$$

$$\hat{\mathcal{K}} = -t \sum_{\langle i,j\rangle,\sigma} (\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}) - \mu \sum_i (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}) \qquad \hat{\mathcal{V}} = U \sum_i \left(\hat{n}_{i\uparrow} - \frac{1}{2}\right)\left(\hat{n}_{i\downarrow} - \frac{1}{2}\right)$$

- Sum of quadratic and quartic terms of fermionic operators

$$\mathcal{Z} = \mathrm{Tr}_{\{n\}}\left(e^{-\beta(\hat{\mathcal{K}}+\hat{\mathcal{V}})}\right) = \mathrm{Tr}_{\{n\}}\left(\prod_{l=1}^{N_t} e^{-\Delta\tau(\hat{\mathcal{K}}+\hat{\mathcal{V}})}\right) \approx \mathrm{Tr}_{\{n\}}\left(\prod_{l=1}^{N_t} e^{-\Delta\tau\hat{\mathcal{K}}}e^{-\Delta\tau\hat{\mathcal{V}}}\right) + \mathcal{O}[(\Delta\tau)^2]$$

- This approximation is exact in the limit that $\Delta\tau \to 0$ and constitutes **the only single approximation** in determinant quantum Monte Carlo methods.

Integrating out free fermions – quadratic terms

- Suppose we have a Hamiltonian with only quadratic terms in fermionic operators

$$\Rightarrow \hat{\mathcal{H}} = \vec{c}^{\dagger}\,\mathrm{H}\,\vec{c} \quad \text{, where} \quad \vec{c}^{\dagger} = \left[c_1^{\dagger}, c_2^{\dagger}, \ldots, c_{N_s}^{\dagger}\right] \quad \text{and} \quad \vec{c} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_{N_s} \end{bmatrix}$$

$$[\mathrm{H}] \equiv \begin{pmatrix} h_{11} & h_{12} & h_{13} & \cdots \\ h_{21} & h_{22} & h_{23} & \cdots \\ h_{31} & h_{32} & h_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \xrightarrow{\text{Unitary transformation}} [\tilde{\mathrm{H}}] \equiv \begin{pmatrix} \lambda_{k_1} & 0 & 0 & \cdots \\ 0 & \lambda_{k_2} & 0 & \cdots \\ 0 & 0 & \lambda_{k_3} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\mathcal{H} = \vec{\tilde{c}}^{\dagger}\,\mathrm{H}\,\vec{\tilde{c}} = \vec{\tilde{c}}^{\dagger}\,\mathrm{diag}\left(\lambda_{k_1}, \lambda_{k_2}, \ldots \lambda_{k_N}\right)\vec{\tilde{c}} = \sum_{i=1}^{N_s} \lambda_{k_i} n_{k_i}$$

$$\Rightarrow \mathcal{Z}_{\Delta\tau} = \mathrm{Tr}_{\{n\}} e^{-\Delta\tau\mathcal{H}} = \mathrm{Tr}_{\{n\}} e^{\sum_{i=1}^{N_s} \lambda_{k_i} n_{k_i}}$$

- Occupation numbers… for femions: $n_{ki} \in 0 \,\mathrm{or}\, 1$

$$\mathcal{Z}_{\Delta\tau} = \mathrm{Tr}_{\{n\}} e^{-\Delta\tau\mathcal{H}} \overset{!}{=} \prod_{i=1}^{N_s} \left(1 + e^{-\Delta\tau\lambda_{k_i}}\right) = \det(\hat{I} + e^{-\Delta\tau\hat{H}})$$

But the Hubbard Hamiltonian has quartic terms…

$$\hat{\mathcal{V}} \propto \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} = \hat{c}^{\dagger}_{i\uparrow}\hat{c}_{i\uparrow}c^{\dagger}_{j\uparrow}\hat{c}_{j\uparrow}$$

- Hubbard-Stratonovich transformation:
  - The part on the partition function related to this term is:

$$e^{-\Delta\tau\mathcal{V}} = e^{-\Delta\tau U\sum_{i=1}^{N_s}\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)} = \prod_{i=1}^{N_s} e^{-U\Delta\tau\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)}$$

  - Let's take one term of this independent products for site i: $e^{-U\Delta\tau\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)}$

- Is there a transformation that can take this term and make it quadratic in fermion ops.?

$$e^{\frac{1}{2}A^2} \equiv \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\frac{1}{2}x^2 - xA}\,dx$$

: Gaussian integration

- For fermions: $n^2_{i,\sigma} = n_{i,\sigma} = 0 \,\text{or}\, 1$

$$\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right) \overset{!}{=} -\frac{1}{2}\left(n_{i\uparrow}-n_{i\downarrow}\right)^2 + \frac{1}{4}$$

$$e^{-U\Delta\tau\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)} = \frac{e^{\frac{-U\Delta\tau}{4}}}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\frac{1}{2}x^2-\sqrt{U\Delta\tau}\left(n_{i\uparrow}-n_{i\downarrow}\right)x}\,dx$$

Auxiliary field!

$$e^{-U\Delta\tau\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)} = \frac{e^{\frac{-U\Delta\tau}{4}}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{2}x^2-\sqrt{U\Delta\tau}(n_{i\uparrow}-n_{i\downarrow})x} dx \quad U > 0$$

- The repulsive Coulomb interaction has been replaced by a bosonic (scalar) field which couples to the **magnetization** in a given site!

- But what if $U < 0$? → Another transformation…

$$\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right) \overset{!}{=} \frac{1}{2}(n_{i\uparrow}+n_{i\downarrow}-1)^2-\frac{1}{4} \qquad e^{\frac{1}{2}A^2} \equiv \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\frac{1}{2}x^2-xA}dx$$

$$\Rightarrow \quad e^{-U\Delta\tau\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)} = \frac{e^{\frac{-U\Delta\tau}{4}}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{2}x^2-\sqrt{|U|\Delta\tau}(n_{i\uparrow}+n_{i\downarrow}-1)x} dx$$

- The auxiliary field couples to the **charge** at a given site… Physically it creates charge fluctuations in that orbital

- This is all great but having a continuous (scalar field) is still complicated when dealing with actual simulations…

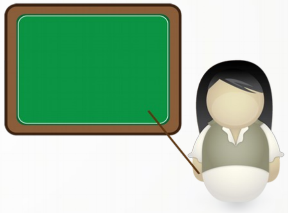
Discrete auxiliary field!

$U > 0$

$$e^{-U\Delta\tau\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)} = \frac{e^{\frac{-U\Delta\tau}{4}}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{2}x^2 - \sqrt{U\Delta\tau}(n_{i\uparrow}-n_{i\downarrow})x} dx$$

$U < 0$

$$e^{-U\Delta\tau\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)} = \frac{e^{\frac{-U\Delta\tau}{4}}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{2}x^2 - \sqrt{|U|\Delta\tau}(n_{i\uparrow}+n_{i\downarrow}-1)x} dx$$



$$e^{-U\Delta\tau\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)} = \frac{e^{\frac{-U\Delta\tau}{4}}}{2} \sum_{x=\pm 1} e^{\alpha x(n_{i\uparrow}-n_{i\downarrow})}$$

Ising-like field!

$$e^{-U\Delta\tau\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)} = \frac{e^{\frac{-|U|\Delta\tau}{4}}}{2} \sum_{x=\pm 1} e^{\alpha x(n_{i\uparrow}+n_{i\downarrow}-1)}$$

$$\cosh\alpha = \exp\left(\Delta\tau|U|/2\right)$$

$$\Bigg($$

Discrete auxiliary field – checking its validity

$U > 0$

$$e^{-U\Delta\tau\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)} = \frac{e^{\frac{-U\Delta\tau}{4}}}{2}\sum_{x=\pm 1} e^{\alpha x(n_{i\uparrow}-n_{i\downarrow})}$$

$$\cosh\alpha = \exp\left(\Delta\tau|U|/2\right)$$

- Possibilities of occupation of a single site:

$\lvert a\rangle$	$\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)$	$(n_{i\uparrow}-n_{i\downarrow})$
$\lvert\,\rangle$	$\frac{1}{4}\lvert\,\rangle$	$0\lvert\,\rangle$
$\lvert\uparrow\rangle$	$-\frac{1}{4}\lvert\uparrow\rangle$	$\lvert\uparrow\rangle$
$\lvert\downarrow\rangle$	$-\frac{1}{4}\lvert\downarrow\rangle$	$\lvert\downarrow\rangle$
$\lvert\uparrow\downarrow\rangle$	$\frac{1}{4}\lvert\uparrow\downarrow\rangle$	$0\lvert\uparrow\downarrow\rangle$

LHS:

$e^{-\frac{U\Delta\tau}{4}}\lvert a\rangle$ if $\lvert a\rangle = \lvert\,\rangle$ or $\lvert\uparrow\downarrow\rangle$

$e^{\frac{U\Delta\tau}{4}}\lvert a\rangle$ if $\lvert a\rangle = \lvert\uparrow\rangle$ or $\lvert\downarrow\rangle$

RHS:

$2\cdot\frac{e^{-\frac{U\Delta\tau}{4}}}{2}\lvert a\rangle$ if $\lvert a\rangle = \lvert\,\rangle$ or $\lvert\uparrow\downarrow\rangle$

$\frac{e^{\frac{-U\Delta\tau}{4}}}{2}\underbrace{(e^{\alpha}+e^{-\alpha})}_{2\cosh(\alpha)}\lvert a\rangle$ if $\lvert a\rangle = \lvert\uparrow\rangle$ or $\lvert\downarrow\rangle$

Few notes:

- There are other forms of discrete Hubbard Stratonovich transformation (HST)
- Some are symmetric in the charge and spin coupling [SU(2) symmetry is always present]

Two fields:

$$e^{-\Delta\tau U n_\uparrow n_\downarrow} = \frac{1}{4} \sum_{\sigma_1,\sigma_2=\pm 1} e^{\lambda\sigma_1(n_\uparrow - n_\downarrow) + i\lambda\sigma_2(n_\uparrow + n_\downarrow)}$$

where: $$\tanh^2 = 1 - \frac{e^{-\Delta\tau U}}{2}$$

Side note: In spite of some early attempts [Phys. Rev. B 42, 2282 (1990)], different HST were not seen to substantially affect the sign problem (more on this later)

$$\Bigg)$$

Let's pick up where we left...

$$e^{-\Delta\tau\mathcal{V}} = e^{-\Delta\tau U\sum_{i=1}^{N_s}\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)} = \prod_{i=1}^{N_s} e^{-U\Delta\tau\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)}$$

Hubbard-Stratonovich tranformation→

$$= \prod_{i=1}^{N_s}\frac{e^{\frac{-U\Delta\tau}{4}}}{2}\sum_{x=\pm1} e^{\alpha x(n_{i\uparrow}-n_{i\downarrow})}$$

$$= \left(\frac{e^{\frac{-U\Delta\tau}{4}}}{2}\right)^{N_s}\mathrm{Tr}_{\{x\}} e^{\sum_{i=1}^{N_s}\alpha x_i(n_{i\uparrow}-n_{i\downarrow})}$$

$$= \left(\frac{e^{\frac{-U\Delta\tau}{4}}}{2}\right)^{N_s}\mathrm{Tr}_{\{x\}} e^{\sum_{i=1}^{N_s}\alpha x_i n_{i\uparrow}} e^{-\sum_{i=1}^{N_s}\alpha x_i n_{i\downarrow}}$$

$$= \left(\frac{e^{\frac{-U\Delta\tau}{4}}}{2}\right)^{N_s}\mathrm{Tr}_{\{x\}} e^{\mathcal{V}_\uparrow} e^{\mathcal{V}_\downarrow}$$

$\mathcal{V}_\sigma = \sigma\sum_{i=1}^{N}\alpha x_i n_{i\sigma}$ is a diagonal matrix

$$[\mathcal{V}_\sigma] \equiv \begin{pmatrix} e^{\sigma\alpha x_1} & & & 0 \\ & e^{\sigma\alpha x_2} & & \\ & & \ddots & \\ 0 & & & e^{\sigma\alpha x_{N_s}} \end{pmatrix}$$

Let's pick up where we left...

