Finite-T QMC

QMC ≠ Quantized MC, but MC of QM!

Equilibrium:

quantum & thermal ave

$$Z = \mathrm{Tr}\, e^{-\beta H} \qquad \langle O \rangle = \frac{1}{Z} \mathrm{Tr}\left(e^{-\beta H} O\right)$$

The QMC method works like a Dream! (But... more later)

Focus on 1d quantum XY-model (N sites with P.b.c.)

0 1 2 ... N-1 0

spin-flips

$$H = -\sum_{i=0}^{N-1} \Big[2J \underbrace{\left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right)}_{\frac{1}{2}\left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right)} + d_{i,i+1} \Big] = -\sum_{k=0}^{3N-1} H_k$$

$$S^{\pm} = S^x \pm i S^y$$

diag $\{ H_0 = d_{0,1}, \quad H_3 = d_{1,2}, \quad H_6 = d_{2,3}$

offd $\begin{cases} H_1 = J S_0^+ S_1^- & H_4 = J S_1^+ S_2^- & \vdots \\ H_2 = J S_0^- S_1^+ & H_5 = J S_1^- S_2^+ & \end{cases}$

Basis choice: S^z eigenstates

$$\left.\begin{array}{l} |\uparrow\uparrow \cdots \uparrow\uparrow\rangle \\ |\uparrow\uparrow \cdots \uparrow\downarrow\rangle \\ |\uparrow\uparrow \cdots \downarrow\uparrow\rangle \\ \vdots \end{array}\right\} 2^N \text{ states}$$

$$S^+|\downarrow\rangle = |\uparrow\rangle, \quad S^-|\downarrow\rangle = 0$$

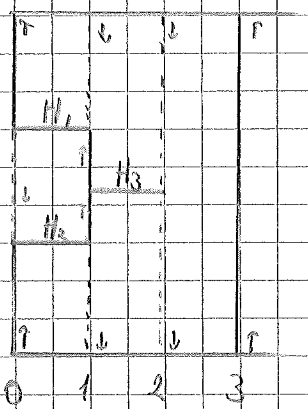
$$S^+|\uparrow\rangle = 0, \quad S^-|\uparrow\rangle = |\downarrow\rangle$$

$$(\hbar = 1)$$

$$Z = \underset{\substack{\uparrow \\ \text{Basis states}}}{\sum_{S}} \langle S| e^{-\beta H} |S\rangle \overset{\substack{\text{SSE} \\ \downarrow}}{=} \sum_{S} \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \langle S| H^n |S\rangle$$

$$= \underbrace{\sum_{S=0}^{2^N-1} \sum_{n=0}^{\infty} \sum_{k_1=0}^{3N-1} \cdots \sum_{k_n=0}^{3N-1}}_{\sum_c} \underbrace{\frac{\beta^n}{n!} \langle S| H_{k_n} H_{k_{n-1}} \cdots H_{k_1} |S\rangle}_{W_{\underbrace{S,\, n,\, \{k_i\}}_{C \,\leftarrow\, \text{a "configuration"}}}}$$

A configuration with $n=3$:



$$\left.\begin{array}{l} |S\rangle = |\uparrow\downarrow\downarrow\uparrow\ldots\rangle \\ n = 3 \\ k_1 = 2 \\ k_2 = 3 \\ k_3 = 1 \end{array}\right\} \quad W_c = \frac{\beta^3}{3!} J J J$$

assumed to be a diag op in S^z-basis.

$$\langle O\rangle = \frac{1}{Z} \mathrm{Tr}\left(e^{-\beta H} O\right) = \frac{\sum_c W_c O_c}{\sum_c W_c}$$

MC: Sample the distribution using detailed balance:

$$P_{c\to c'} W_c = P_{c'\to c} W_{c'}$$

$\uparrow$ Prob. that MC engine picks new config c' given the old config c.

(for unlikely configs c': $W_{c'} \ll W_c$ so $P_{c\to c'} \ll P_{c'\to c}$)

$1 \geq P_{c \to c'} \geq 0$ as it is a probability

However $W_c < 0$ for some systems : Sign Problem!

Sign Problem (Nightmare!)

