Introduction to Path Integral Monte Carlo method

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Outline

Generic many-particle Hamiltonian

For N particles of same charge and of mass m:

$$\hat{\mathrm{H}} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i=1}^{N} V_{\mathrm{ext}}(\hat{\mathbf{r}}_i) + \sum_{i<j} V_{\mathrm{int}}(\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j)$$

- Single-particle terms
  - kinetic energy term
  - external potential V_{ext}
- Pair interaction V_{int},
  typically (screened) (repulsive) instantaneous[1] Coulomb interaction

[1] Instantaneous = frequency independent

Density matrix

Macrostate represented by a set of microstates $|x\rangle$ with probabilities $p(x)$
Mean of a physical quantity A ($\leftrightarrow \hat{A}$): $\sum_x p(x) \langle x| \hat{A} |x\rangle$
Density matrix: $\hat{\rho} = \sum_x |x\rangle p(x) \langle x|$

$$\Rightarrow \qquad \bar{A} = \mathrm{Tr}\left(\hat{\rho}\hat{A}\right) \equiv \sum_n \langle n| \hat{\rho}\hat{A} |n\rangle$$

Property: $\mathrm{Tr}\,(\hat{\rho}) = \sum_x p(x) = 1$

For a pure state $|\Psi\rangle$: $\hat{\rho}_\Psi = |\Psi\rangle \langle\Psi|$
is the density matrix idempotent: $\hat{\rho}^2 = \hat{\rho}$

Q: Does the density matrix $\begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$ represent a pure state?

Finite temperature formalism

Example of a mixed state density matrix

$$\begin{pmatrix} p & 0 \\ 0 & 1-p \end{pmatrix}, \qquad p \in (0,1)$$

Properly normalized density matrix of a canonical ensemble

$$\hat{\rho} = \sum_n |n\rangle \frac{e^{-\beta E_n}}{Z} \langle n| = \frac{e^{-\beta \hat{\mathrm{H}}}}{Z}$$

with $\beta = \frac{1}{k_B T}$ and the partition sum

$$Z = \sum_n e^{-\beta E_n} = \mathrm{Tr}\left(e^{-\beta \hat{\mathrm{H}}}\right)$$

Dimensionality problem for multi-particle problems

Classical mechanics in D dimensions with N particles:
$\rightarrow$ dimensionality: $2DN - (\#\ \mathrm{of\ constraints})$

Quantum–mechanical model problem:

- N-particle system
- M relevant single particle states

$\rightarrow$ dimensionality[2]: M^N

Direct approach is thus inapplicable for more than a few of particles (recall that a complex vector of size $2^{30} \approx 10^9$ needs $16\,\mathrm{GB}$ of memory)

[2] Disregarding the proper bosonic/fermionic quantum statistics

Product property of the density matrix

Density matrix in coordinate representation ($\mathbf{R} \equiv (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$):
$\rho(\mathbf{R}, \mathbf{R}'; \beta) = \langle \mathbf{R} | \, \hat{\rho} \, | \mathbf{R}' \rangle$
Product property: $e^{-(\beta_1+\beta_2)\hat{\mathrm{H}}} = e^{-\beta_1\hat{\mathrm{H}}} e^{-\beta_2\hat{\mathrm{H}}}$

$$\Rightarrow \qquad \rho(\mathbf{R}, \mathbf{R}'', \beta_1 + \beta_2) = \frac{Z_1 Z_2}{Z} \int \mathrm{d}\mathbf{R}' \, \rho(\mathbf{R}, \mathbf{R}', \beta_1) \rho(\mathbf{R}', \mathbf{R}'', \beta_2)$$

Useful variant: $e^{-\beta\hat{\mathrm{H}}} = \left(e^{-\tau\hat{\mathrm{H}}}\right)^M$ for $\tau = \frac{\beta}{M}$ in combination with a suitable approximation for $e^{-\tau\hat{\mathrm{H}}}$ for small τ
In coordinate basis:

$$\rho(\mathbf{R}_0, \mathbf{R}_M, \beta) = \mathrm{const} \int \mathrm{d}\mathbf{R}_1 \int \mathrm{d}\mathbf{R}_2 \ldots \int \mathrm{d}\mathbf{R}_{M-1} \, \rho(\mathbf{R}_0, \mathbf{R}_1, \tau) \, \rho(\mathbf{R}_1, \mathbf{R}_2, \tau) \ldots \rho(\mathbf{R}_{M-1}, \mathbf{R}_M, \tau)$$