- Remember that all this *craziness* was for a given imaginary time slice....

$$\mathcal{Z} \approx \mathrm{Tr}_{\{n\}} \left(\prod_{l=1}^{N_t} e^{-\Delta\tau \hat{\mathcal{K}}} e^{-\Delta\tau \hat{\mathcal{V}}} \right)$$

- So the auxiliary discrete field can be then generalized for different imaginary times $x_i \to x_{i,\tau}$

$$\Rightarrow \quad [\mathcal{V}_\sigma^\tau] \equiv \begin{pmatrix} e^{\sigma\alpha x_{1,\tau}} & & & 0 \\ & e^{\sigma\alpha x_{2,\tau}} & & \\ & & \ddots & \\ 0 & & & e^{\sigma\alpha x_{N_s,\tau}} \end{pmatrix}$$

- Hopping matrix – 1d Hubbard model:

$$K_{ij} = \begin{cases} -t & i,j \text{ nearest neighbors} \\ -\mu & i=j \\ 0 & \text{otherwise} \end{cases} \qquad \mathsf{K}_x = \begin{pmatrix} -\mu & -t & 0 & \cdots & 0 & -t \\ -t & -\mu & -t & \cdots & 0 & 0 \\ 0 & -t & -\mu & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -t & 0 & \cdots & 0 & -t & -\mu \end{pmatrix}$$

- Plugging back everything and changing the order of the traces:

$$\mathcal{Z} = \left(\frac{e^{\frac{-U\Delta\tau}{4}}}{2} \right)^{N_s N_t} \mathrm{Tr}_{\{x\}} \mathrm{Tr}_{\{n\}} \left(\prod_{\tau=1}^{N_t} e^{-\Delta\tau \mathcal{K}_\uparrow} e^{\mathcal{V}_\uparrow^\tau} \right) \left(\prod_{\tau=1}^{N_t} e^{-\Delta\tau \mathcal{K}_\downarrow} e^{\mathcal{V}_\downarrow^\tau} \right)$$

We are almost there!

$$\mathcal{Z} = \left(\frac{e^{\frac{-U\Delta\tau}{4}}}{2}\right)^{N_s N_t} \mathrm{Tr}_{\{x(\tau)\}} \mathrm{Tr}_{\{n\}} \left(\prod_{\tau=1}^{N_t} e^{-\Delta\tau\hat{\mathcal{K}}_\uparrow} e^{\hat{\mathcal{V}}_\uparrow^\tau}\right) \left(\prod_{\tau=1}^{N_t} e^{-\Delta\tau\hat{\mathcal{K}}_\downarrow} e^{\hat{\mathcal{V}}_\downarrow^\tau}\right)$$

- We need to be able to integrate out the fermions… But we know how to do that in the case of quadratic terms in fermionic operators
- In this case with two exponentials:

$$\begin{aligned}\mathrm{Tr}_{\{n\}} e^{-c_i^\dagger A_{ij} c_j} e^{-c_i^\dagger B_{ij} c_j} = \mathrm{Tr}_{\{n\}} e^{-\sum_\nu -c_\nu^\dagger l_\nu c_\nu} = \mathrm{Tr}_{\{n\}} e^{-\sum_\nu n_\nu l_\nu} &= \mathrm{Tr}_{\{n\}} \prod_\nu e^{-n_\nu l_\nu} \\ &= \prod_\nu \left(1 + e^{-l_\nu}\right) \\ &= \det\left(1 + e^{-A} e^{-B}\right)\end{aligned}$$

- For many exponentials:

$$\mathrm{Tr}_{\{n\}} \left(e^{-\hat{\mathcal{H}}_1} e^{-\hat{\mathcal{H}}_2} \cdots e^{-\hat{\mathcal{H}}_{N_t}}\right) = \det\left(\mathsf{I} + e^{-\mathsf{H}_{N_t}} e^{-\mathsf{H}_{N_t-1}} \cdots e^{-\mathsf{H}_1}\right)$$

$$Z_{\{x\}} = \left(\frac{e^{\frac{-U\Delta\tau}{4}}}{2}\right)^{N_s N_t} \mathrm{Tr}_{\{x(\tau)\}} \det\left[\mathsf{M}_\uparrow(\{x(\tau)\})\right] \det\left[\mathsf{M}_\downarrow(\{x(\tau)\})\right]$$

$$\mathsf{M}_\sigma(\{x\}) = \mathsf{I} + \mathsf{B}_{N_t,\sigma}(x_{N_t}) \mathsf{B}_{N_t-1,\sigma}(x_{N_t-1}) \cdots \mathsf{B}_{1,\sigma}(x_1) \qquad \mathsf{B}_{\tau,\sigma}(x_\tau) = e^{\Delta\tau \mathsf{K}} e^{\sigma\alpha \mathsf{V}_\tau^\sigma(x_\tau)}$$

Summary – Physical picture

$$\mathcal{Z} = \mathrm{Tr}_{\{n\}} e^{-\beta \hat{\mathcal{H}}}$$: grand-canonical partition function

[Blankenbecler *et al.*1981]

Suzuki-Trotter decomposition

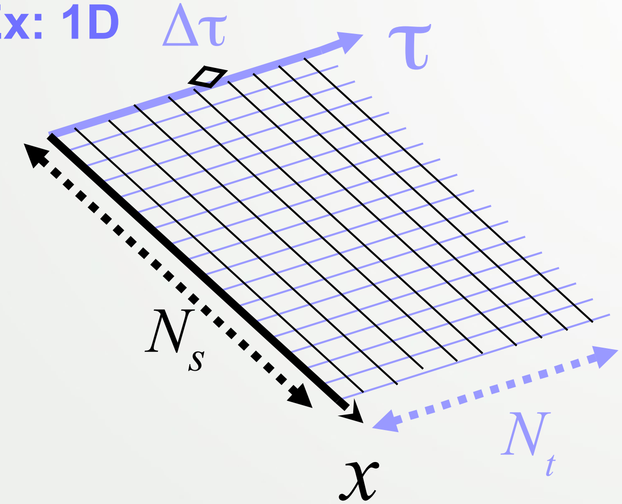
Discretization in β

$$\beta = \Delta\tau N_t$$

$$\mathcal{Z}_{\Delta\tau} \approx \mathrm{Tr}_{\{n\}} \prod_{\tau=1}^{N_t} e^{-\Delta\tau \hat{\mathcal{K}}} e^{-\Delta\tau \hat{\mathcal{V}}}$$

$$\hat{\mathcal{K}} = -t \sum_{\langle i,j\rangle,\sigma} (\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma}) - \mu \sum_i (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow})$$ and $$\hat{\mathcal{V}} = U \sum_i \left(\hat{n}_{i\uparrow} - \frac{1}{2}\right)\left(\hat{n}_{i\downarrow} - \frac{1}{2}\right)$$

Ex: 1D



$0 \leq \tau \leq \beta$

- Hubbard-Stratonovich transformation

$$Z_{\{x\}} = \left(\frac{e^{\frac{-U\Delta\tau}{4}}}{2}\right)^{N_s N_t} \mathrm{Tr}_{\{x(\tau)\}} \det\left[\mathsf{M}_{\uparrow}(\{x(\tau)\})\right] \det\left[\mathsf{M}_{\downarrow}(\{x(\tau)\})\right]$$

- Interacting fermions in D dimensions ➡ Non-interacting fermions coupled to an external **Ising-like** and fluctuating field in (D+1) dimensions

- Field $x_i(\tau)$ is spanned as in an usual classical Monte Carlo Method – ***importance sampling***

Computing things – Green's functions

Central quantity!

$$\langle \hat{c}_{i\sigma}\hat{c}^{\dagger}_{j\sigma}\rangle_{\{x(\tau)\}} = \frac{\mathrm{Tr}_{\{n\}}\hat{c}_{i\sigma}\hat{c}^{\dagger}_{j\sigma}D_{N_t}\dots D_1}{\mathrm{Tr}_{\{n\}}D_{N_t}\dots D_1}$$ where $$D_\tau = \prod_{\sigma=\uparrow,\downarrow}\left(e^{-\Delta\tau\hat{\mathcal{K}}_\sigma}e^{\hat{\mathcal{V}}^\tau_\sigma}\right)$$

- Computing the fermionic trace, one can show that

$$\langle c_{i\sigma}c^{\dagger}_{j\sigma}\rangle_{\{x(\tau)\}} = \left[\frac{1}{1+\mathsf{B}_{N_t,\sigma}\dots\mathsf{B}_{1,\sigma}}\right]_{ij} = G^{\sigma}_{ij} \qquad \mathsf{B}_{\tau,\sigma}(x_\tau) = e^{\Delta\tau\mathsf{K}}e^{\sigma\alpha\mathsf{V}^\sigma_\tau(x_\tau)}$$

- But how about other observables?
  - Density on site i with spin σ

$$\rho_{i,\sigma} = \langle\hat{n}_{i,\sigma}\rangle = \langle\hat{c}^{\dagger}_{i,\sigma}\ \hat{c}_{i,\sigma}\rangle = 1-\langle\hat{c}_{i,\sigma}\hat{c}^{\dagger}_{i,\sigma}\rangle = 1-G^{\sigma}_{ii}$$

  - Total density:

$$\rho = \frac{1}{2N}\sum_{\sigma=\uparrow,\downarrow}\sum_{i=1}^{N}\rho_{i,\sigma} = \frac{1}{2N}\sum_{\sigma=\uparrow,\downarrow}\sum_{i=1}^{N}(1-G^{\sigma}_{ii})$$

Computing things – Green's functions

Central quantity!

$$\langle c_{i\sigma} c^\dagger_{j\sigma} \rangle_{\{x(\tau)\}} = \left[\frac{1}{1 + \mathsf{B}_{N_t,\sigma} \ldots \mathsf{B}_{1,\sigma}} \right]_{ij} = G^\sigma_{ij} \qquad \mathsf{B}_{\tau,\sigma}(x_\tau) = e^{\Delta\tau \mathsf{K}} e^{\sigma\alpha \mathsf{V}^\sigma_\tau(x_\tau)}$$

- Kinetic energy:

$$\langle \hat{\mathcal{K}} \rangle = -t \sum_{\langle i,j \rangle,\sigma} \left(\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma} \right) = +t \sum_{\langle i,j \rangle,\sigma} \left(G^\sigma_{ij} + G^\sigma_{ij} \right)$$

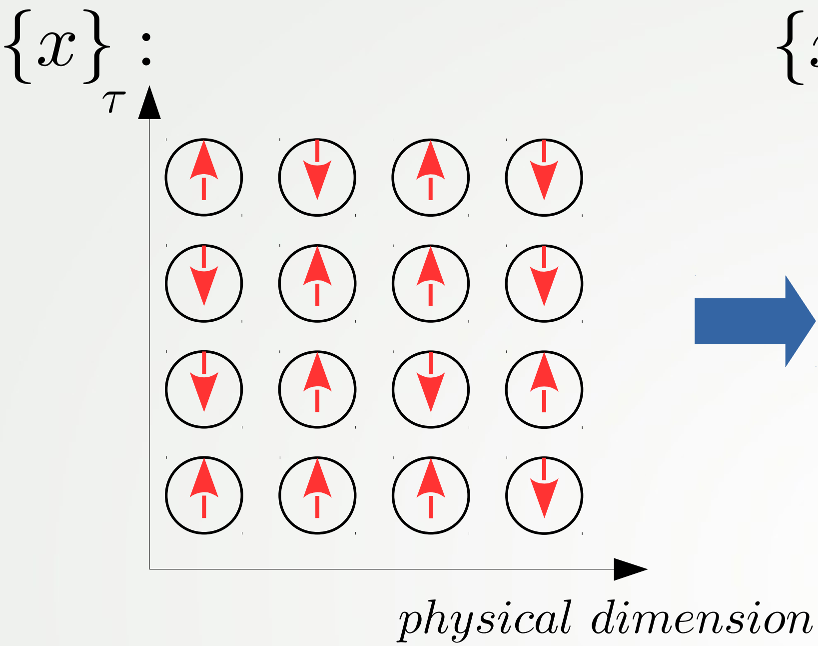
- More complicated ones Wick's theorem:

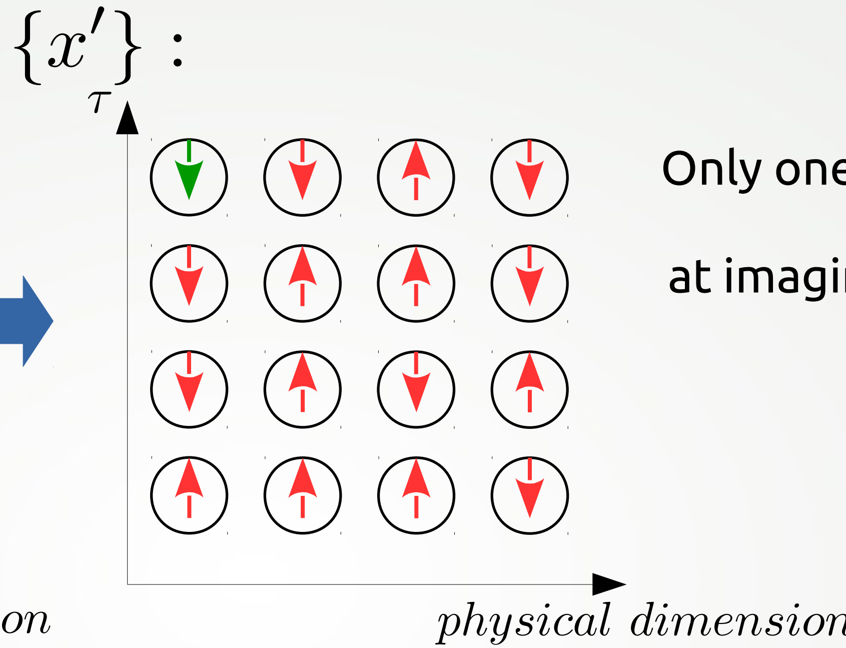
$$\langle c^\dagger_{i_1} c_{i_2} c^\dagger_{i_3} c_{i_4} \rangle_{\{x(\tau)\}} = \langle c^\dagger_{i_1} c_{i_2} \rangle_{\{x(\tau)\}} \langle c^\dagger_{i_3} c_{i_4} \rangle_{\{x(\tau)\}} + \langle c^\dagger_{i_1} c_{i_4} \rangle_{\{x(\tau)\}} \langle c^\dagger_{i_2} c_{i_3} \rangle_{\{x(\tau)\}}$$

- Example – z component of spin-spin correlation:

$$\begin{aligned}
\langle \hat{m}^z_i \hat{m}^z_j \rangle &= \langle (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})(\hat{n}_{j\uparrow} - \hat{n}_{j\downarrow}) \rangle \\
&= \left(1 - G^\uparrow_{ii}\right)\left(1 - G^\uparrow_{jj}\right) + \left(1 - G^\uparrow_{ij}\right) G^\uparrow_{ij} \\
&- \left(1 - G^\uparrow_{ii}\right)\left(1 - G^\downarrow_{jj}\right) - \left(1 - G^\downarrow_{ii}\right)\left(1 - G^\uparrow_{jj}\right) \\
&+ \left(1 - G^\downarrow_{ii}\right)\left(1 - G^\downarrow_{jj}\right) + \left(1 - G^\downarrow_{ij}\right) G^\downarrow_{ij}
\end{aligned}$$

Importance sampling – Metropolis for the scalar field





Only one component of the field
at imaginary-time τ at site i
is updated

- How to accept or reject this move?

- Ratio of “Boltzmann weights”:

$$\mathcal{R} = \mathcal{R}^{\uparrow}\mathcal{R}^{\downarrow} = \frac{\det\left[\mathsf{M}_{\uparrow}(\{x'(\tau)\})\right]\det\left[\mathsf{M}_{\downarrow}(\{x'(\tau)\})\right]}{\det\left[\mathsf{M}_{\uparrow}(\{x(\tau)\})\right]\det\left[\mathsf{M}_{\downarrow}(\{x(\tau)\})\right]}$$

- This seems too expensive… Is there a simple way of computing it?

Importance sampling – Metropolis for the scalar field

$\{x\} \rightarrow \{x'\}$ Only one component of the field at imaginary-time τ at site i is updated

$$[V_\sigma(\tau)] \rightarrow \begin{pmatrix} e^{\sigma\alpha x_{1,\tau}} & & & & 0 \\ & \ddots & & & \\ & & e^{\sigma\alpha x'_{i,\tau}} & & \\ & & & \ddots & \\ 0 & & & & e^{\sigma\alpha x_{N_s,\tau}} \end{pmatrix} = \left(\hat{1} + \Delta^\sigma(\mathrm{i},\tau)\right) \mathrm{V}_\sigma(\tau)$$

where

$$[\Delta_\sigma(i,\tau)] \rightarrow \begin{pmatrix} 0 & & & & 0 \\ & \ddots & & & \\ & & e^{\sigma\alpha(x'_{i,\tau}-x_{i,\tau})} - 1 & & \\ & & & \ddots & \\ 0 & & & & 0 \end{pmatrix}$$

- How does that affect the Green's function?

- Single-particle propagators:

$$\mathrm{B}_{N_t,\sigma}(x_{N_t})\mathrm{B}_{N_t-1,\sigma}(x_{N_t-1})\cdots\mathrm{B}_{1,\sigma}(x_1) \equiv \mathrm{B}^\sigma(\beta,0) = \mathrm{B}^\sigma(\beta,\tau)\mathrm{B}^\sigma(\tau,0)$$

$$\rightarrow \mathrm{B}^\sigma(\beta,\tau)\left(\hat{1} + \Delta^\sigma(\mathrm{i},\tau)\right)\mathrm{B}^\sigma(\tau,0)$$

Importance sampling – Metropolis for the scalar field

$\{x\} \to \{x'\}$ Only one component of the field at imaginary-time τ at site i is updated

Spin-dependent ratio of Boltzmann weights:

$$\mathcal{R}^\sigma = \frac{\det\left[1 + \mathsf{B}^\sigma(\beta,\tau)((1+\Delta^\sigma(i,\tau))\mathsf{B}^\sigma(\tau,0)\right]}{\det\left[1+\mathsf{B}^\sigma(\beta,0)\right]}$$

$$= \frac{\det\left[1 + \mathsf{B}^\sigma(\beta,0) + \mathsf{B}^\sigma(\beta,\tau)\Delta^\sigma(i,\tau)\mathsf{B}^\sigma(\tau,0)\right]}{\det\left[1+\mathsf{B}^\sigma(\beta,0)\right]}$$

$$= \det\left[1 + (1+\mathsf{B}^\sigma(\beta,0))^{-1}\mathsf{B}^\sigma(\beta,\tau)\Delta^\sigma(i,\tau)\mathsf{B}^\sigma(\tau,0)\right]$$

$$= \det\left[1 + \Delta^\sigma(\mathsf{i},\tau)\mathsf{B}^\sigma(\tau,0)(1+\mathsf{B}^\sigma(\beta,0))^{-1}\mathsf{B}^\sigma(\beta,\tau)\right]$$

$$= \det\left[1 + \Delta^\sigma(\mathsf{i},\tau)(1 - \mathsf{G}^\sigma(\tau,\tau))\right]$$

- Since the matrix Δ^σ has only one non-zero element, one can show that

$$\mathcal{R} = \mathcal{R}^\uparrow\mathcal{R}^\downarrow = \prod_{\sigma=\uparrow,\downarrow}\left(1 + \Delta^\sigma_{ii}(i,\tau)\left(1 - G^\sigma_{ii}(\tau,\tau)\right)\right)$$

Just a scalar!

Updating the Green's functions

$\{x\} \to \{x'\}$ Only one component of the field at imaginary-time τ at site i is updated

- Note, however, that although we know how to compute the acceptance ratio, the Green's functions would require to compute an inverse for every new field configuration...

$$\mathsf{G}^\sigma(\tau,\tau) = [1 + \mathsf{B}^\sigma(\tau,0)\mathsf{B}^\sigma(\beta,\tau)]^{-1}$$

$\longrightarrow \mathcal{O}(N^3)$ process (very expensive...)

- Is there a cheaper (exact) way to promote the update?

Let's take a single "time"-slice and define:

$$\mathsf{G} \equiv \mathsf{M}^{-1}$$

Let M_1 and M_2 such that they differ by a single diagonal element at position i

$$\mathsf{M}_1 = \mathbb{I} + \mathsf{F}\mathsf{V}_1 \text{ and } \mathsf{M}_2 = \mathbb{I} + \mathsf{F}\mathsf{V}_2, \text{ with } \mathsf{F} = e^{\Delta\tau \mathsf{K}}$$

Updating the Green's functions

$$\mathsf{V}_1{}^{-1}\mathsf{V}_2 = \mathbb{I} + \delta_i \mathsf{e}_i \mathsf{e}_i^{\mathsf{T}}$$

where, $\mathsf{e}_i = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$ → "i-th" position

$$\Rightarrow \quad \delta_i = \frac{\mathsf{V}_2{}^{ii}}{\mathsf{V}_1{}^{ii}} - 1 = e^{\sigma\alpha(x'_{i\tau} - x_{i\tau})} - 1$$

Note that,

$$\begin{aligned}
\mathsf{M}_2 &= \mathbb{I} + \mathsf{F}\mathsf{V}_2 \\
&= \mathbb{I} + \mathsf{F}\mathsf{V}_1 + \mathsf{F}\mathsf{V}_1(\mathsf{V}_1{}^{-1}\mathsf{V}_2 - \mathbb{I}) \\
&= \mathsf{M}_1 + (\mathsf{M}_1 - \mathbb{I})(\cancel{\mathbb{I}} + \delta_i \mathsf{e}_i \mathsf{e}_i^{\mathsf{T}} - \cancel{\mathbb{I}}) \\
&= \mathsf{M}_1 - \delta_i(\mathsf{M}_1 - \mathbb{I})\mathsf{e}_i \mathsf{e}_i^{\mathsf{T}} \\
&= \mathsf{M}_1 \left[\mathbb{I} + \delta_i(\mathbb{I} - \mathsf{M}_1{}^{-1})\mathsf{e}_i \mathsf{e}_i^{\mathsf{T}}\right]
\end{aligned}$$

But we need the inverse of these matrices to obtain the Green's functions:

$$\mathsf{M}_2{}^{-1} = \left[\mathbb{I} + \delta_i(\mathbb{I} - \mathsf{M}_1{}^{-1})\mathsf{e}_i \mathsf{e}_i^{\mathsf{T}}\right]^{-1} \mathsf{M}_1{}^{-1}$$

Updating the Green's functions

- Sherman-Morrison-Woodbury formula come to the rescue!

$$(A+UV^T)^{-1} = A^{-1} - A^{-1}(I+V^T A^{-1} U)^{-1} U^T A^{-1}$$

$$\begin{aligned} \mathsf{M_2}^{-1} &= \left[\mathbb{I} + \delta_i(\mathbb{I} - \mathsf{M_1}^{-1})\mathsf{e}_i\mathsf{e}_i^{\mathsf{T}}\right]^{-1} \mathsf{M_1}^{-1} \\ &= \{\mathbb{I} - \underbrace{[\mathbb{I} + \mathsf{e}_i\mathsf{e}_i^{\mathsf{T}}\delta_i(\mathbb{I} - \mathsf{M_1}^{-1})]^{-1}}_{R_\sigma^{-1}}\delta_i(\mathbb{I} - \mathsf{M_1}^{-1})^{\mathsf{T}}\}\mathsf{M_1}^{-1} \end{aligned}$$

$$\Rightarrow \quad \mathsf{M_2}^{-1} = \mathsf{M_1}^{-1} - \frac{\delta_i}{R_i^\sigma}(1 - \mathsf{M_1}^{-1})^{\mathsf{T}}\mathsf{e}_i\mathsf{e}_i^{\mathsf{T}}\mathsf{M_1}^{-1}$$

$$\Rightarrow \quad \mathsf{G}' = \mathsf{G} - \frac{\delta_i}{R_i^\sigma}(1 - \mathsf{G})^{\mathsf{T}} G_{ii} \quad \Rightarrow \quad \mathcal{O}(N^2) \text{ procedure!}$$

Cake recipe – how to perform simulations

- Establish parameters: $t, U, \mu, \beta = 1/T, \Delta\tau$
- Start the auxiliary Ising-like field randomly $\{x\}_{\rightarrow}$ $x_{i,\tau} = \pm 1$
- Monte Carlo loop (warms + measurement sweeps)
  - Site $(i,\tau) = (1,1)$
  - Loop in space-"time" lattice (i,τ) (*double* loop)
    - Propose field update: $x_{i,\tau} \rightarrow -x_{i,\tau} : \{x'\}$
    - Compute Metropolis ratio – ratio of Boltzmann weights

$$\mathcal{R}_{i,\tau} = \prod_{\sigma=\uparrow,\downarrow} \left(1 + \Delta^{\sigma}_{ii}(i,\tau)\left(1 - G^{\sigma}_{ii}(\tau,\tau)\right)\right)$$

    - Acceptance-rejection: Throw a random number $r \in [0,1]$

      if $r \leq \mathcal{R}_{i,\tau}$ accept the move $\{x\} \rightarrow \{x'\}$ $\rightarrow$ Update the Green's functions

      if $r > \mathcal{R}_{i,\tau}$ reject the move
    - **if** number of loops in imaginary-time is above a certain threshold perform measurements (combinations of Green's functions elements)

Sign problem – life is not that "easy"

- Some configurations of the imaginary time may result in a negative Boltzmann weight...

$$Z_{\{x\}} = \left(\frac{e^{\frac{-U\Delta\tau}{4}}}{2}\right)^{N_s N_t} \mathrm{Tr}_{\{x(\tau)\}} \underbrace{\det\left[\mathrm{M}_{\uparrow}(\{x(\tau)\})\right] \det\left[\mathrm{M}_{\downarrow}(\{x(\tau)\})\right]}$$