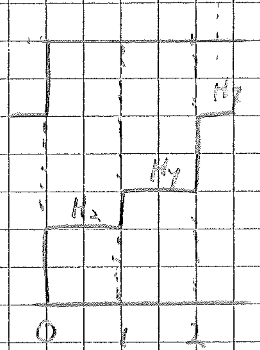
for $J > 0$ & $d > 0$ all $W_c \geq 0$ No sign problem

d can be chosen > 0 so let's do that

for $J < 0$ & $d > 0$ $W_c < 0$ when $n_{offd} = $ odd

$\uparrow$ # of offd. ops.

Example of config with $W_c < 0$:



So the 1d XY-model has a sign problem for $N =$ odd and $J < 0$ (AF)

Attempt to fix it: $W_c = (-1)^{n_{offd}} \underbrace{|W_c|}_{\tilde{W}_c}$

$$\langle O \rangle = \frac{\sum_c (-1)^{n_{offd}} O_c \tilde{W}_c}{\sum_c (-1)^{n_{offd}} \tilde{W}_c} = \frac{\sum_c (-1)^{n_{offd}} O_c \tilde{W}_c}{\sum_c \tilde{W}_c} \cdot \frac{1}{\frac{\sum_c (-1)^{n_{offd}} \tilde{W}_c}{\sum_c \tilde{W}_c}}$$

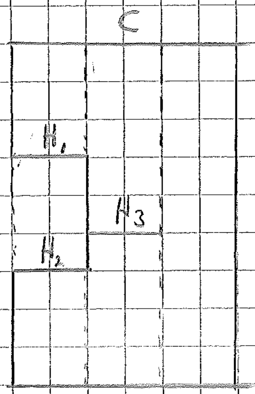
$$= \frac{\langle (-1)' \, O \rangle_{\tilde{W}}}{\langle (-1)' \rangle_{\tilde{W}}} \leftarrow \text{But} \sim e^{-\beta N \overbrace{(f_F - f)}^{\varepsilon}} \to 0$$

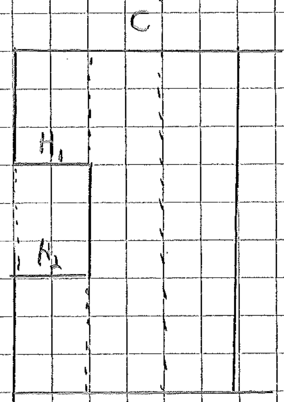
and so $\langle O \rangle$ will be very uncertain for large N at low T.

<u>Solving the sign problem</u> is the <u>holy grail</u> of QMC.

MC updates

- Insert/remove diag ops. : (n changes, but not S & offd ops)





$$W_c = \frac{\beta^3}{3!} J^2 d \qquad\qquad W_{c'} = \frac{\beta^2}{2!} J^2$$

$$P(\text{remove } H_3)\, \frac{\beta^3}{3!} J^2 d = \underbrace{P(\text{insert } H_3)}_{\underbrace{P(\text{choose } H_3)}_{1/N} P(\text{accept insertion})} \frac{\beta^2}{2!} J^2$$

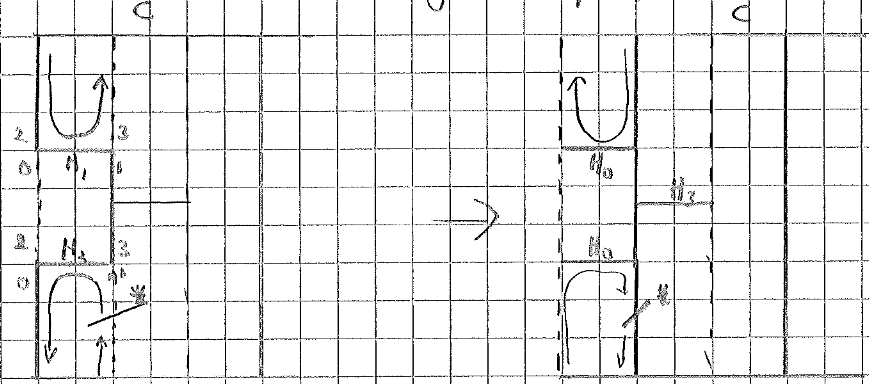
$$\Rightarrow P(\text{remove}) = P(\text{accept ins.}) \frac{n}{\beta N d} \qquad (n = 3 \text{ here})$$

$$\left.\begin{array}{l} P(\text{remove}) = \min\left(1, \dfrac{n}{\beta N d}\right) \\ P(\text{accept ins}) = \min\left(1, \dfrac{\beta N d}{n}\right) \end{array}\right\} \quad n \sim \beta N d$$