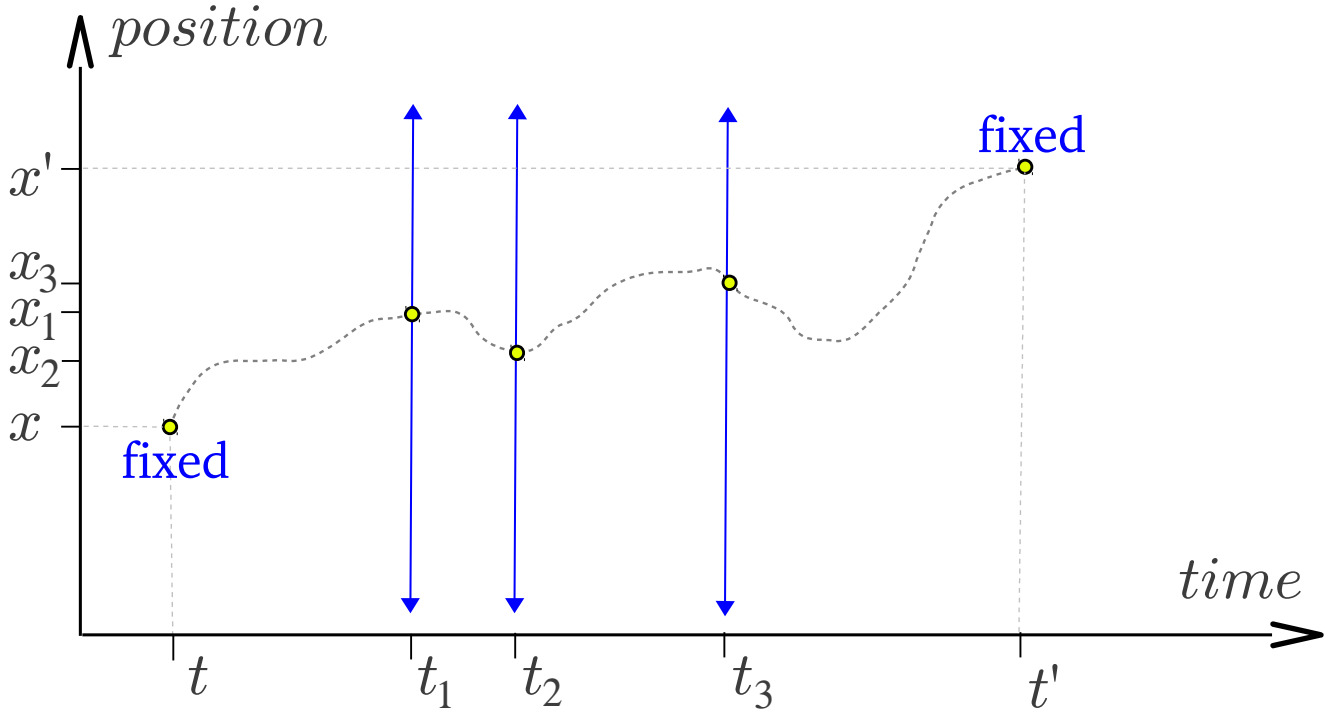
with $\mathbf{R}_k$ being the coordinates of all particles in the k-th time slice τ_k.

Product property schematically

For single particle in 1D, real-time evolution:

$$\tilde{\rho}(x, t=0; x', t') = \text{const} \left\langle x' \right| \underbrace{e^{-\frac{i}{\hbar}\hat{\mathrm{H}}t'} \left| x \right\rangle}_{|x(t')\rangle}$$

$$\tilde{\rho}(x, t; x', t') = \text{const} \int \mathrm{d}x_1 \int \mathrm{d}x_2 \int \mathrm{d}x_3 \, \tilde{\rho}(x, t; x_1, t_1) \times$$
$$\times \tilde{\rho}(x_1, t_1; x_2, t_2) \tilde{\rho}(x_2, t_2; x_3, t_3) \tilde{\rho}(x_3, t_3; x', t')$$



High-temperature approximations

Task: to approximate the high-temperature (small τ) density matrix

Assumption: $\hat{\mathrm{H}} = \hat{T} + \hat{V}$

Baker–Campbell–Hausdorff relation:

$$\exp\left\{-\tau\left(\hat{T}+\hat{V}\right)+\frac{\tau^2}{2}\left[\hat{T},\hat{V}\right]+\ldots\right\}=\exp\left(-\tau\hat{T}\right)\exp\left(-\tau\hat{V}\right)$$

Primitive approximation:

$$\exp\left[-\tau\left(\hat{T}+\hat{V}\right)\right]=\exp\left(-\tau\hat{T}\right)\exp\left(-\tau\hat{V}\right)+O\left(\tau^2\right)$$

alternative higher order scheme:

$$\exp\left[-\tau\left(\hat{T}+\hat{V}\right)\right]=\exp\left(-\frac{\tau}{2}\hat{V}\right)\exp\left(-\tau\hat{T}\right)\exp\left(-\frac{\tau}{2}\hat{V}\right)+O\left(\tau^3\right)$$

and many more.

Suzuki–Trotter formula

For any $\hat{T}$, $\hat{V}$ bounded from below

$$\exp\left[-\beta\left(\hat{T}+\hat{V}\right)\right] = \lim_{M\to+\infty}\left[\exp\left(-\tau\hat{T}\right)\exp\left(-\tau\hat{V}\right)\right]^{M}$$

Ref.:
Masuo Suzuki: Progress of Theoretical Physics, Vol. **56**, No. 5, 1454, November 1976.
Masuo Suzuki: Commun. math. Phys. **51**, 183–190 (1976).
(original reference for bounded operators)

Q: is the formula applicable for a simulation of atom of Helium?

Note: the proof does not apply for a real-time simulation.