Should always be positive to be interpreted as a Boltzmann weight

- In fact one can introduce a measure of when this is positive

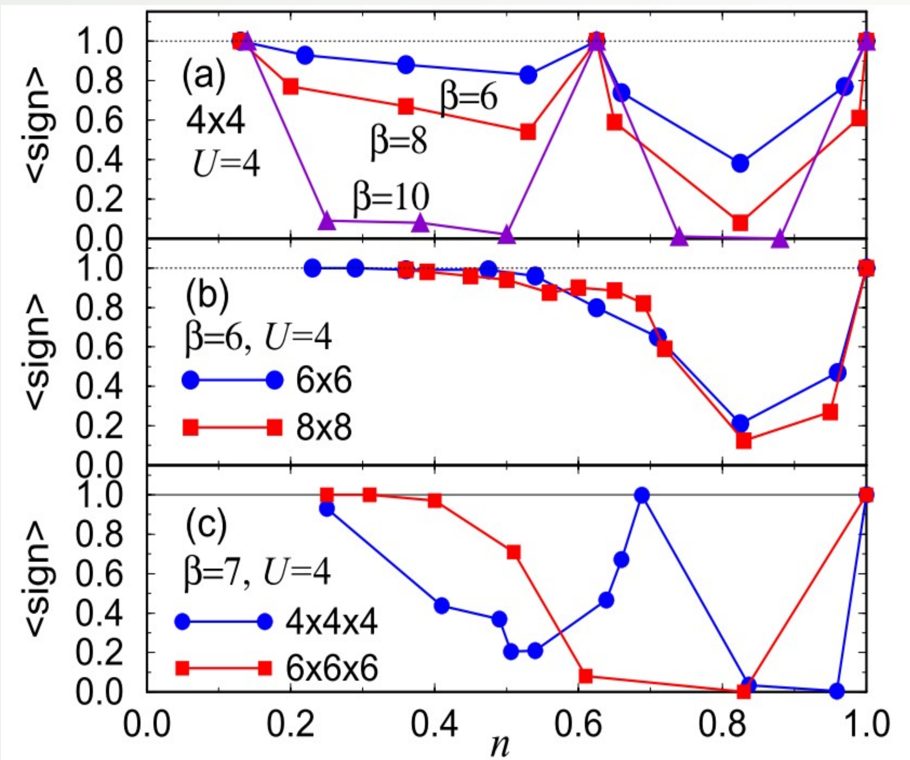
$$Z_{\{x\}} \equiv \sum_x p(x) \quad \Rightarrow \quad p(x) \equiv s(x)|p(x)| \qquad s(x) = \pm 1$$

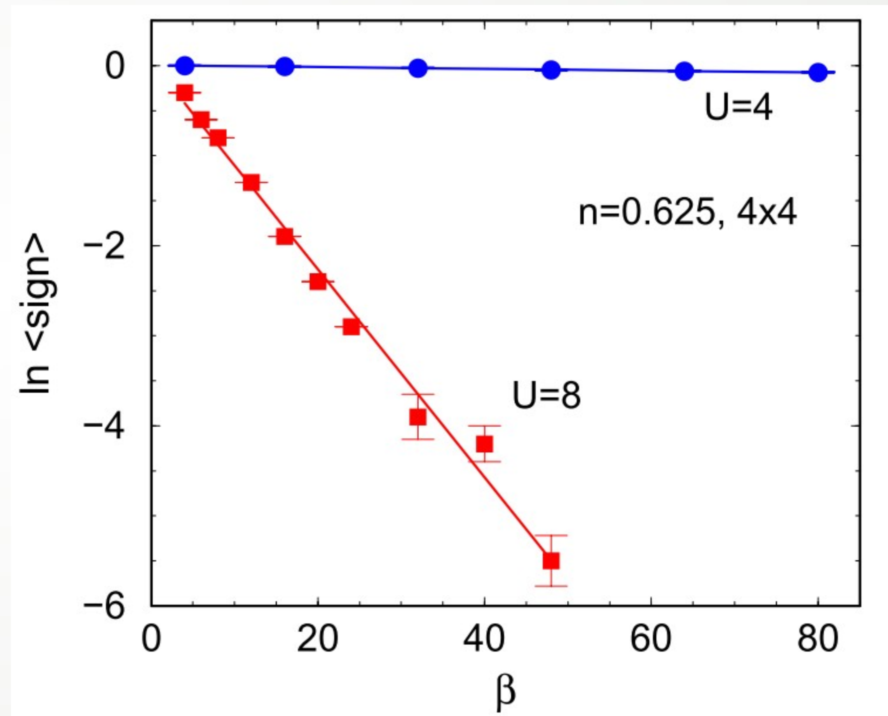
$$\begin{aligned}
\langle \hat{A} \rangle &= \frac{\sum_x A(x)p(x)}{\sum_x p(x)} = \frac{\sum_x A(x)|p(x)|s(x)}{\sum_x |p(x)|s(x)} \\
&= \frac{\left[\sum_x A(x)|p(x)|s(x)\right] / \sum_x |p(x)|}{\left[\sum_x |p(x)|s(x)\right] / \sum_x |p(x)|} \\
&= \frac{\sum_x p'(x)[s(x)A(x)]}{\sum_x p'(x)[s(x)]} \equiv \frac{\langle sA \rangle_{p'}}{\langle s \rangle_{p'}}
\end{aligned}$$

Sign problem – life is not that "easy"

- Dependence of the sign with parameters...

$$\langle sign \rangle = \frac{\sum_{\{x\}} \det[\mathrm{M}_\uparrow(\{x(\tau)\})] \det[\mathrm{M}_\downarrow(\{x(\tau)\})]}{\sum_{\{x\}} |\det[\mathrm{M}_\uparrow(\{x(\tau)\})] \det[\mathrm{M}_\downarrow(\{x(\tau)\})]|}$$





At half-filling there is no sign problem

$$\mu = 0 \rightarrow \rho = 1$$

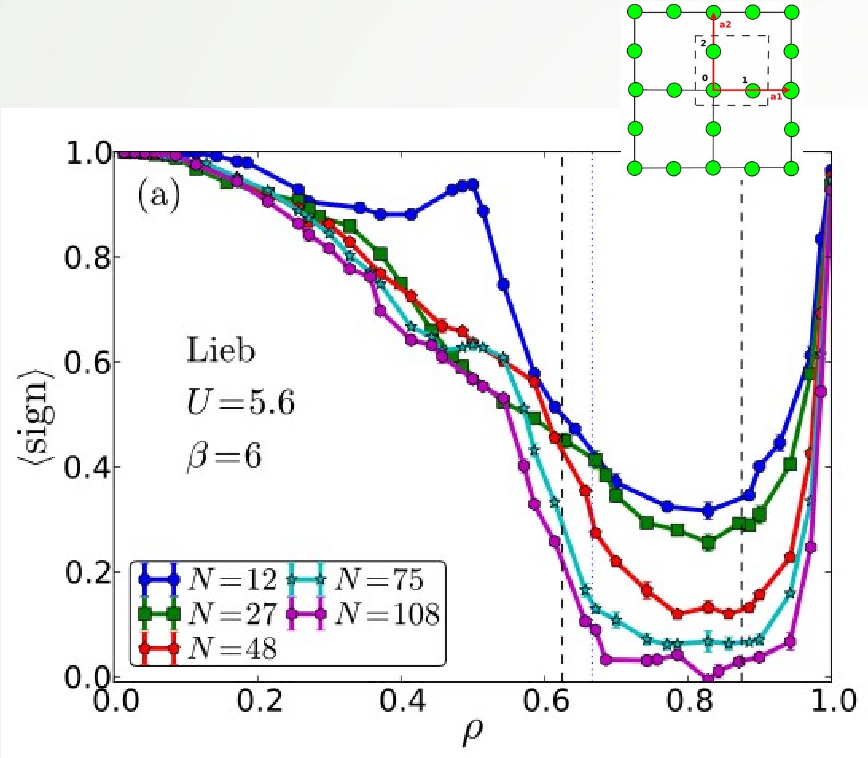
$$\det \mathrm{M}^\uparrow \cdot \det \mathrm{M}^\downarrow > 0$$

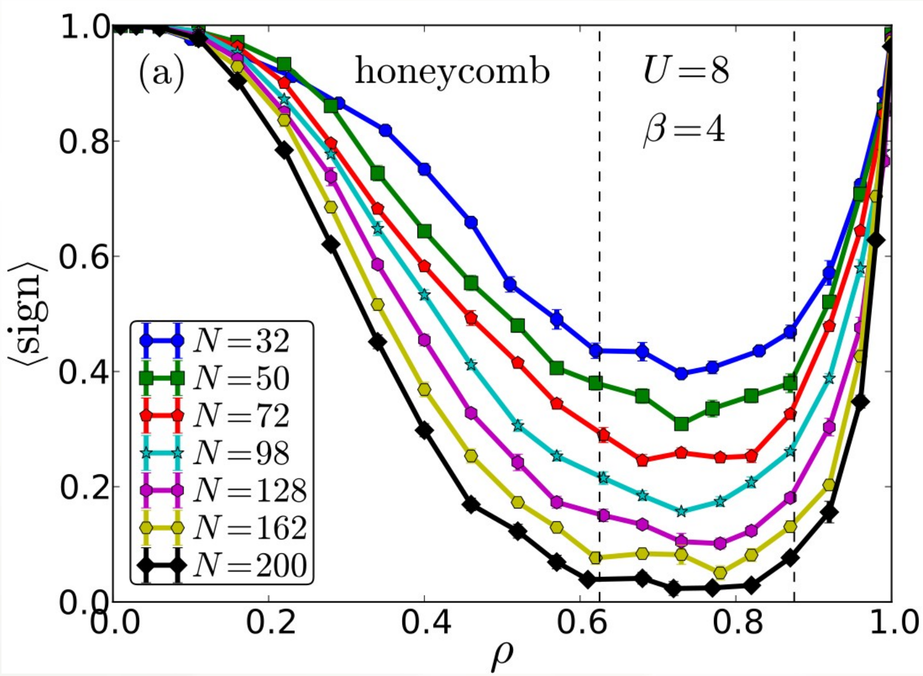
$$\langle \mathrm{sign} \rangle \sim e^{-\beta N U \gamma}$$

$$\gamma = \gamma(n)$$

Sign problem – life is not that “easy”

- Other types of lattices



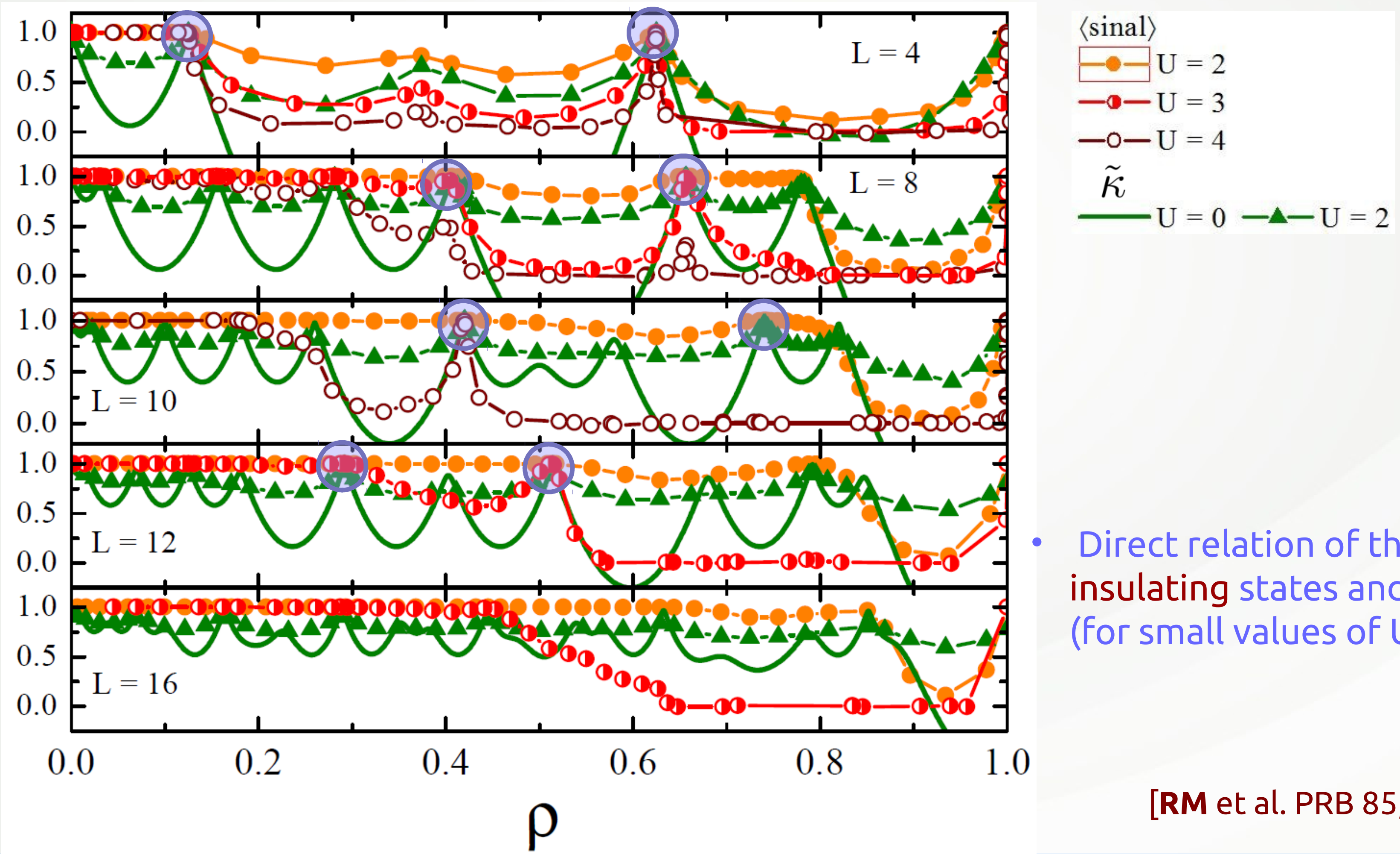


[Iglovikov et al. PRB 92, 045110 (2015)]