(n refers to # ops before removal / or after insertion
If one instead set n to be the # of ops before remove / bef. ins.
$P(\text{accept}) = \min\left(1, \frac{\beta N d}{n+1}\right)$)

• Directed loop update (S & off-diag ops changes, but not n)

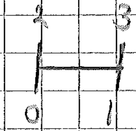
Flip along a loop path



$W_c = \frac{\beta^3}{3!} J^2 d$ $\qquad$ $W_{c'} = \frac{\beta^3}{3!} d^3$

What about detailed balance?

Label "legs" of each operator vertex:



in-leg $\qquad$ out-leg

$W_c \quad P(c \to c') = P(\text{start at } *, \text{go up})\; P(1, H_2 \to 0, H_0)\, J \quad P(2, H_1 \to 3, H_0)\, J \quad \frac{\beta^3}{3!} d$

$\parallel$

$W_{c'} \quad P(c' \to c) = P(\text{start at } *, \text{go down})\; P(3, H_0 \to 2, H_1)\, d \quad P(0, H_0 \to 1, H_2)\, d \quad \frac{\beta^3}{3!} d$

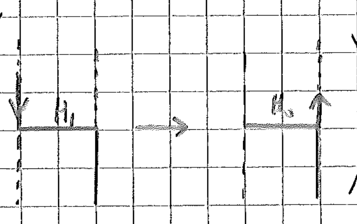
Detailed balance if

$P(\text{start at } *, \text{up}) = P(\text{start at } *, \text{down})$

$P(1, H_2 \to 0, H_0)\, J = P(0, H_0 \to 1, H_2)\, d$ $\qquad$ Detailed balance for each vertex move

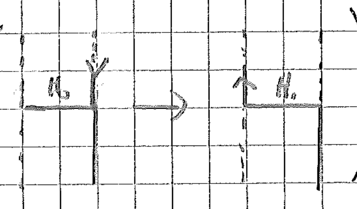
$P(2, H_1 \to 3, H_0)\, J = P(3, H_0 \to 2, H_1)\, d$

In pictures

$J\cdot\rho(2,H_1 \to 3,H_0) = J\cdot\rho\Big($ 

$\Big)$

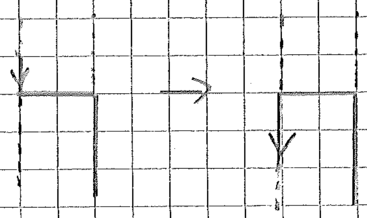
"

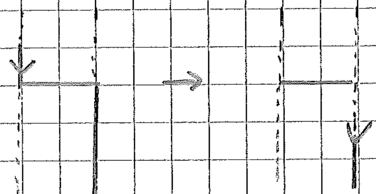
$J\cdot\rho(3,H_0 \to 2,H_1) = J\,\rho\Big($ 

$\Big)$

Opposite processes are related

There are also

$\rho\Big($  $\Big) = 0$ as it leads to a not allowed vertex SS'

$\rho\Big($  $\Big) = \rho(2,H_1 \to 1\,H_0)$

What comes in, goes out $\Rightarrow$

$$\rho(2,H_1 \to 1,H_0) + \rho(2\,H_1 \to 3\,H_0) = 1$$

$\Rightarrow$ a set of lin. eqs. for the ρ's which can be solved.

Dynamics

$$\tilde{S}(\tau) \equiv \langle S_0^z(\tau) S_0^z(0) \rangle = \frac{1}{Z} \mathrm{Tr}\left(e^{-\beta H} \underbrace{e^{\tau H} S_0^z e^{-\tau H}}_{e^{iHt} S_0^z e^{-iHt} \text{ with } \tau = it} S_0^z \right)$$

$\uparrow$ Imaginary time

QMC "needs" imaginary time, otherwise lots of oscillations $\rightarrow$ sign problem.