Mapping of the quantum problem onto a classical

By insertion of closure relation:

$$\hat{\mathbb{I}} = \int \mathrm{d}\mathbf{R} \; |\mathbf{R}\rangle \langle \mathbf{R}|$$

into the Suzuki–Trotter formula

$$\begin{aligned}
\langle \mathbf{R}| \, e^{-\beta\left(\hat{T}+\hat{V}\right)} \, \left|\mathbf{R}'\right\rangle \quad = \quad & \lim_{M\to+\infty} \int \mathrm{d}\mathbf{R}_1 \ldots \int \mathrm{d}\mathbf{R}_{2M-1} \; \times \\
& \times \langle \mathbf{R}| \, e^{-\tau \hat{T}} \, |\mathbf{R}_1\rangle \langle \mathbf{R}_1| \, e^{-\tau \hat{V}} \, |\mathbf{R}_2\rangle \; \times \\
& \times \langle \mathbf{R}_2| \, e^{-\tau \hat{T}} \, |\mathbf{R}_3\rangle \langle \mathbf{R}_3| \, e^{-\tau \hat{V}} \, |\mathbf{R}_4\rangle \; \times \\
& \times \ldots \times \\
& \times \langle \mathbf{R}_{2M-2}| \, e^{-\tau \hat{T}} \, |\mathbf{R}_{2M-1}\rangle \langle \mathbf{R}_{2M-1}| \, e^{-\tau \hat{V}} \, \left|\mathbf{R}'\right\rangle
\end{aligned}$$

Free particle density matrix

The density matrix corresponding to

$$\hat{T} \equiv -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 = \frac{1}{2m}\sum_i \hat{\mathbf{p}}_i^2$$

for a single particle in D dimensions

$$\begin{aligned}\rho^{\text{free}}(\mathbf{r},\mathbf{r}',\tau) &= \frac{1}{Z^{\text{free}}}\int \mathrm{d}\mathbf{p}\int \mathrm{d}\mathbf{p}'\,\langle\mathbf{r}|\mathbf{p}\rangle\,\langle\mathbf{p}|\,e^{-\tau\hat{T}}\,|\mathbf{p}'\rangle\,\langle\mathbf{p}'|\mathbf{r}'\rangle \\ &= \frac{1}{Z^{\text{free}}}\frac{1}{(2\pi\hbar)^D}\int \mathrm{d}\mathbf{p}\, e^{i(\mathbf{r}-\mathbf{r}')\cdot\mathbf{p}/\hbar}e^{-\frac{\tau}{2m}\mathbf{p}^2}\end{aligned}$$

Thus for N particles:

$$\rho^{\text{free}}(\mathbf{R},\mathbf{R}',\tau) = \left(\frac{m}{2\pi\tau\hbar^2}\right)^{ND/2}\exp\left[-\frac{m}{2\tau\hbar^2}\sum_i\left(\mathbf{r}_i-\mathbf{r}_i'\right)^2\right]$$

Note: $Z^{\text{free}} = 1 \Leftrightarrow \rho^{\text{free}}(\mathbf{R},\mathbf{R}',\tau) = \langle\mathbf{R}|\,e^{-\tau\hat{T}}\,|\mathbf{R}\rangle$

Potential density matrix

The density matrix corresponding to

$$\hat{V} \equiv \sum_i V_{\rm ext}(\hat{\mathbf{r}}_i) + \sum_{i<j} V_{\rm int}(\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j)$$

is diagonal in coordinate representation

$$\begin{aligned} \rho^{\rm pot}(\mathbf{R}, \mathbf{R}', \tau) &= \frac{1}{Z^{\rm pot}} \left\langle \mathbf{R} \right| \exp\left(-\tau \hat{V}\right) \left| \mathbf{R}' \right\rangle \\ &= \frac{1}{Z^{\rm pot}} \exp\left(-\tau V(\mathbf{R})\right) \delta(\mathbf{R} - \mathbf{R}') \end{aligned}$$

with

$$V(\mathbf{R}) = \sum_i V_{\rm ext}(\mathbf{r}_i) + \sum_{i<j} V_{\rm int}(\mathbf{r}_i - \mathbf{r}_j)$$

and

$$Z^{\rm pot} = \int {\rm d}\mathbf{R}\, e^{-\tau V(\mathbf{R})} \qquad (1)$$

Putting it together

Primitive approximation:

$$\rho(\mathbf{R}, \mathbf{R}', \tau) \approx \rho^{\text{free}}(\mathbf{R}, \mathbf{R}', \tau) \frac{e^{-\tau V(\mathbf{R}')}}{Z^{\text{pot}}}$$