Sign problem – life is not that “easy”

- Defining: $\boxed{\tilde{\kappa} \equiv 1 - \rho^2 \kappa}$
- Pseudo-insulating states $\kappa \approx 0$ ➡ $\tilde{\kappa} \approx 1$

- Closed-shell (U=0) and the sign problem



- Direct relation of the pseudo-insulating states and the sign (for small values of U)

[**RM** et al. PRB 85, 125127 (2012)]

Technical Issues: Stabilization

- Round-off errors associated with matrix manipulations
- Product of matrices $\boldsymbol{B}_l$ could be ill-behaved
- It has a mix of scales which are exponentially diverging and exponentially decaying

$$\frac{\lambda_{\max}}{\lambda_{\min}} \propto e^{c' \beta U}$$

- Partial products of the B matrices can be performed by decomposing the matrix in a UDV form, or in a singular-value decomposition scheme (SVD)

This step is fundamental!

$$\mathbf{UDV} = \begin{pmatrix} x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{pmatrix} \begin{pmatrix} X & & & \\ & X & & \\ & & X & \\ & & & x \end{pmatrix} \begin{pmatrix} x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{pmatrix}$$
$$= \begin{pmatrix} X & X & X & X \\ X & X & X & X \\ X & X & X & X \\ X & X & X & X \end{pmatrix}.$$

- Small scales can never be recovered

Technical Issues: Stabilization

- Round-off errors associated with matrix manipulations
- Product of matrices $\boldsymbol{B}_l$ could be ill-behaved
- It has a mix of scales which are exponentially diverging and exponentially decaying

$$\frac{\lambda_{\max}}{\lambda_{\min}} \propto e^{c'\beta U}$$

- Partial products of the B matrices can be performed by decomposing the matrix, or in a singular-value decomposition scheme (SVD)

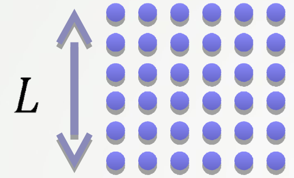
This step is fundamental!

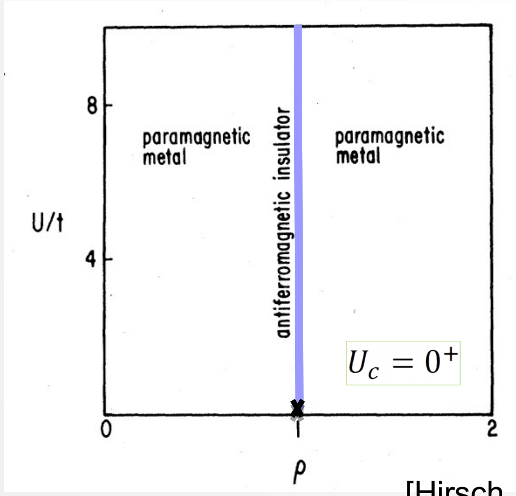
$$\begin{aligned}
\mathbf{B}(\tau+\tau_0,0) &= \mathbf{B}(\tau+\tau_0,\tau)\mathbf{UDV} = (\mathbf{B}(\tau+\tau_0,\tau)\mathbf{UD})\mathbf{V} \\
&= \left(\mathbf{B}(\tau+\tau_0,\tau)\mathbf{U} \begin{pmatrix} X & & & \\ & X & & \\ & & x & \\ & & & x \end{pmatrix} \right) \mathbf{V} \\
&= \begin{pmatrix} X & X & x & x \\ X & X & x & x \\ X & X & x & x \\ X & X & x & x \end{pmatrix} \mathbf{V} \\
&= (\mathbf{U'D'V'})\mathbf{V} = \mathbf{U'D'}(\mathbf{V'V}),
\end{aligned}$$

Famous results

- **Phase diagrams obtained with DQMC**

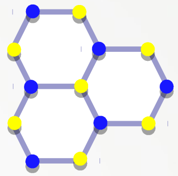
- Square lattice

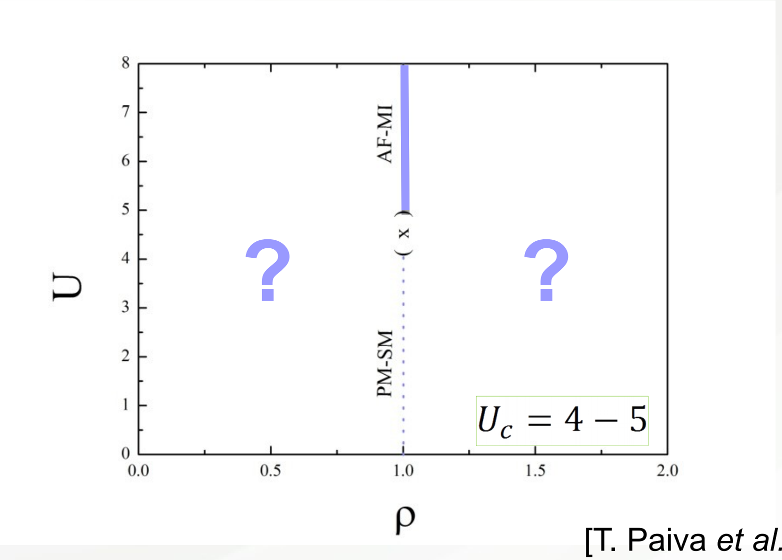




[Hirsch 1985]

- Honeycomb lattice



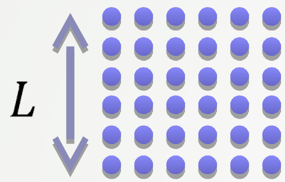


[T. Paiva *et al.*2005]

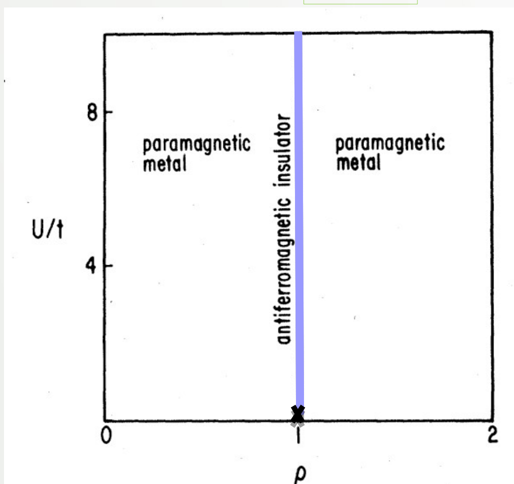
- Away from half-filling is very hard to get low-temperature results due to the sign problem

Famous results

- **Square lattice**



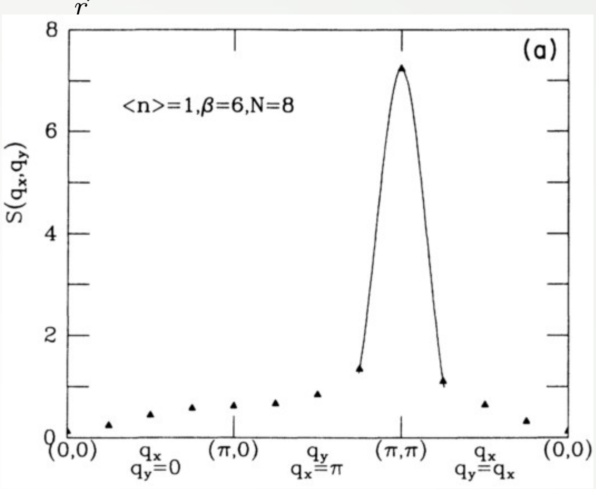
$U_c = 0^+$



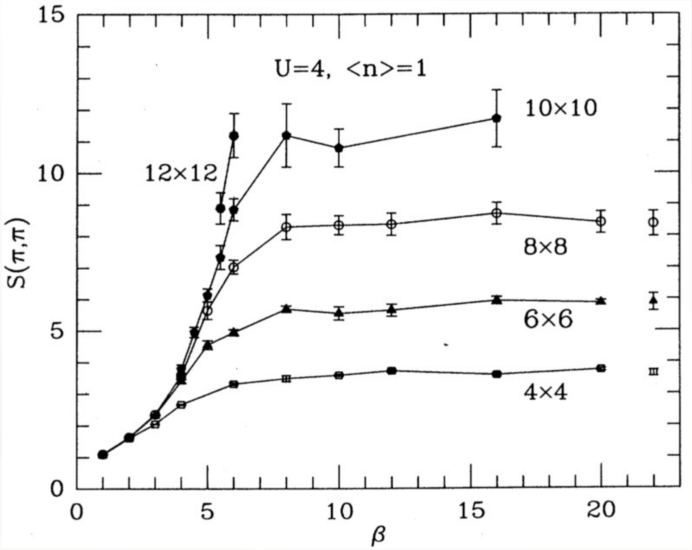
[Hirsch, PRB 31, 4403 1985]

- Structure factor

$$S(\vec{q}) = \frac{1}{N}\sum_{\vec{r}} e^{i\vec{q}\cdot\vec{r}} \left(n_{i\uparrow} - n_{i\downarrow}\right)\left(n_{i+\vec{r},\uparrow} - n_{i+\vec{r},\downarrow}\right)$$



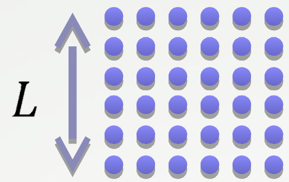
[Moreo et al. PRB 41 2313, 1990]



[White et al. PRB 40 506, 1989]