Expand

$$\tilde{S}(\tau) = \frac{1}{Z} \sum_s \sum_{n_2} \sum_{n_1} \sum_{\{k\}} \frac{(\beta-\tau)^{n_2}}{n_2!} \frac{\tau^{n_1}}{n_1!} \langle s | H_{k_{n_1+n_2}} \dots H_{k_{n_1+1}} S_0^z H_{k_{n_1}} \dots H_{k_1} S_0^z | s \rangle$$

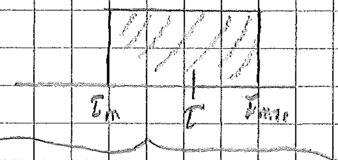
Set $m = n_1$, $n = n_1 + n_2 \Rightarrow n_2 = n - m$

$$\hookrightarrow \tilde{S}(\tau) = \frac{1}{Z} \sum_s \sum_{n=0}^{\infty} \sum_{m=0}^{n} \frac{(\beta-\tau)^{n-m}}{(n-m)!} \frac{\tau^m}{m!} \langle s | H_{k_n} \dots H_{k_{m+1}} S_0^z H_{k_m} \dots H_{k_1} S_0^z | s \rangle$$

Integral id:

$$\frac{(\beta-\tau)^{n-m}}{(n-m)!} \frac{\tau^m}{m!} = \underbrace{\int_0^\beta d\tau_n \int_0^{\tau_n} d\tau_{n-1} \dots \int_0^{\tau_2} d\tau_1}_{0 \le \tau_1 \le \tau_2 \le \dots \le \beta} \left(\Theta(\tau_{m+1} - \tau) - \Theta(\tau_m - \tau) \right)$$

(Works also for
$m = 0$ with $\tau_0 = 0$
$m = n$ with $\tau_{n+1} = \beta$)



Proof:

$$I=\int_0^{\beta} d\tau_n \int_0^{\tau_n} d\tau_{n-1} \dots \int_0^{\tau_{m+2}} d\tau_{m+1} \int_0^{\tau_{m+1}} d\tau_m \dots \dots \int_0^{\tau_2} d\tau_1 \left(\Theta(\tau_{m+1}-\tau)-\Theta(\tau_m-\tau)\right)$$

The Θ-functions only contributes when $\tau_m \le \tau \le \tau_{m+1}$. Therefore we may replace the upper limit on τ_m by τ and the lower limit on τ_{m+1} (and τ_{m+2}, τ_{m+3} etc as they are all bigger than τ_{m+1}) by τ so

$$I=\int_{\tau}^{\beta} d\tau_n \int_{\tau}^{\tau_n} d\tau_{n-1} \dots \int_{\tau}^{\tau_{m+2}} d\tau_{m+1} \int_0^{\tau} d\tau_m \dots \int_0^{\tau_2} d\tau_1 \cdot 1$$

Then set $\tilde{\tau}_i = \tau_i - \tau$ for $i = m+1 \dots n$ (The $n-m$ left integrals)

$$I=\underbrace{\int_0^{\beta-\tau} d\tilde{\tau}_n \int_0^{\tilde{\tau}_n} d\tilde{\tau}_{n-1} \dots \int_0^{\tilde{\tau}_{m+2}} d\tilde{\tau}_{m+1}}_{\frac{(\beta-\tau)^{n-m}}{(n-m)!}} \underbrace{\int_0^{\tau} d\tau_m \dots \underbrace{\int_0^{\tau_3} d\tau_2 \underbrace{\int_0^{\tau_2} d\tau_1}_{\tau_2}}_{\frac{\tau_3^2}{2!}}}_{\frac{\tau^m}{m!}}$$

($n-m$ integrals) $\qquad$ (m integrals)

Also note

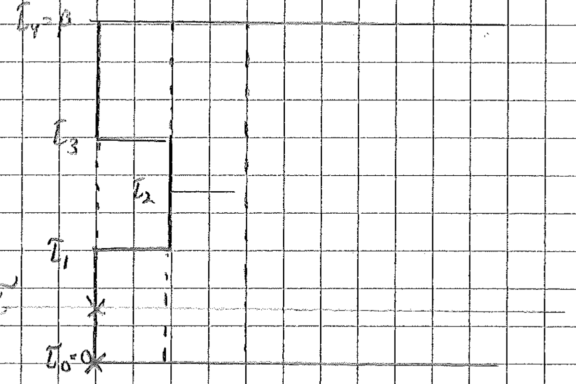
$$\int_0^\beta d\tau_n \int_0^{\tau_n} d\tau_{n-1} \ldots \int_0^{\tau_2} d\tau_1 = \frac{\beta^n}{n!}$$