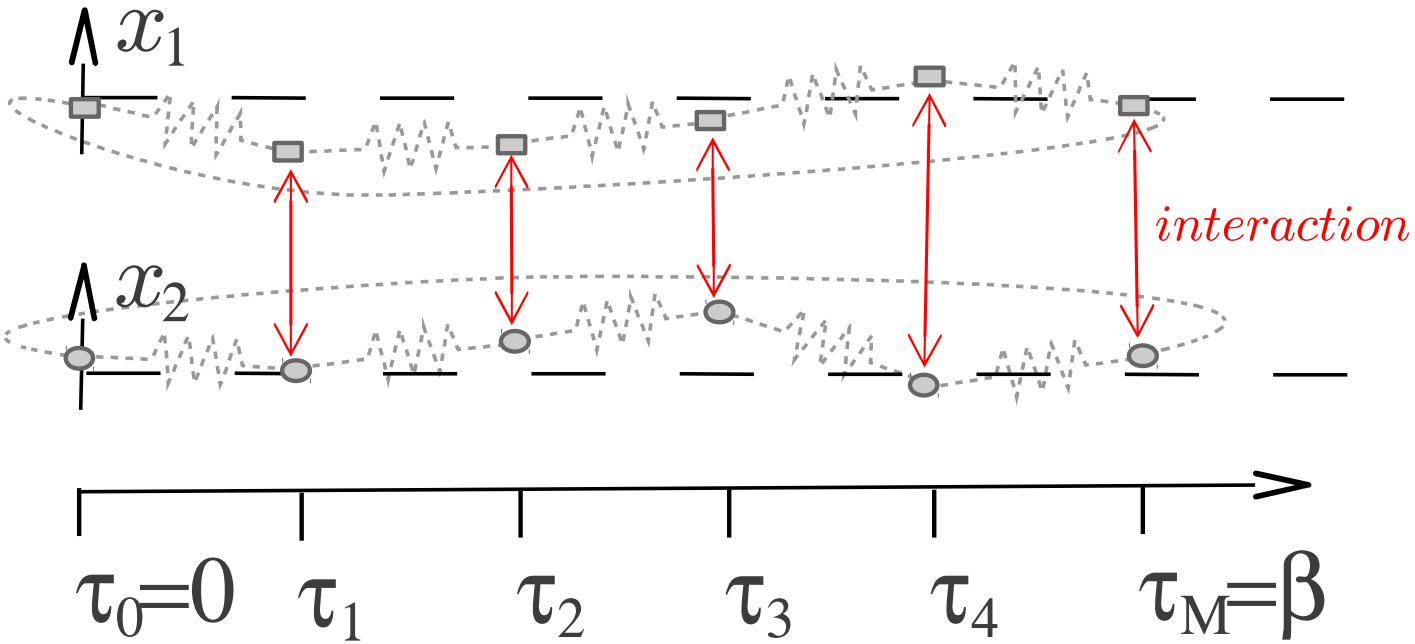
Then

$$\begin{aligned}
\rho(\mathbf{R}_0, \mathbf{R}_M, \beta) \approx & \frac{1}{(Z^{\text{pot}})^M} \int \mathrm{d}\mathbf{R}_1 \int \mathrm{d}\mathbf{R}_2 \ldots \int \mathrm{d}\mathbf{R}_{M-1} \times \\
& \times \rho^{\text{free}}(\mathbf{R}_0, \mathbf{R}_1, \tau) e^{-\tau V(\mathbf{R}_1)} \times \\
& \times \rho^{\text{free}}(\mathbf{R}_1, \mathbf{R}_2, \tau) e^{-\tau V(\mathbf{R}_2)} \times \\
& \times \ldots \times \\
& \times \rho^{\text{free}}(\mathbf{R}_{M-1}, \mathbf{R}_M, \tau) e^{-\tau V(\mathbf{R}_M)}
\end{aligned}$$

Partition sum for distinguishable particles

$$
\begin{aligned}
Z(N,V,T) &= \mathrm{Tr}\left(e^{-\beta\hat{\mathrm{H}}}\right) = \int \mathrm{d}\mathbf{R}\ \langle\mathbf{R}|\, e^{-\beta\hat{\mathrm{H}}}\,|\mathbf{R}\rangle \\
&= \int \ldots \int \Pi_{k=0}^{M-1} \mathrm{d}\mathbf{R}_k \times \\
&\qquad \times \Pi_{l=0}^{M-1} \left\{ \rho^{\mathrm{free}}\left(\mathbf{R}_l, \mathbf{R}_{l+1}, \tau\right) e^{-\tau V(\mathbf{R}_{l+1})} \right\}
\end{aligned}
$$

with boundary condition $\mathbf{R}_M = \mathbf{R}_0$.



Bose/fermionic symmetry

Symmetry under particle exchange has to be built in

$$\rho_{\mathrm{Bose}}(\mathbf{R}, \mathbf{R}', \beta) = \frac{\mathrm{const}}{N!} \sum_P \rho(\mathbf{R}, P\mathbf{R}', \beta)$$