Famous results

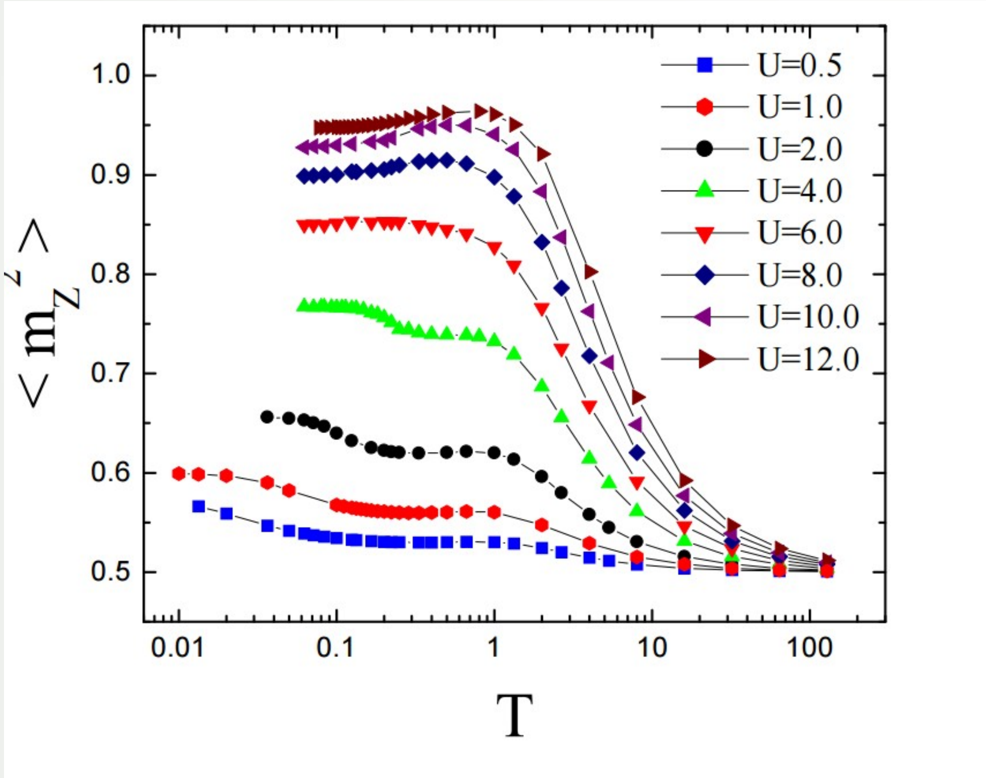
- Square lattice

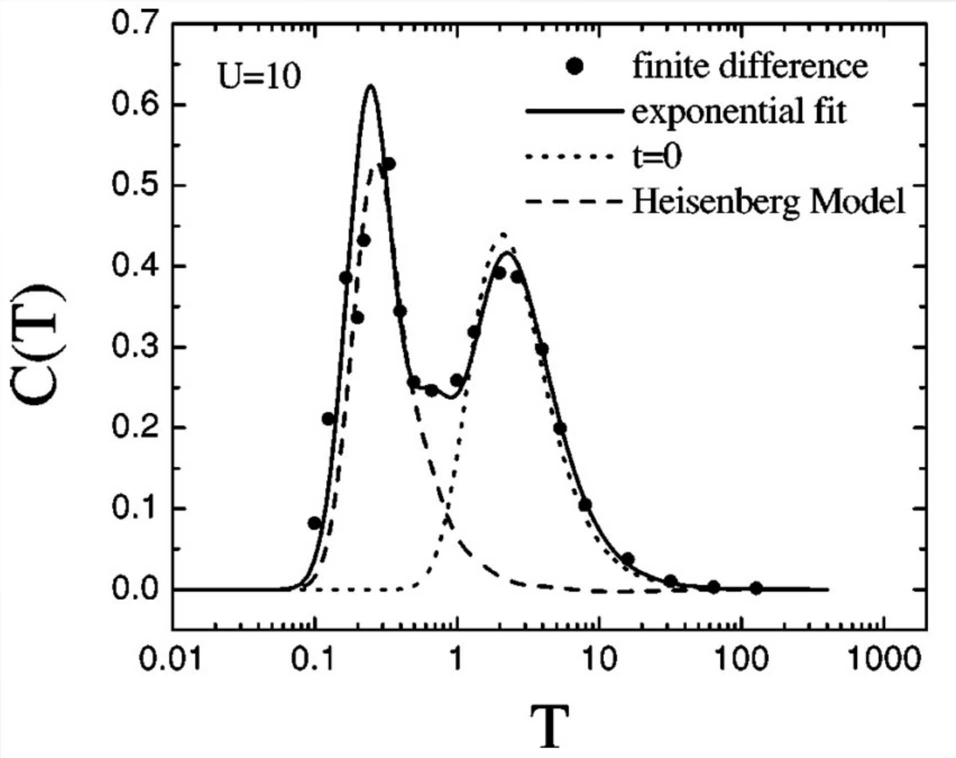


$$\langle m_z^2 \rangle = \langle (n_{i\uparrow} - n_{i\downarrow})^2 \rangle$$

$$E_e(T) = E(0) + \sum_{l=1}^{M} c_l e^{-\beta l \Delta}$$

$$C(T) = \frac{dE(T)}{dT}$$



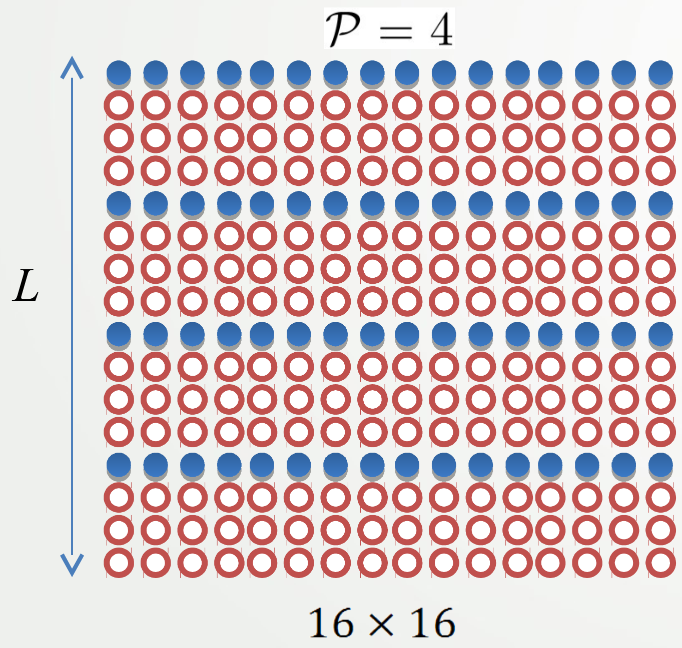


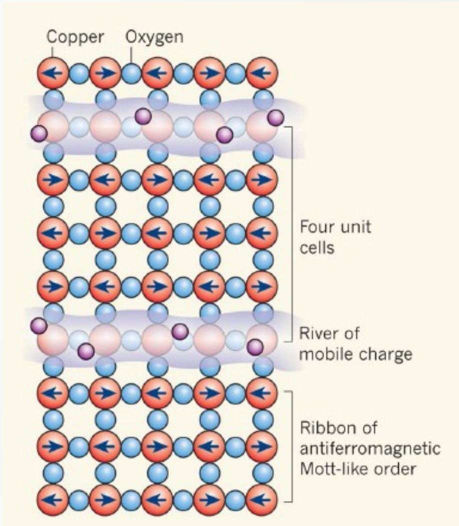
Not so famous results – stripes and SC fluctuations

- **2D** repulsive Hubbard Hamiltonian

$$\hat{\mathcal{H}} = -t \sum_{\langle \mathbf{i}\,\mathbf{j}\rangle\,\sigma} (c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + c^{\dagger}_{\mathbf{j}\sigma} c_{\mathbf{i}\sigma}) + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} - \mu \sum_{\mathbf{i}} (n_{\mathbf{i}\uparrow} + n_{\mathbf{i}\downarrow}) + V_0 \sum_{i_y \in \mathcal{P}} (n_{\mathbf{i}\uparrow} + n_{\mathbf{i}\downarrow})$$

- Formation of hole rich stripe regions ⟹ increasing the onsite energy in certain rows
- Instead of being **spontaneous**, the striped formation is **induced**



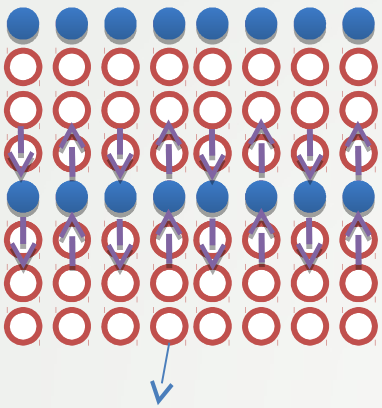


[K.A. Moler Nature **468**, 643–644 (2010)]

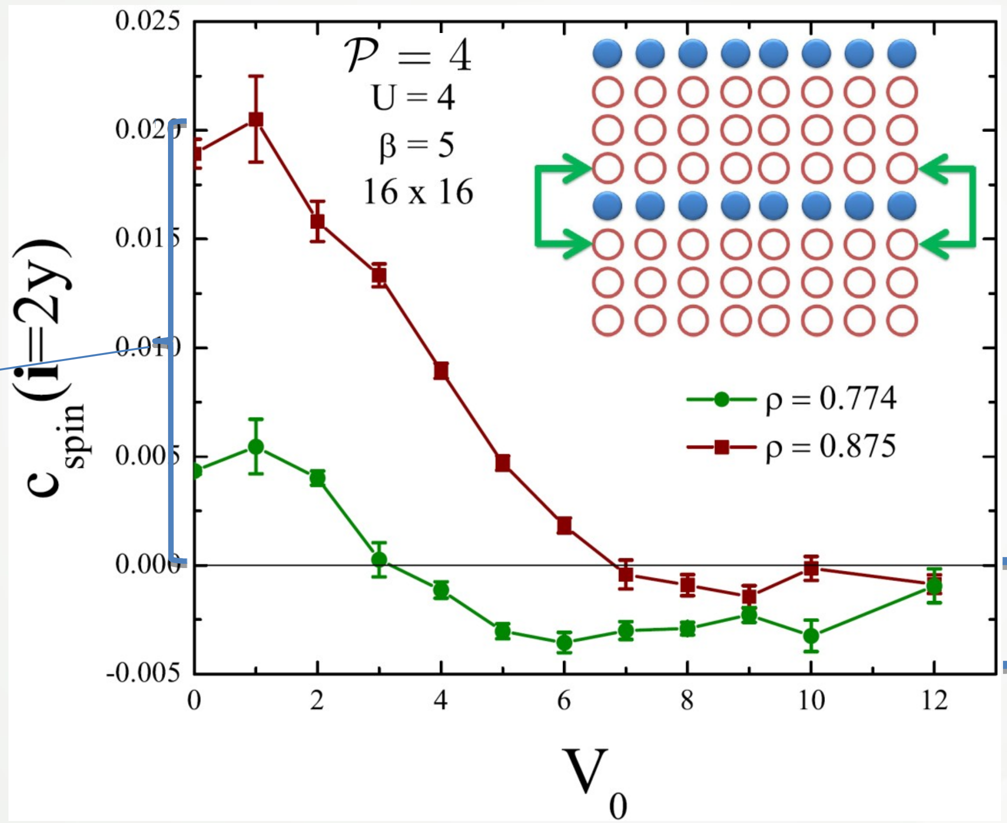
- Simulations using **DQMC** performed in the underdoped regime: $\left\{ \begin{array}{l} \rho = 0.774 \\ \rho = 0.875 \end{array} \right.$

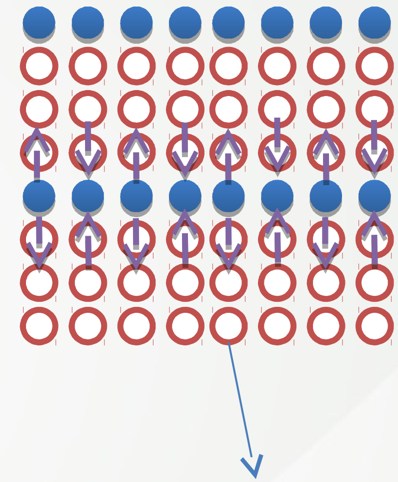
Not so famous results – stripes and SC fluctuations

$$\boxed{c_{spin}(\mathbf{i}) \equiv \langle m^z_{\mathbf{j}+\mathbf{i}} m^z_{\mathbf{i}} \rangle}$$



- absence of phase shift





- π - phase shift

- As experimentally observed

Not so famous results – stripes and SC fluctuations

Pair formation

- d-wave pair creation operator: $\Delta^{\dagger}_{d\,\mathbf{j}} = c^{\dagger}_{\mathbf{j}\uparrow}(c^{\dagger}_{\mathbf{j}+\hat{x}\downarrow} - c^{\dagger}_{\mathbf{j}+\hat{y}\downarrow} + c^{\dagger}_{\mathbf{j}-\hat{x}\downarrow} - c^{\dagger}_{\mathbf{j}-\hat{y}\downarrow})$
- d-wave pair corr. function: $c_{d\,\mathrm{pair}}(\mathbf{i}) = \langle \Delta_{d\,\mathbf{j}+\mathbf{i}} \Delta^{\dagger}_{d\,\mathbf{j}} \rangle$
  - Pair-field susceptibility

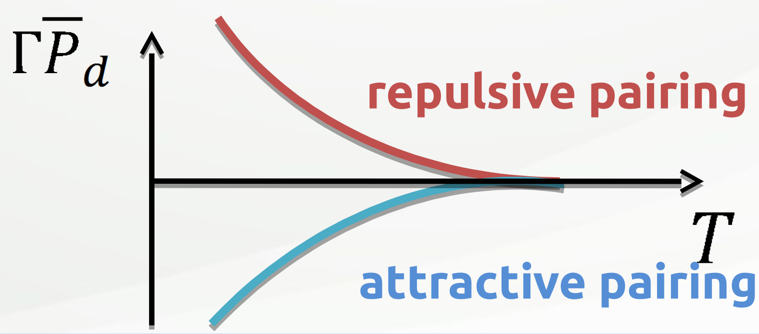
$$P_d = \frac{1}{N}\sum_{\mathbf{j}}\int_0^{\beta} d\tau \langle \Delta_{d\mathbf{j}+\mathbf{i}}(\tau)\, \Delta^{\dagger}_{d\mathbf{j}}(0)\rangle$$

