Intro to auxiliary field Quantum Monte Carlo methods

Rubem Mondaini

Beijing Computational Science Research Center

CSRC

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

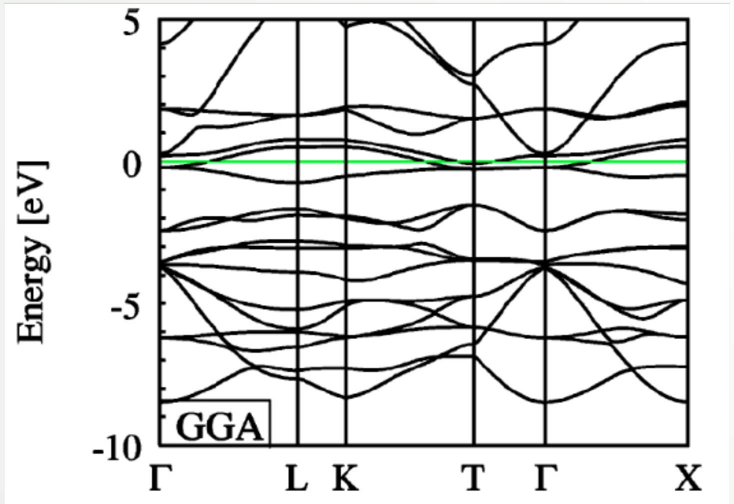
Fermionic systems in nature

- 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



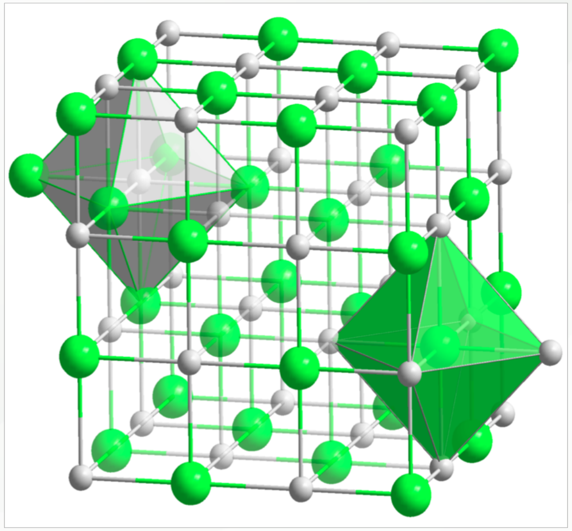
Metal!

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

Experimentally

Insulating and antiferromagnetic

$T_{Ne\acute{e}l} = 200K$



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

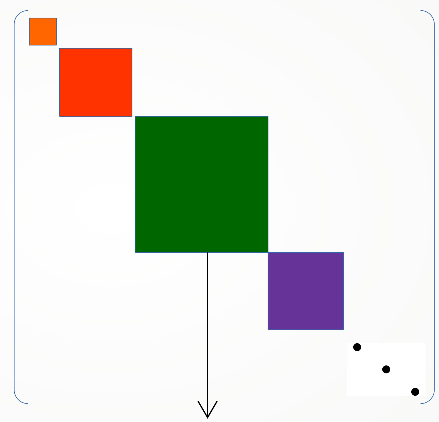
- Typical Fock state (occupation basis): $|\uparrow\ \uparrow\downarrow\ \downarrow\ \downarrow\ldots\rangle$
- How are the thermodynamical properties of the Hubbard model? $\mathcal{Z}=\sum_\alpha e^{-\beta E_\alpha}$
- Physical observables: $\langle\hat{\mathcal{O}}\rangle=\dfrac{\mathrm{Tr}\hat{\mathcal{O}}e^{-\beta\hat{H}}}{\mathcal{Z}}$

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

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

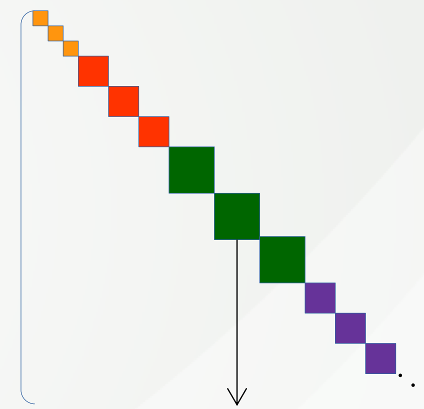
$[\mathcal{H},n_e]=0$

$[\mathcal{H},S_z]=0$



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

$[\mathcal{H},T_{\vec{R}}]=0$



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

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 com

- 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 : Occurrence 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***?