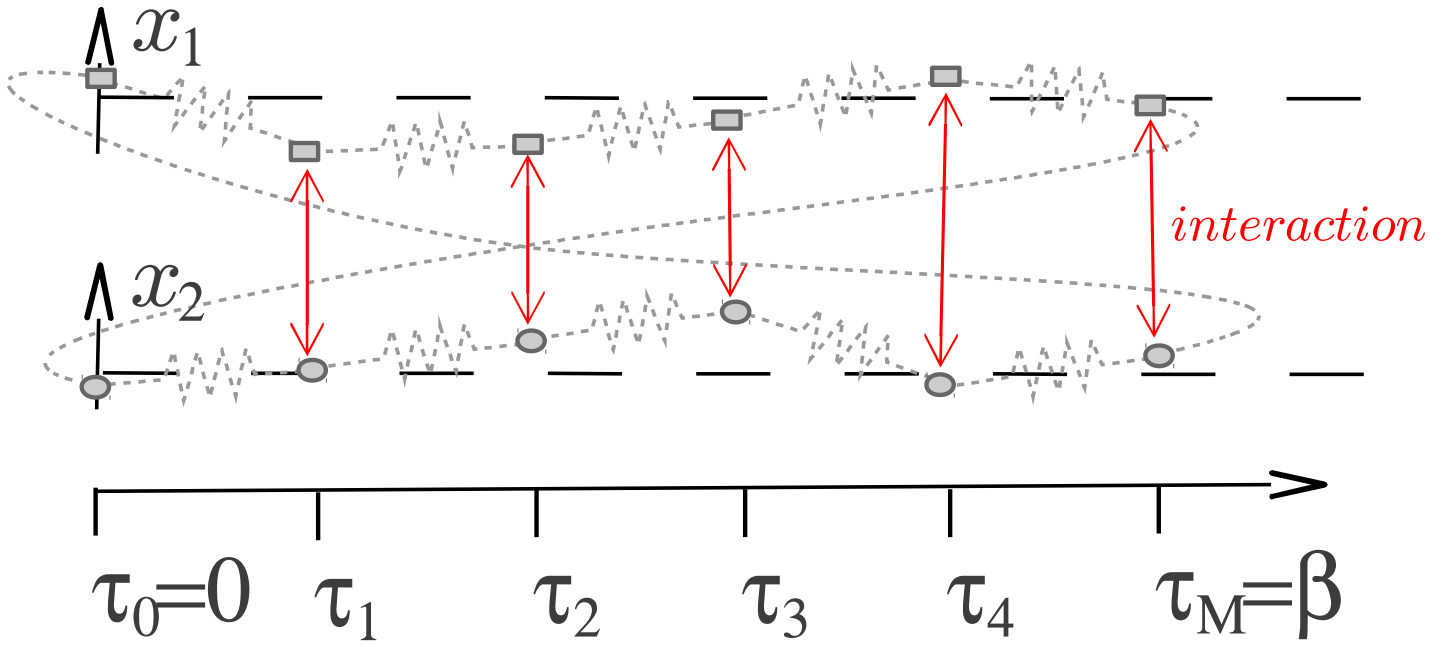
$$\rho_{\mathrm{Fermi}}(\mathbf{R}, \mathbf{R}', \beta) = \frac{\mathrm{const}}{N!} \sum_P \mathrm{sgn}(P)\, \rho(\mathbf{R}, P\mathbf{R}', \beta)$$

Note: for simplicity we deal with spinless particles.

Partition sum for indistinguishable spinless particles

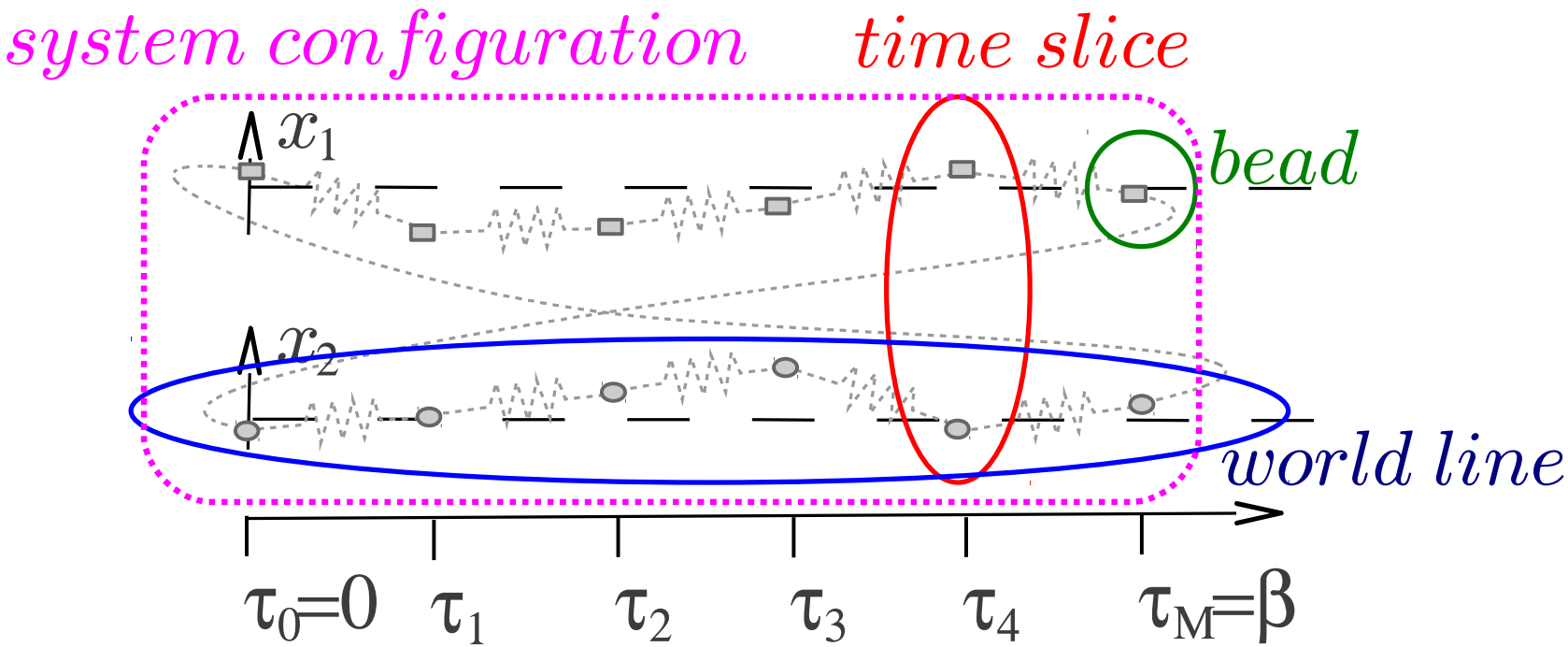
$$
\begin{aligned}
Z(N,V,T) &= \frac{1}{N!}\sum_P (\pm 1)^P \int \mathrm{d}\mathbf{R}\ \langle \mathbf{R}|\, e^{-\beta \hat{\mathrm{H}}}\, |P\mathbf{R}\rangle \\
&= \frac{1}{N!}\sum_P (\pm 1)^P \int \ldots \int \Pi_{k=0}^{M-1} \mathrm{d}\mathbf{R}_k \times \\
&\qquad \times \Pi_{l=0}^{M-1} \left\{ \rho^{\mathrm{free}}\left(\mathbf{R}_l, \mathbf{R}_{l+1}, \tau\right) e^{-\tau V(\mathbf{R}_{l+1})} \right\}
\end{aligned}
$$