  - Uncorrelated pair-field susceptibility

$$\overline{P_d} = \frac{1}{N}\sum_{\mathbf{j}}\int_0^{\beta} d\tau \langle \Delta_{d\mathbf{j}+\mathbf{i}}(\tau)\rangle \langle \Delta^{\dagger}_{d\mathbf{j}}(0)\rangle$$

- Interaction vertex:

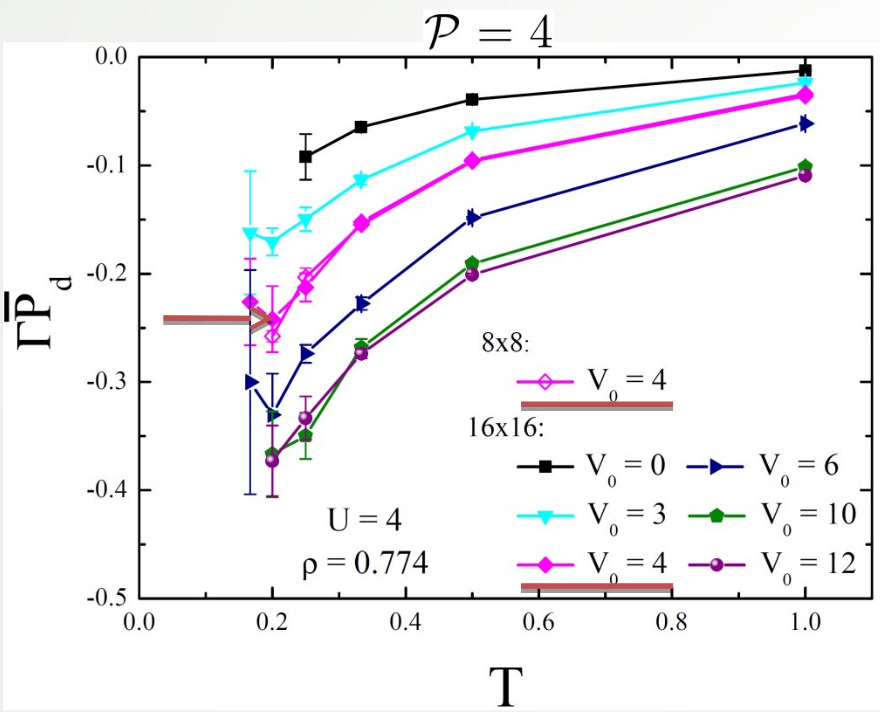
$$\Gamma_d = \frac{1}{P_d} - \frac{1}{\overline{P_d}} \Longrightarrow P_d = \frac{\overline{P}_d}{1+\Gamma_d \overline{P}_d} \Longrightarrow \underbrace{\Gamma_d \overline{P}_d \to -1}_{\text{SC instability}}$$

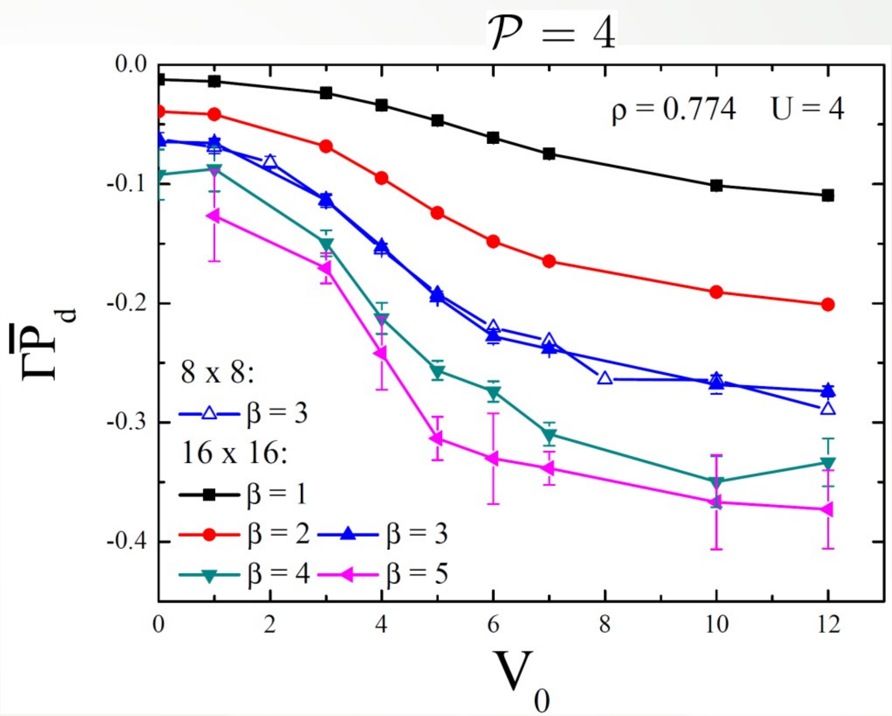


Not so famous results – stripes and SC fluctuations

❑ **Pair formation –** $\rho = 0.774$

- Sign problem prevents direct establishment of T_c
- The observed trend indicates that stripe formation favors **SC**





- Small finite size effects
- Charge domains (by increasing V_0) enhance the ***d*** -wave pairing

Summary – Physical picture

Suzuki-Trotter decomposition

$$\mathcal{Z} = \mathrm{Tr}_{\{n\}} e^{-\beta \hat{\mathcal{H}}}$$: grand-canonical partition function

[Blankenbecler *et al.*1981]

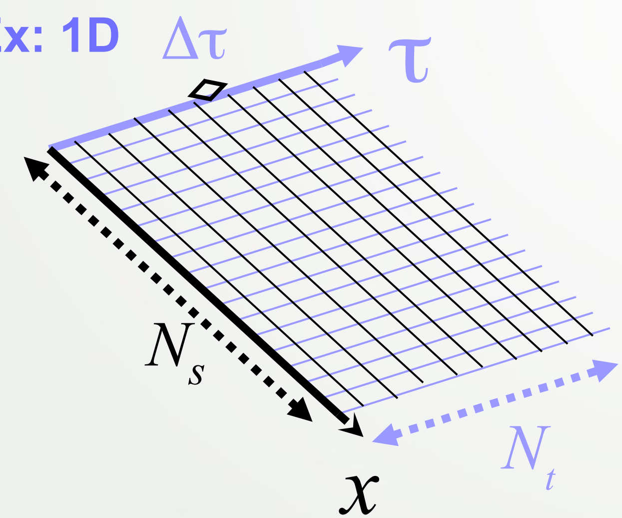
Discretization in β

$$\beta = \Delta\tau N_t$$

$$\mathcal{Z}_{\Delta\tau} \approx \mathrm{Tr}_{\{n\}} \prod_{\tau=1}^{N_t} e^{-\Delta\tau \hat{\mathcal{K}}} e^{-\Delta\tau \hat{\mathcal{V}}}$$

$$\hat{\mathcal{K}} = -t \sum_{\langle i,j \rangle,\sigma} (\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma}) - \mu \sum_i (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow})$$ and $$\hat{\mathcal{V}} = U \sum_i \left(\hat{n}_{i\uparrow} - \frac{1}{2}\right)\left(\hat{n}_{i\downarrow} - \frac{1}{2}\right)$$

Ex: 1D



$0 \leq \tau \leq \beta$

- Hubbard-Stratonovich transformation

$$Z_{\{x\}} = \left(\frac{e^{\frac{-U\Delta\tau}{4}}}{2}\right)^{N_s N_t} \mathrm{Tr}_{\{x(\tau)\}} \det\left[\mathrm{M}_{\uparrow}(\{x(\tau)\})\right] \det\left[\mathrm{M}_{\downarrow}(\{x(\tau)\})\right]$$

- Interacting fermions in D dimensions → Non-interacting fermions coupled to an external **Ising-like** and fluctuating field in (D+1) dimensions

- Field $x_i(\tau)$ is spanned as in an usual classical Monte Carlo Method – ***importance sampling***

Are there more QMC methods?

YES! Many more…

One simple variation is the **Projector QMC** which tackles the GS directly

Rationale:

$$\mathcal{Z} = \mathrm{Tr}_{\{n\}} e^{-\beta\hat{\mathcal{H}}} = \sum_{|\psi\rangle} \langle\psi|e^{-\beta\hat{\mathcal{H}}}|\psi\rangle$$

- Sum in all closed paths in imaginary time at a given temperature $\beta = 1/k_B T$

- If β is really large, one may argue that the boundary condition in imaginary time becomes unimportant

$$\mathcal{Z} = \langle\psi_{\mathrm{L}}|e^{-\beta\hat{\mathcal{H}}}|\psi_{\mathrm{R}}\rangle$$

- Who are now the endpoints $|\psi_{\mathrm{L}}\rangle$ and $|\psi_{\mathrm{R}}\rangle$?

- Let’s do it in a more appropriate form

Basic formulation - PQMC

- Suppose one is interested in computing an observable $\mathcal{O}$ of a given Hamiltonian $\hat{\mathcal{H}}$

$$\langle \mathcal{O} \rangle = \frac{\langle \Psi_0 | \mathcal{O} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = \lim_{\Theta \to \infty} \frac{\langle \Psi_T | e^{-\Theta \hat{\mathcal{H}}} \mathcal{O} e^{-\Theta \hat{\mathcal{H}}} | \Psi_T \rangle}{\langle \Psi_T | e^{-2\Theta \hat{\mathcal{H}}} | \Psi_T \rangle}$$

  - $|\psi_T\rangle$ Is a trial wave functions that gets projected out if the parameter Θ is large
  - If the projection parameter is large enough, we can take the endpoints to be equal

- $|\Psi_T\rangle$ can be the the ground-state of the non-interacting part of the Hamiltonian, the mean-field solution of the problem, etc.. In reality, what matters is how fast the GS is approached with the smallest possible number of steps

State can be written as: $|\Psi_R\rangle = |\Psi_R^\uparrow\rangle |\Psi_R^\downarrow\rangle$

where

$$\begin{aligned} |\Psi_R^\sigma\rangle &= (P_{11} c_{1\sigma}^\dagger + P_{21} c_{2\sigma}^\dagger + \cdots + P_{N1} c_{N\sigma}^\dagger) \\ &= (P_{12} c_{1\sigma}^\dagger + P_{22} c_{2\sigma}^\dagger + \cdots + P_{N2} c_{N\sigma}^\dagger) \\ &\cdots \\ &= (P_{1N_\sigma} c_{1\sigma}^\dagger + P_{2N_\sigma} c_{2\sigma}^\dagger + \cdots + P_{NN_\sigma} c_{N\sigma}^\dagger)|0\rangle \end{aligned}$$

P's are coefficients of the many body-state in the single-particle basis, for example.