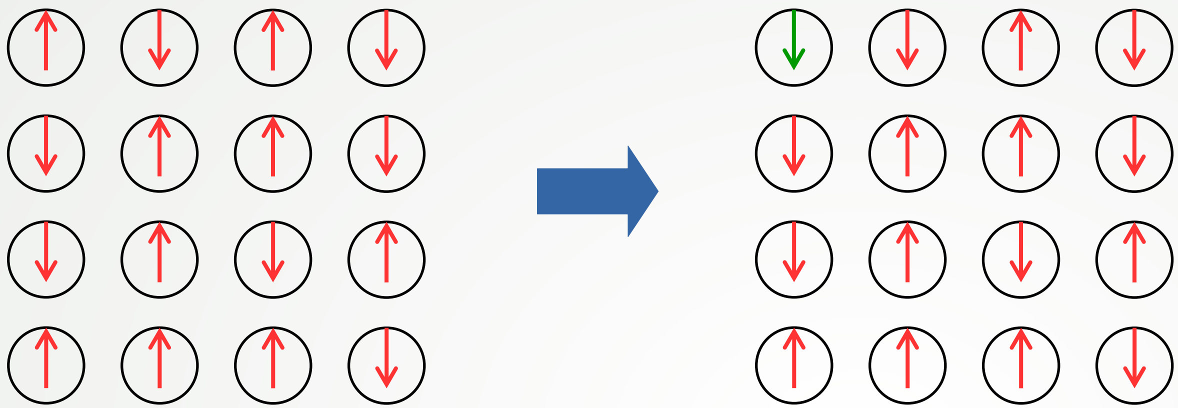
- Start from a random spin configuration $\alpha = |\sigma_1^z \sigma_2^z \ldots \sigma_{N_s}^z\rangle$

- 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 : $\qquad\qquad\qquad$ 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: $r \equiv \dfrac{p(\alpha')}{p(\alpha)} = e^{-\Delta E/k_b T}$

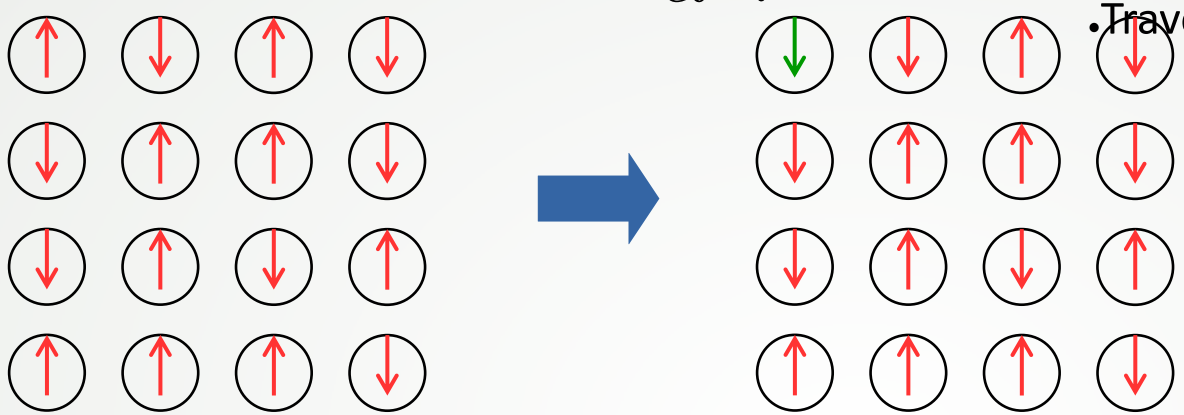
- **Metropolis algorithm:**
  - If $\Delta E < 0$ accept the move
  - If $\Delta E > 0$ accept it with probability $r = e^{-\Delta E/k_b T}$: accounts for fluctuations