with boundary condition $P\mathbf{R}_M = \mathbf{R}_0$.



Nomenclature

- System configuration (or many-particle path): $\mathbf{X} = (P, \mathbf{R}_0, \mathbf{R}_1, \ldots, \mathbf{R}_{M-1})$ of DNM coordinates
- Time slice $\mathbf{R}_k = (\mathbf{r}_1(\tau_k), \mathbf{r}_2(\tau_k), \ldots, \mathbf{r}_N(\tau_k))$
- World line i: $(\mathbf{r}_i(\tau_0), \mathbf{r}_i(\tau_1), \ldots, \mathbf{r}_i(\tau_{M-1}))$
- Bead of i-th world line for k-th time slice: $\mathbf{r}_i(\tau_k)$



High-dimensional integrals

Task: efficiently calculate an integral in high dimension d

Note: simulation with M time slices, N particles in a D-dimensional space $\rightarrow d = MND$

Deterministic methods perform poorly in high dimension d, error for the Simpson method

$$\text{error} \propto (\#\ \text{of grid-points})^{-4/d}.$$

Stochastic sampling:

$$\text{statistical error} \propto \sqrt{\frac{\text{variance of the integrand}}{\#\ \text{of measurements} - 1}}.$$

More effective for integrands with large variance: non-uniform sampling ($\rightarrow$ *importance sampling*)

Monte Carlo method for a classical system

Task: calculate various properties for a canonical ensemble with degrees of freedom $\mathbf{X}$

Probability distribution: $\pi(\mathbf{X})$

Mean of a quantity A: $\bar{A} = \int \mathrm{d}\mathbf{X}\, A(\mathbf{X})\, \pi(\mathbf{X})$

- Perform a random walk $\mathbf{X}_0 \to \mathbf{X}_1 \to \mathbf{X}_2 \to \ldots$ (Markov chain)
- With $P(\mathbf{X}, \mathbf{X}')$ being the probability to go from $\mathbf{X}$ to $\mathbf{X}'$
- Satisfying the detailed balance condition

$$\pi(\mathbf{X})P(\mathbf{X}, \mathbf{X}') = \pi(\mathbf{X}')P(\mathbf{X}', \mathbf{X})$$

- Ergodicity: it shall be possible to reach any point $\mathbf{X}'$ from any $\mathbf{X}$ (in a finite number of steps)

$\Rightarrow$ the random walk samples the points $\mathbf{X}$ with probability $\pi(\mathbf{X})$:

$$\bar{A} \approx \frac{1}{N} \sum_{t=1}^{N} A(\mathbf{X}_t)$$

Metropolis algorithm

Is a flexible algorithm satisfying the detailed balance

- Update proposal: from a configuration $\mathbf{X}$ randomly generate a new $\mathbf{X}'$ with probability $T(\mathbf{X}, \mathbf{X}')$
- The acceptance probability of the proposed update is[3]

$$A(\mathbf{X}, \mathbf{X}') = \min\left(1, \frac{\pi(\mathbf{X}')T(\mathbf{X}', \mathbf{X})}{\pi(\mathbf{X})T(\mathbf{X}, \mathbf{X}')}\right)$$

  In case of rejection stay in configuration $\mathbf{X}$.

Ref.: N. Metropolis, *et al*: J. of Chem. Phys. **21**, 1087 (1953).