PQMC method

In matrix form:

$$\mathsf{P}_R^\sigma = \begin{pmatrix} P_{11} & P_{12} & P_{13} & \cdots & P_{1N_\sigma} \\ P_{21} & P_{22} & P_{23} & \cdots & P_{2N_\sigma} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ P_{N1} & P_{N2} & P_{N3} & \cdots & P_{NN_\sigma} \end{pmatrix} \qquad \text{and} \qquad \mathsf{P}_L^\sigma = (\mathsf{P}_R^\sigma)^\dagger$$

Finally, the partitition function can be written as:

$$\mathcal{Z} = \mathrm{Tr}_{\{x\}} \left(\mathsf{P}_L^\uparrow \mathsf{B}^\uparrow(\beta, 0) \mathsf{P}_R^\uparrow \right) \left(\mathsf{P}_L^\downarrow \mathsf{B}^\downarrow(\beta, 0) \mathsf{P}_R^\downarrow \right)$$

$\mathsf{B}^\sigma(\beta, 0)$ Is the single particle propagator (as before)

$$\mathsf{B}^\sigma(\tau, \tau - \Delta\tau) \approx \mathsf{A}^\sigma(\tau) \exp(\Delta\tau \mathsf{K})$$

But yet, we don’t know how to compute the central quantity, the Green’s functions…

PQMC method – computing Green's functions

- Computing Green's function matrix element (for a given configuration x of the imaginary-time field):

$$G^{\sigma}_{ij;x}(\tau) = \langle c_{i\sigma}(\tau)c^{\dagger}_{j\sigma}(\tau)\rangle_x = \delta_{ij} - \langle c^{\dagger}_{j\sigma}(\tau)c_{i\sigma}(\tau)\rangle_x$$

with

$$\langle c^{\dagger}_{j\sigma}(\tau)c_{i\sigma}(\tau)\rangle_x = \langle \Psi^{\sigma}_T|\mathsf{B}^{\sigma}(\beta,\tau)c^{\dagger}_{j\sigma}c_{i\sigma}B^{\sigma}(\tau,0)|\Psi^{\sigma}_T\rangle/p[x]$$

Let's define the probability of a given configuration x of the imaginary-time field as

$$p_h[x] = \det(\mathsf{P}^{\sigma}_{\mathrm{L}}\mathsf{B}^{\sigma}(\beta,\tau)e^{h\mathsf{O}}\mathsf{B}^{\sigma}(\tau,0)\mathsf{P}^{\sigma}_{\mathrm{R}})\det(\mathsf{P}^{\sigma}_{\mathrm{L}}{}'\mathsf{B}^{\sigma}{}'(\beta,\tau)\mathsf{B}^{\sigma}{}'(\tau,0)\mathsf{P}^{\sigma}_{\mathrm{R}}{}')$$

We have introduced a source term which will be taken to zero in the following and O has a single nonzero element $O_{ji} = 1$

- Using the definitions $\mathsf{L}^{\sigma}(\tau) = \mathsf{P}^{\sigma}_{\mathrm{L}}\mathsf{B}^{\sigma}(\beta,\tau)$ and $\mathsf{R}^{\sigma}(\tau) = \mathsf{B}^{\sigma}(\tau,0)\mathsf{P}^{\sigma}_{\mathrm{R}}$

The expectation value becomes:

$$\begin{aligned}\langle c^{\dagger}_{j\sigma}(\tau)c_{i\sigma(\tau)}\rangle &= \frac{\partial}{\partial h}\ln p_h[x]|_{h=0} = \mathrm{Tr}\frac{\partial}{\partial h}\ln(\mathsf{L}^{\sigma}e^{h\mathsf{O}}\mathsf{R}^{\sigma})]|_{h=0} \\ &= \mathrm{Tr}(\mathsf{L}^{\sigma}\mathsf{R}^{\sigma})^{-1}\mathsf{L}^{\sigma}\mathsf{O}\mathsf{R}^{\sigma} = \left(\mathsf{R}^{\sigma}(\mathsf{L}^{\sigma}\mathsf{R}^{\sigma})^{-1}\mathsf{L}^{\sigma}\right)_{ij}\end{aligned}$$

PQMC method – computing Green's functions

Finally, the Green's functions at equal times can be written as:

$$\mathsf{G}^{\sigma}(\tau,\tau) = \mathsf{I} - \mathsf{R}^{\sigma}(\tau)(\mathsf{L}^{\sigma}(\tau)\mathsf{R}^{\sigma}(\tau))^{-1}\mathsf{L}^{\sigma}(\tau)$$

- Once the Green's functions are obtained, the previous formalism essentially works in the same way.

- Even the updates are similar, and one has to focus in how the observables approach an equilibrium value once the projection parameter is increased

PQMC method – some basic results

- Convergence of quantities with the projection parameter

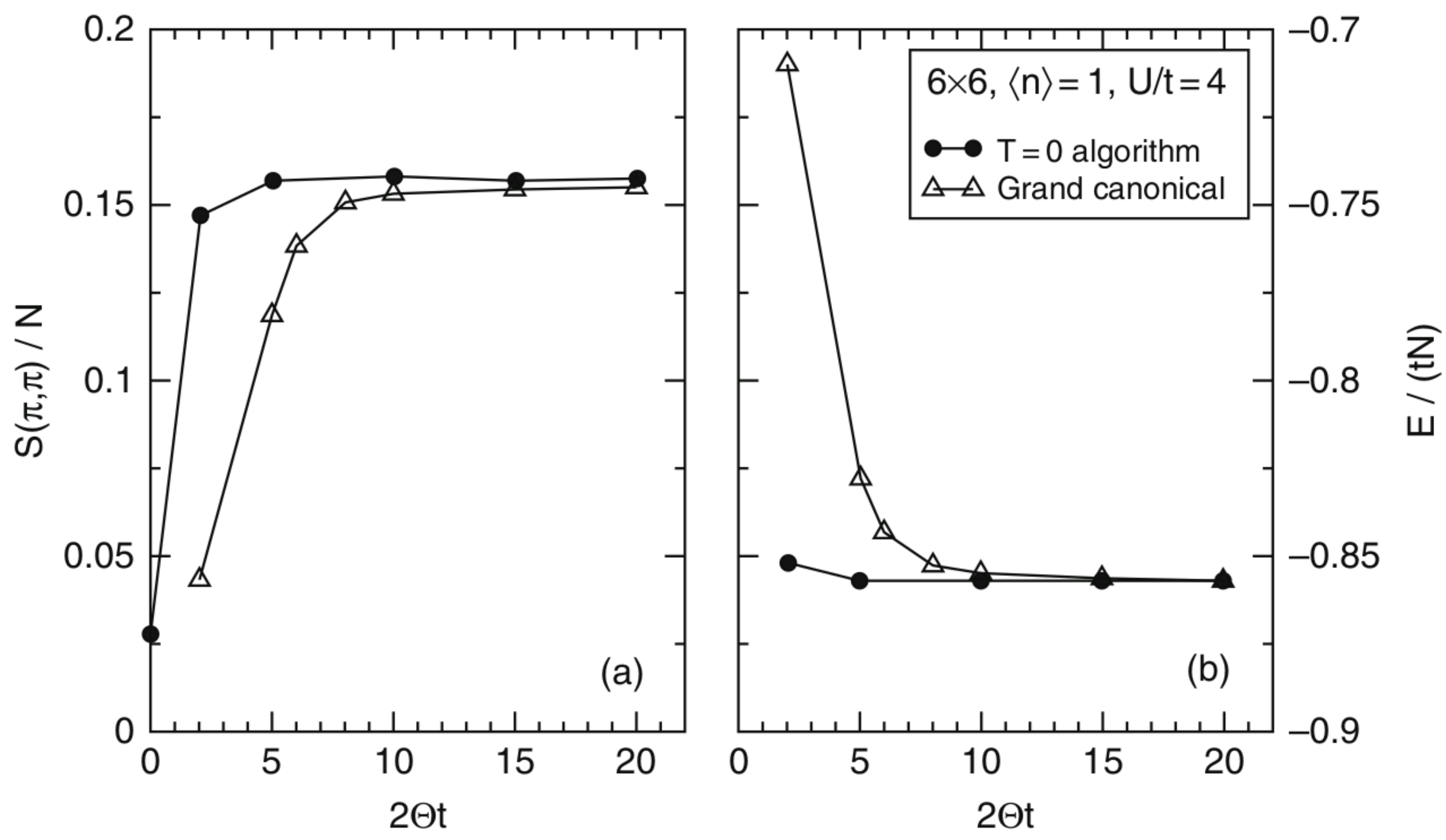
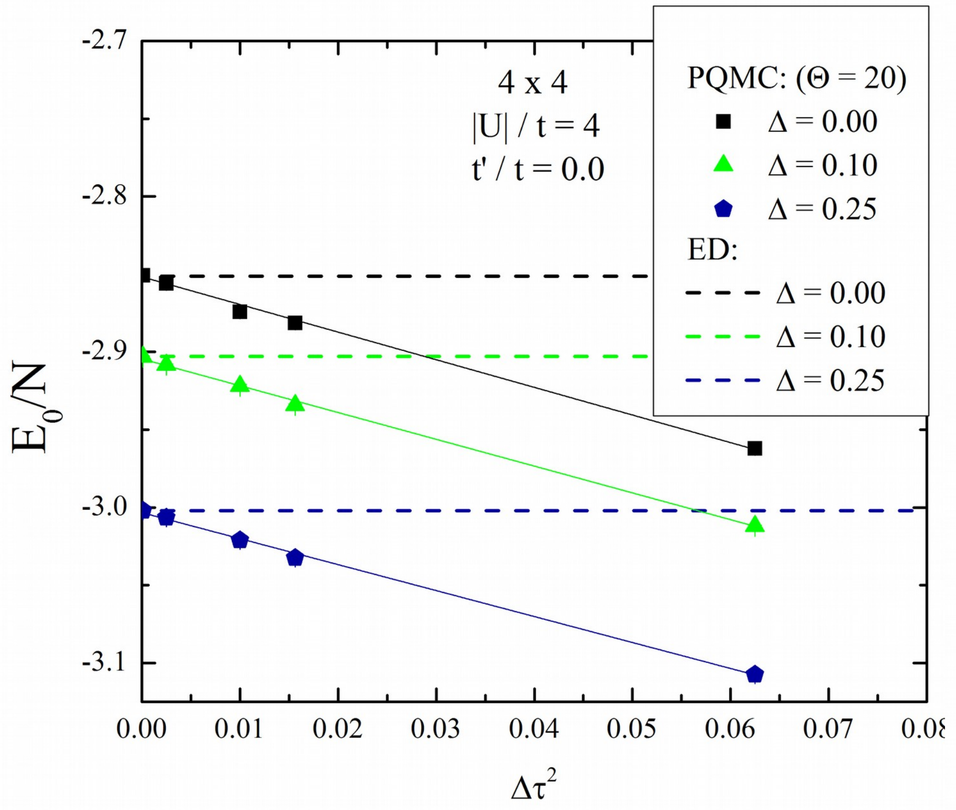
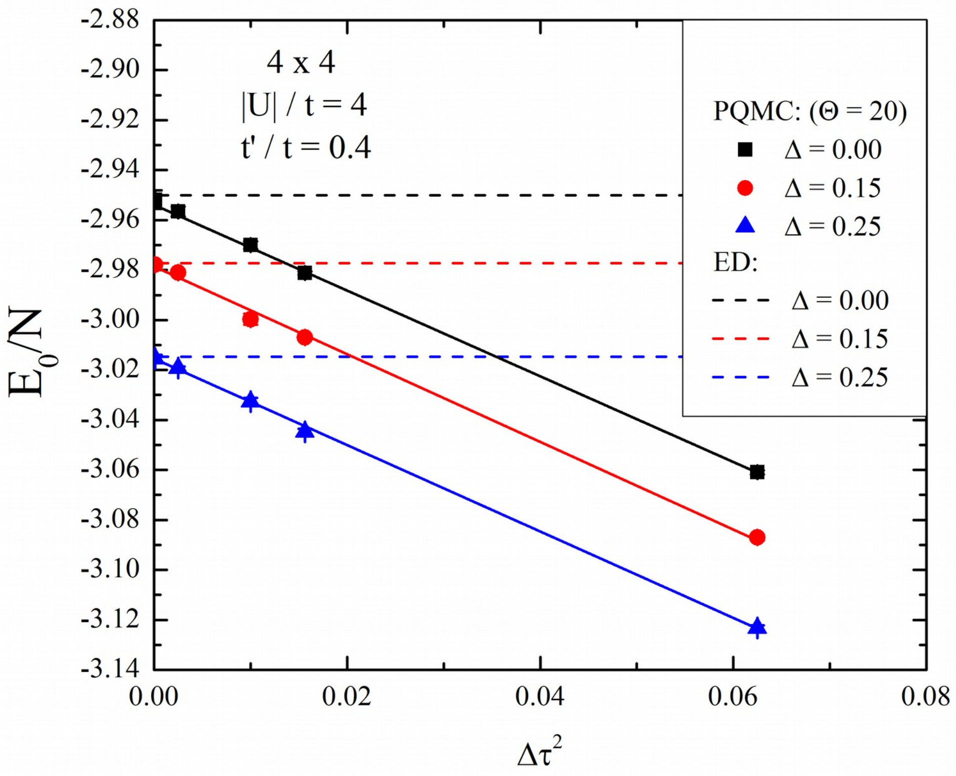


Fig. 10.15. Fourier transform of the spin-spin correlation functions at $\boldsymbol{Q} = (\pi, \pi)$ (**a**) and energy (**b**) for the half-filled Hubbard model (10.90). •: PQMC algorithm. △: FTQMC algorithm at $\beta = 2\Theta$

PQMC method – some basic results

- Convergence of quantities with the projection parameter
- Attractive Hubard model with NNN hopping and staggered potential





Summary

- Interacting fermionic problem in a lattice can be solved either in finite or zero temperature if special conditions are met.

- Sign problem appears in many classes of fermionic problems and there is no simple solution to it.

- In some special classes of Hamiltonian, one can circumvent the sign problem by working on a different basis, called the Majorana basis. → These results were obtained recently by Tsinghua researchers!

- This is just a small and simplified introduction to the method of QMC for the case of auxiliary fields… There are many more “QMC” methods as the

- Wordline algorithm
- Stochastic Series Expansions
- Stochastic Green’s functions
- etc.

That’s all folks!