Spin on site 0 after op m in op strg.

at op 0.

$$\tilde{S}(\tau) = \frac{\sum_S \sum_{n=0}^{\infty} \sum_{\{k_i\}} \int_0^\beta d\tau_n \ldots \int_0^{\tau_2} d\tau_1 \sum_{m=0}^{n} \left(\Theta(\tau_{m+1}-\tau) - \Theta(\tau_m - \tau) \right) S^z_{0m} S^z_{00} \; W(S, n, \{k_i\})}{\sum_S \sum_{n=0}^{\infty} \sum_{\{k_i\}} \int_0^\beta d\tau_n \ldots \int_0^{\tau_2} d\tau_1 \; \underbrace{\langle S | H_{k_n} \ldots H_{k_1} | S \rangle}_{W(S,n,\{k_i\})}} \qquad \begin{pmatrix} \tau_0 = 0 \\ \tau_{n+1} = \beta \end{pmatrix}$$

$$= \left\langle \sum_{m=0}^{n} \left(\Theta(\tau_{m+1}-\tau) - \Theta(\tau_m - \tau) \right) S^z_{0m} S^z_{00} \right\rangle$$



Which value contribute depends on m which is determined by the number of random numbers smaller than τ

- Draw n random numbers between 0 & β
- Sort them
- Assign these random times to the ops beginning from the bottom.

So the configuration can be interpreted as a

Space - Imaginary time snapshot !

Real time & freqs

We are more interested in

$$S(t) = \frac{1}{Z} \operatorname{Tr}\left(e^{-\beta H} \underbrace{e^{itH}}_{\sum_n |n\rangle\langle n|} S_0^z \underbrace{e^{-itH}}_{\sum |m\rangle\langle m|} S_0^z \right) \leftarrow \text{energy eigenstates}$$

and its Fourier-transform

$$S(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} S(t) = \frac{2\pi}{Z} \sum_{nm} e^{-\beta E_n} |\langle m| S_0^z |n\rangle|^2 \delta(\omega - (E_m - E_n))$$

energy eigenstates

for low-T only n=0 contributes. Then $S(\omega)$ has peaks at the excitation energies of the system.

The inverse transform is

$$S(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega\, e^{-i\omega t} S(\omega) = \frac{1}{2\pi} \int_0^{\infty} d\omega \left(e^{-i\omega t} + e^{-\beta\omega} e^{i\omega t} \right) S(\omega)$$

Where we used $S(-\omega) = e^{-\beta\omega} S(\omega)$

(let $\omega \to -\omega$, $n \leftrightarrow m$ and use δ-func $e^{-\beta E_m} = e^{-\beta(E_n+\omega)}$)

Do the analytic cont: $it = \tau$ or $t = -i\tau$

$$\tilde{S}(\tau) = \int_0^{\infty} d\omega \left(\frac{e^{-\omega\tau} + e^{-\omega(\beta-\tau)}}{2\pi} \right) S(\omega)$$

$\uparrow$ Known from QMC $\qquad \uparrow$?

$$\tilde{S}(\tau) = \int_0^\infty d\omega \, K(\tau,\omega) \, S(\omega)$$

Want to invert this

But hard! (Bad dream, not nightmare though)

Viewed as a matrix K is almost singular.
This is caused by its insensitiveness to high ω
(K is exp small then) so many $S(\omega)$ that differs
for high ω give almost the same $\tilde{S}(\tau)$. This
makes the inversion ill-defined.

Attempts: Guess $S(\omega)$ so that

$$\int_0^\beta d\tau \left[\frac{\tilde{S}(\tau) - \int d\omega \, K(\tau,\omega) \, S(\omega)}{\sigma(\tau)} \right]^2$$

$\leftarrow$ QMC errors

is minimized.

Bayesian Problem: Given QMC Data and prior knowledge on $S(\omega)$, find the most likely $S(\omega)$.