- **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

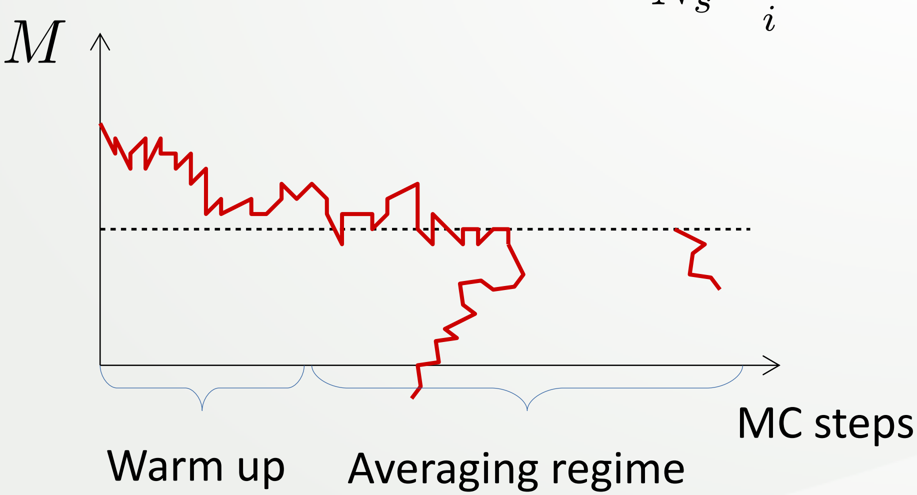
- Attempting local spin flips

$\alpha :$ $\qquad\qquad$ $\alpha' :$



- Traversing the whole lattice constitutes a s
- or one MC step

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



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

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

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

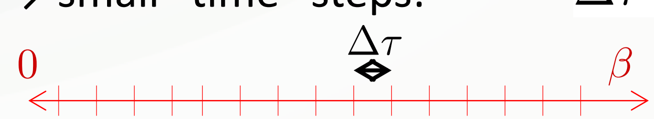
- As before, is it possible to devise an ***importance sampling*** mechanism that will prevent us to average over all possible configurations? In this case ***all possible states*** ?

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

- 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

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

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

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

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

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

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

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

Auxiliary field!

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

- 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...

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

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

- 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...

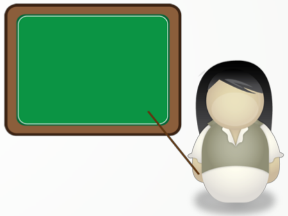
Discrete auxiliary field!

$U > 0$

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

$U < 0$

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



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

Ising-like field!

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

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

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→

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

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

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

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

$$\mathcal{V}_\sigma = \sigma \sum_{i=1}^{N} \alpha x_i n_{i\sigma}$$ 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:

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

- 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:

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

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

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

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

$$\langle c_{i\sigma}c^\dagger_{j\sigma}\rangle_{\{x(\tau)\}} = \left[\frac{1}{1+\mathsf{B}_{N_t,\sigma}\dots\mathsf{B}_{1,\sigma}}\right]_{ij} = G^\sigma_{ij}$$

$$\mathsf{B}_{\tau,\sigma}(x_\tau) = e^{\Delta\tau\mathsf{K}}e^{\sigma\alpha\mathsf{V}^\sigma_\tau(x_\tau)}$$

- 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:

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

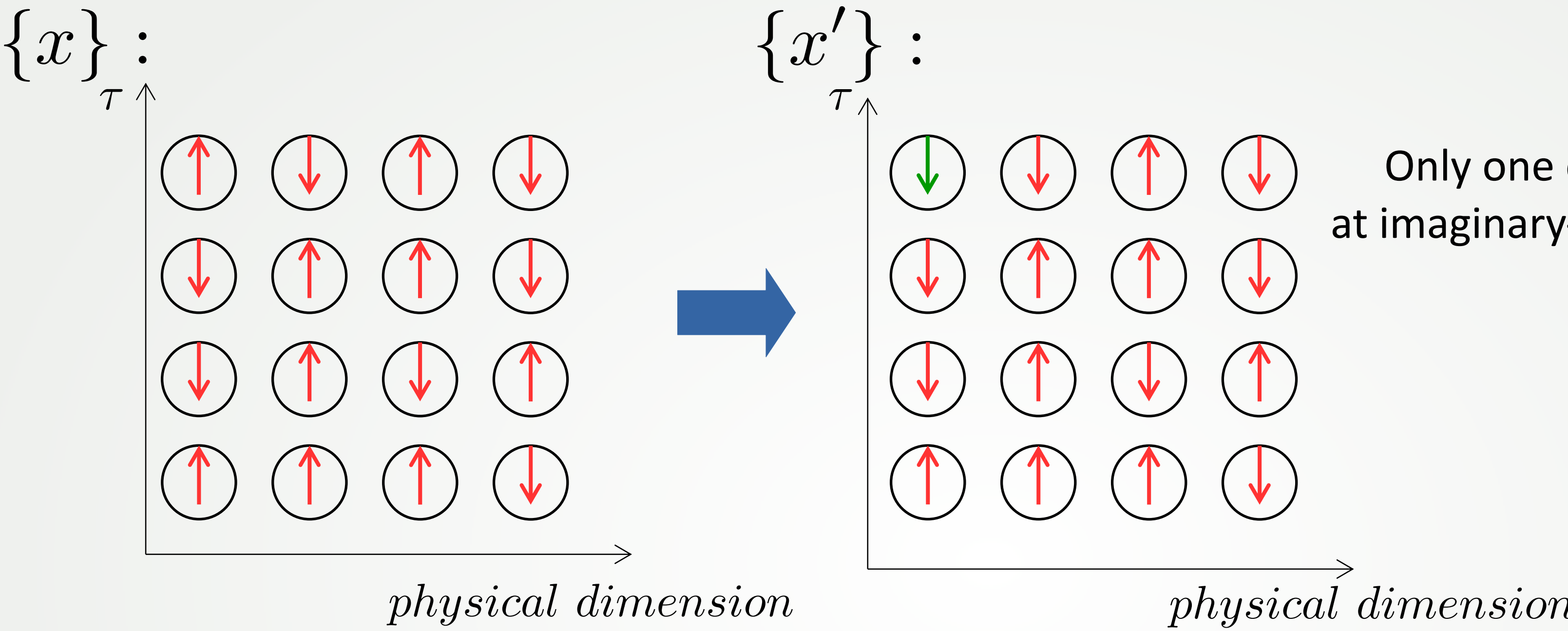
- More complicated ones Wick's theorem:

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

- 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 update

- 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 τ imaginary-time at site i is u

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

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 u

Spin-dependent ratio of Boltzmann weights:

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

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

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

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

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

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

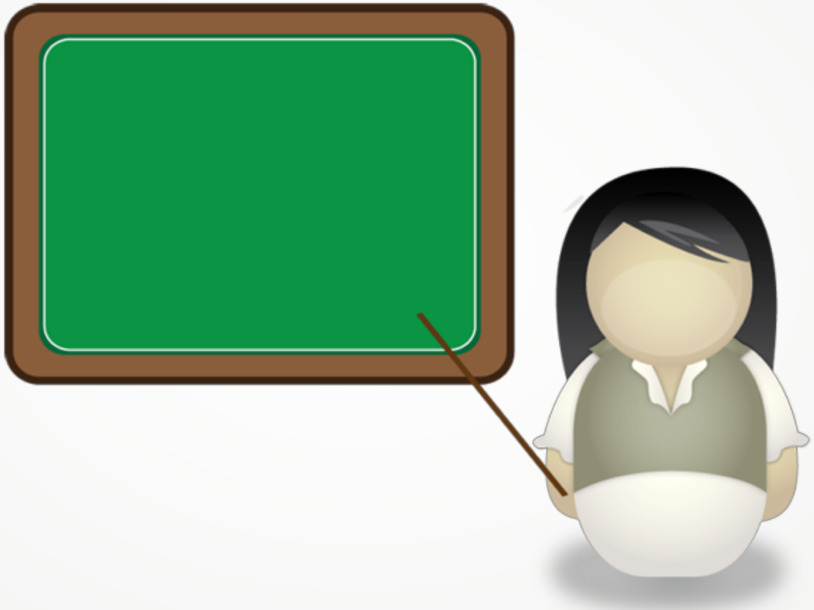
$$\mathcal{R} = \mathcal{R}^\uparrow\mathcal{R}^\downarrow = \prod_{\sigma=\uparrow,\downarrow}\left(1+\Delta^\sigma_{ii}(i,\tau)\left(1-G^\sigma_{ii}(\tau,\tau)\right)\right)$$

Just a scalar!

Updating the Green's functions

$$\{x\} \rightarrow \{x'\}$$

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



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 $r \in [0,1]$

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

$\text{if } r > \mathcal{R}_{i,\tau} \text{ reject the move}$

- **if** number of loops in imaginary-time is above a certain threshold perform measure