[3] $P(\mathbf{X}, \mathbf{X}') = T(\mathbf{X}, \mathbf{X}')A(\mathbf{X}, \mathbf{X}')$

Metropolis algorithm for a clasical canonical ensemble

Boltzmann probability distribution: $\pi(\mathbf{X}) = \frac{1}{Z} e^{-\beta E(\mathbf{X})}$

Metropolis algorithm:

- starting with configuration $\mathbf{X}$ propose an update to $\mathbf{X}'$
- calculate $\Delta E = E(\mathbf{X}') - E(\mathbf{X})$ and
  - if $\Delta E < 0$: accept the update
  - if $\Delta E > 0$: accept the update with probability $e^{-\beta \Delta E}$, otherwise stay in $\mathbf{X}$

  (assuming $T(\mathbf{X}, \mathbf{X}') = T(\mathbf{X}', \mathbf{X})$)
- perform measurements in current configuration

Measuring after each update attempt may be inefficient
$\rightarrow$ do multiple update attempts between measurements

Simulation of bosons

$$Z(N,V,T) = \frac{1}{N!}\sum_P \int \dots \int \Pi_{k=0}^{M-1} \mathrm{d}\mathbf{R}_k \times \\ \times \Pi_{l=0}^{M-1} \left\{ \rho^{\mathrm{free}}\left(\mathbf{R}_l, \mathbf{R}_{l+1}, \tau\right) e^{-\tau V(\mathbf{R}_{l+1})} \right\}$$

with boundary condition $P\mathbf{R}_M = \mathbf{R}_0$

Sampling over configurations $\mathbf{X} \equiv (P, \mathbf{R}_0, \mathbf{R}_1, \dots, \mathbf{R}_{M-1})$

Weight:
$w(\mathbf{X}) = \frac{1}{N!}\Pi_{k=0}^{M-1}\mathrm{d}\mathbf{R}_k \Pi_{l=0}^{M-1} \left\{ \rho^{\mathrm{free}}\left(\mathbf{R}_l, \mathbf{R}_{l+1}, \tau\right) e^{-\tau V(\mathbf{R}_{l+1})} \right\}$

Local update

In our case:
$\pi(\mathbf{X}) = \frac{1}{Z} w(\mathbf{X}) = const \times \Pi_{l=0}^{M-1} \left\{ \rho^{\text{free}} \left(\mathbf{R}_l, \mathbf{R}_{l+1}, \tau \right) e^{-\tau V(\mathbf{R}_{l+1})} \right\}$
with appropriate boundary condition

The simplest update: randomly pick single bead $\mathbf{r}_i(\tau_k)$ and move it by a (Gaussian) random displacement $\mathbf{\Delta}$ to $\mathbf{r}'_i(\tau_k) = \mathbf{r}_i(\tau_k) + \mathbf{\Delta}$

The proposal probabilities are symmetric: $T(\mathbf{X}, \mathbf{X}') = T(\mathbf{X}', \mathbf{X})$
Thus the acceptance rate: $A(\mathbf{X}, \mathbf{X}') = \min\left(1, \pi(\mathbf{X}')/\pi(\mathbf{X})\right)$

$$\frac{\pi(\mathbf{X}')}{\pi(\mathbf{X})} = \frac{\exp\left\{-\tau\left[V_{\text{ext}}(\mathbf{r}'_i(\tau_k)) + \sum_{j\neq i} V_{\text{int}}(\mathbf{r}'_i(\tau_k) - \mathbf{r}_j(\tau_k))\right]\right\}}{\exp\left\{-\tau\left[V_{\text{ext}}(\mathbf{r}_i(\tau_k)) + \sum_{j\neq i} V_{\text{int}}(\mathbf{r}_i(\tau_k) - \mathbf{r}_j(\tau_k))\right]\right\}} \times$$
$$\times \frac{\exp\left\{-\frac{m}{2\tau\hbar^2}\left[\left(\mathbf{r}'_i(\tau_k) - \mathbf{r}_i(\tau_{k+1})\right)^2 + \left(\mathbf{r}'_i(\tau_k) - \mathbf{r}_i(\tau_{k-1})\right)^2\right]\right\}}{\exp\left\{-\frac{m}{2\tau\hbar^2}\left[\left(\mathbf{r}_i(\tau_k) - \mathbf{r}_i(\tau_{k+1})\right)^2 + \left(\mathbf{r}_i(\tau_k) - \mathbf{r}_i(\tau_{k-1})\right)^2\right]\right\}}$$

Q: does the local update satisfy the ergodicity requirement?

Estimators based on realspace basis

Straightforward when using realspace basis:

$$\begin{aligned}
\bar{f} &= \frac{1}{Z}\frac{1}{N!}\sum_P \int \mathrm{d}\mathbf{R}\,\langle \mathbf{R}|\,\hat{f}(\mathbf{R})e^{-\beta\hat{\mathrm{H}}}\,|P\mathbf{R}\rangle \\
&= \frac{1}{Z}\frac{1}{N!}\sum_P \int \mathrm{d}\mathbf{R}\, f(\mathbf{R})\,\langle \mathbf{R}|\,e^{-\beta\hat{\mathrm{H}}}\,|P\mathbf{R}\rangle \\
&= \sum_P \int \ldots \int \pi(\mathbf{X}) f(\mathbf{R}_0) = \sum_P \int \ldots \int \pi(\mathbf{X}) \frac{1}{M}\sum_{k=0}^{M-1} f(\mathbf{R}_k)
\end{aligned}$$

- Probability distribution histogram
- Single particle potential energy
- Interaction potential energy