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

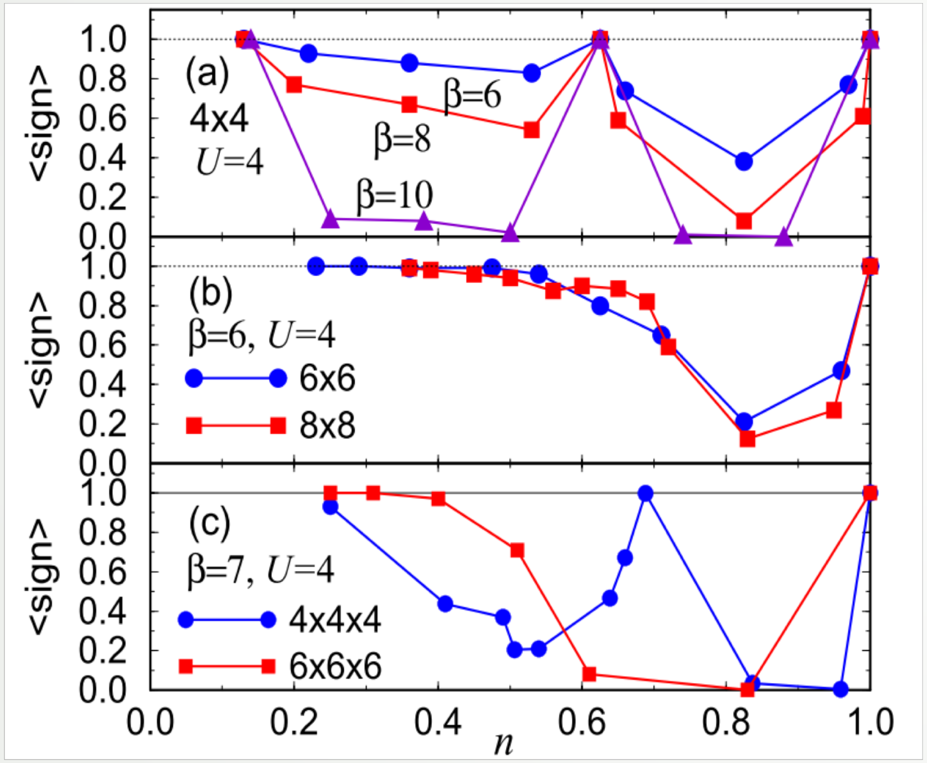
$$Z_{\{x\}} \equiv \sum_x p(x) \quad \Rightarrow \quad p(x) \equiv s(x)|p(x)| \qquad s(x) = \pm 1$$

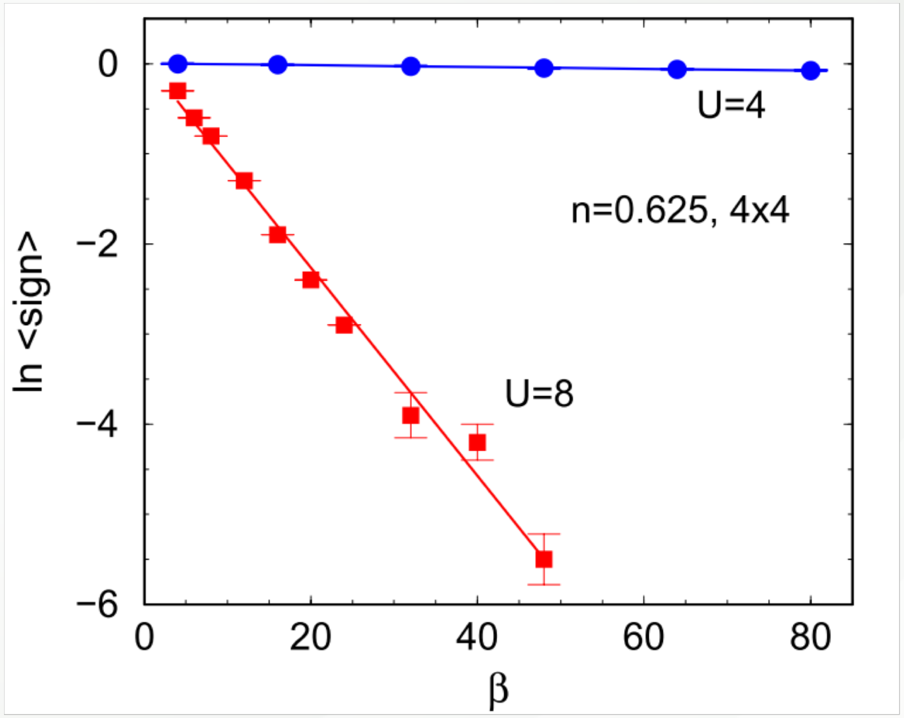
$$\begin{aligned}
\langle \hat{A} \rangle &= \frac{\sum_x A(x)p(x)}{\sum_x p(x)} = \frac{\sum_x A(x)|p(x)|s(x)}{\sum_x |p(x)|s(x)} \\
&= \frac{\left[\sum_x A(x)|p(x)|s(x)\right] / \sum_x |p(x)|}{\left[\sum_x |p(x)|s(x)\right] / \sum_x |p(x)|} \\
&= \frac{\sum_x p'(x)[s(x)A(x)]}{\sum_x p'(x)[s(x)]} \equiv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

Sign problem – life is not that "easy"

- Dependence of the sign with parameters...

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





At half-filling there is no sign problem

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

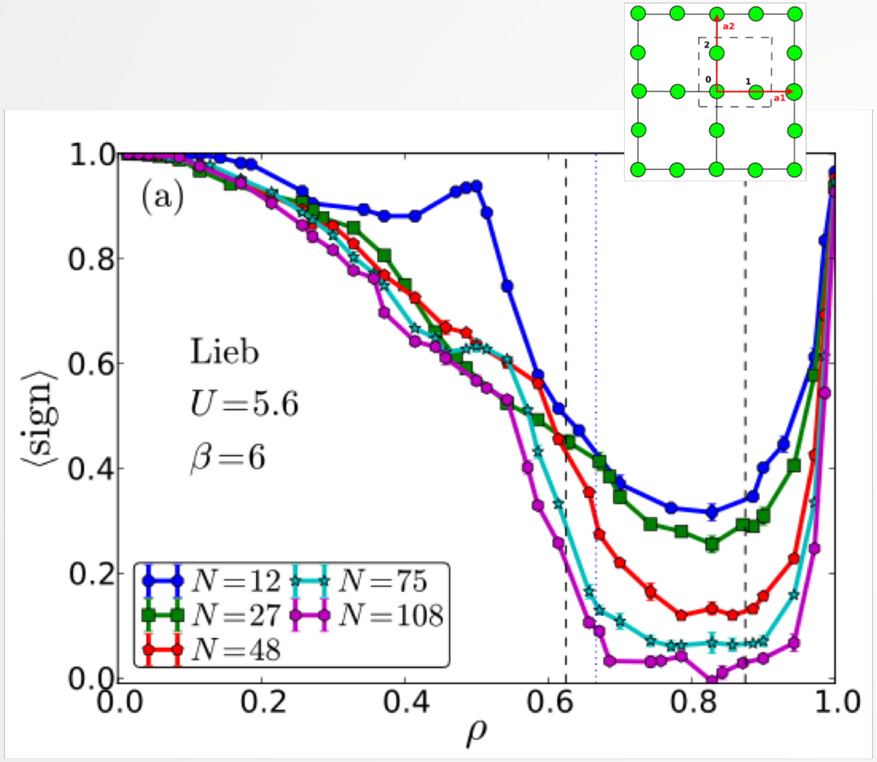
$$\det \mathrm{M}^{\uparrow} \cdot \det \mathrm{M}^{\downarrow} > 0$$

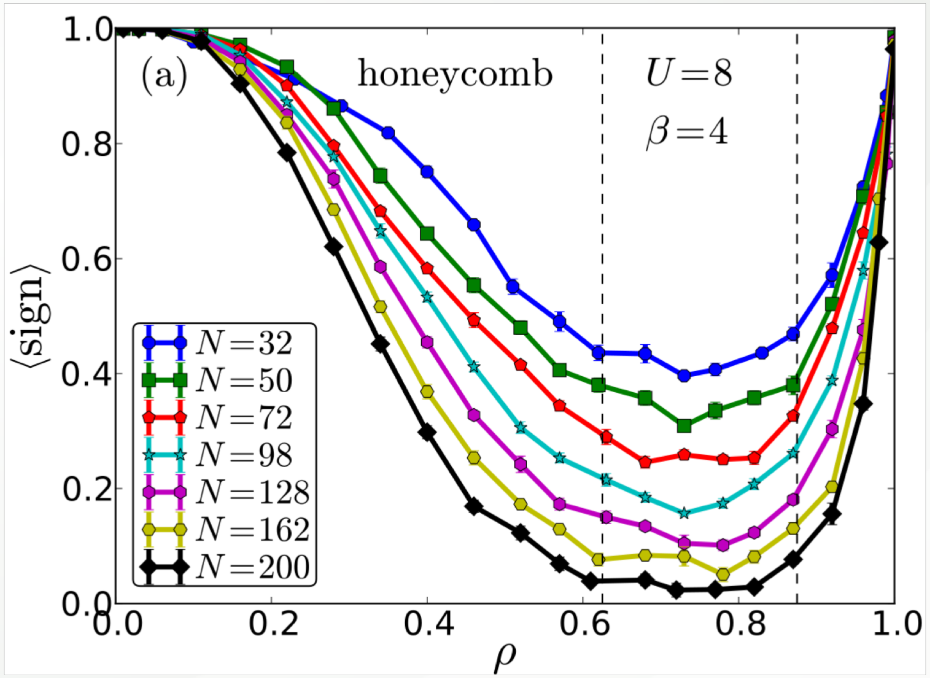
$$\langle \mathrm{sign} \rangle \sim e^{-\beta N U \gamma}$$

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

Sign problem – life is not that "easy"

- Other types of lattices





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

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,

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

where

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

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

PQMC method

In matrix form:

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

and

$$\mathsf{P}_L^\sigma = (\mathsf{P}_R^\sigma)^\dagger$$

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:

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

- Once the Green's fucntions 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 witht the projection parameter

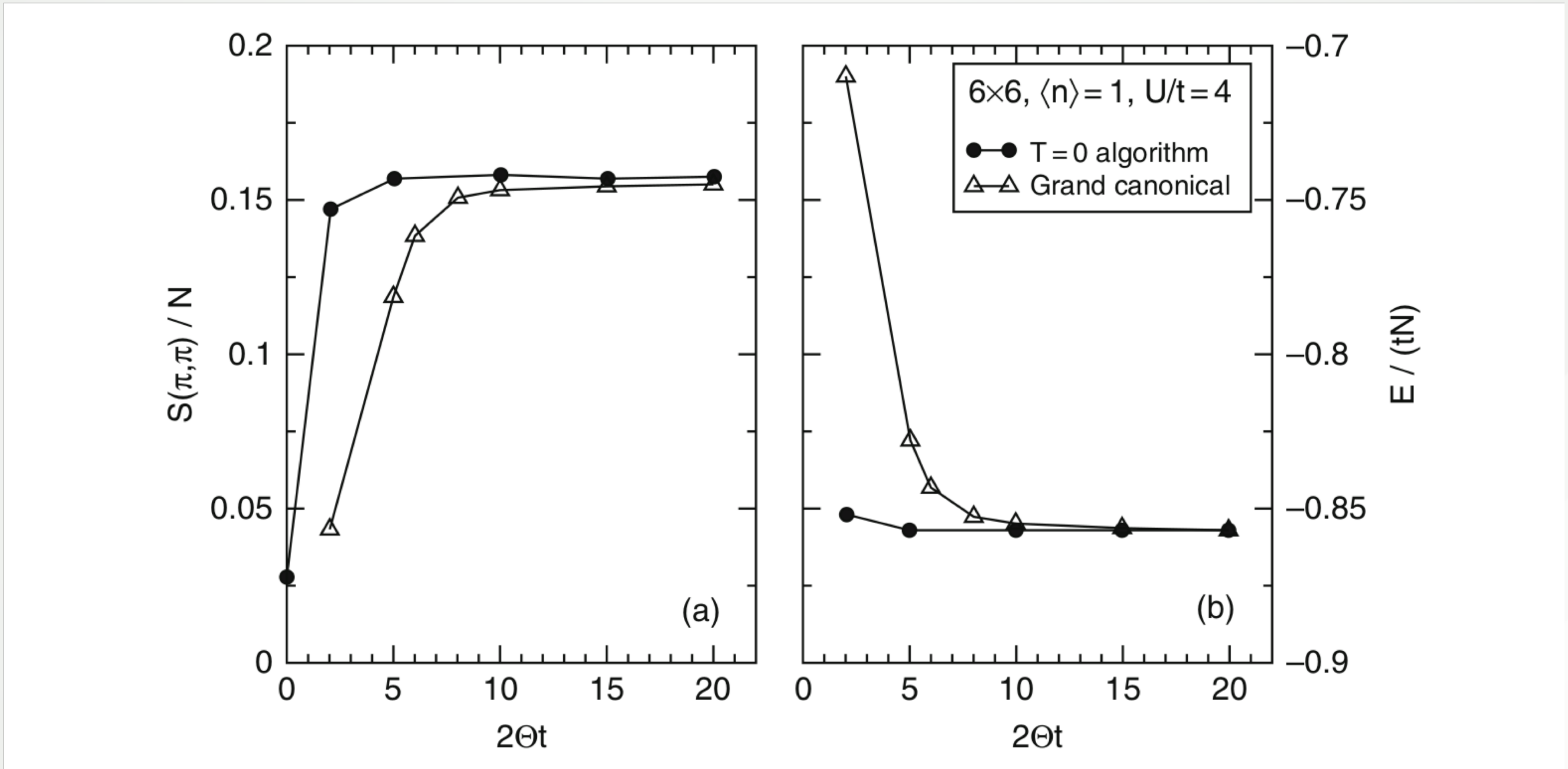
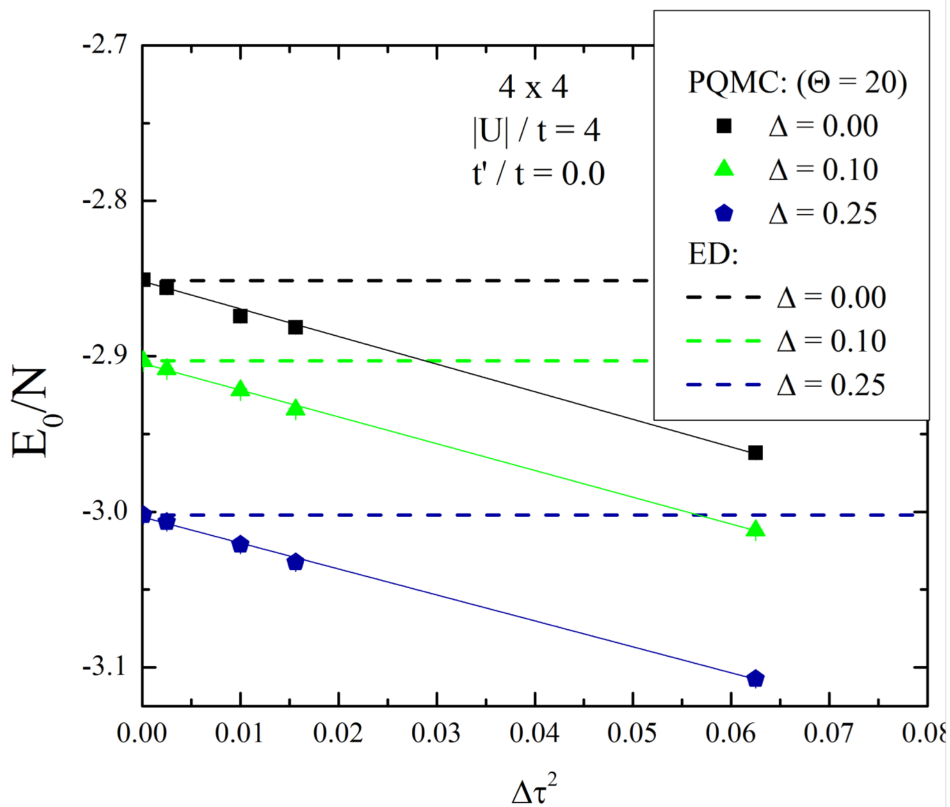
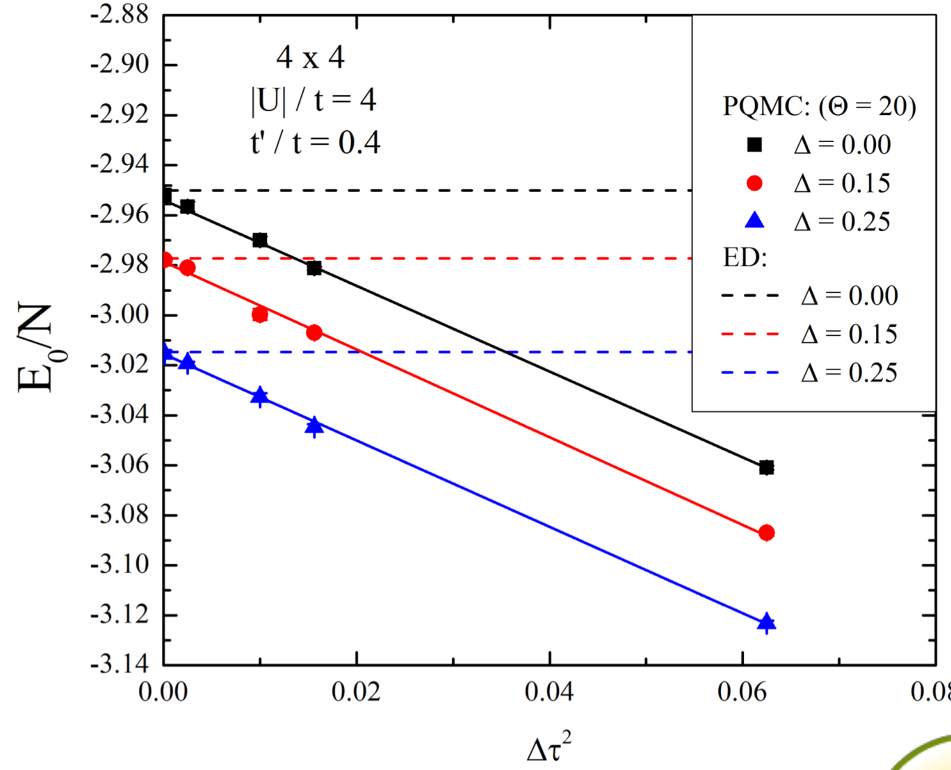


Fig. 10.15. Fourier transform of the spin-spin correlation functions at $\boldsymbol{Q} = (\pi, \pi)$ (**a**) and energy (**b**) for the half-filled Hubbard model (10.90). ●: PQMC algorithm. △: FTQMC algorithm at $\beta = 2\Theta$

PQMC method – some basic results

- Convergence of quantities witht 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!