Note: information about phase not available

Thermodynamic estimator for the total energy

For the energy (per particle) we have estimator based on thermodynamic equation

$$\frac{E(N,V,\beta)}{N} = -\frac{1}{NZ}\frac{\partial Z(N,V,\beta)}{\partial \beta},$$

which gives the thermodynamic estimator

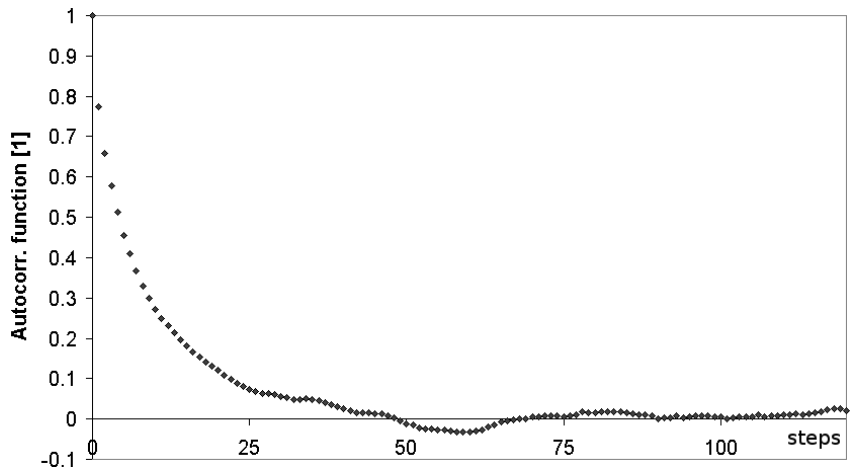
$$\begin{aligned}\frac{E_{\rm th}}{N} &= -\sum_P \int \cdots \int \frac{1}{N}\partial_\beta \pi(\mathbf{X};\beta) \\ &= \left\langle \frac{D}{2\tau} - \frac{m}{2\hbar^2\tau^2 MN}\sum_{j=0}^{M-1}(\mathbf{R}_j - \mathbf{R}_{j+1})^2 + \frac{1}{MN}\sum_{j=0}^{M-1} V(\mathbf{R}_j)\right\rangle.\end{aligned}$$

Statistical analysis of the measurements

The Metropolis measurements are not independent, as the new configuration is generated out of the previous $\Rightarrow$ autocorrelations

$$R_A(k) = \frac{1}{(N-k)\sigma_A^2} \sum_{i=1}^{N-k} (A_i - \bar{A})(A_{i+k} - \bar{A})$$

with $\sigma_A^2 = \frac{1}{N}\sum_i A_i^2 - \bar{A}^2$



Standard deviation of the mean $\bar{A} \approx \sqrt{\frac{1+2\tau_A}{N}}\sigma_A$ (for $\tau_A \ll N$)

Naive estimate $\frac{1}{\sqrt{N-1}}\sigma_A$ underestimates the errors

Single binning step

The autocorrelation times may be very long + the exponential decay shall be extracted from behaviour at large number of steps
Reliable estimate of τ_A does need a robust method

Binning analysis utilizes the property of independent measurements, that the naive error estimate for the measurements and for the binned measurements is the same

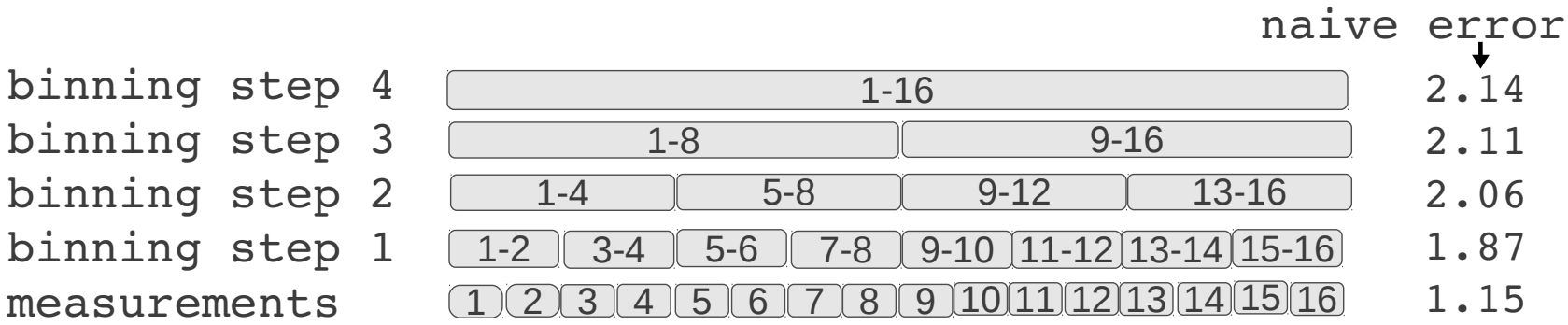
- Assumption: N independent measurements A_i
  Error estimate: $\frac{1}{\sqrt{N-1}}\sqrt{\frac{1}{N}\sum_i A_i^2 - \bar{A}^2}$
- Binned measurements: $A'_i = \frac{A_{2i}+A_{2i+1}}{2}$ for $i = 1, \ldots, N/2$
  Error estimate:

$$\frac{\sqrt{2}}{\sqrt{N}}\sqrt{\frac{2}{N}\sum_i{}' A_i'^2 - \bar{A}^2} = \frac{1}{\sqrt{N}}\sqrt{\frac{1}{N}\sum_i A_i^2 - \bar{A}^2 + \underbrace{\frac{2}{N}\sum_i{}' A_{2i}A_{2i+1} - \bar{A}^2}_{=0 \text{ for independent } A_i}}$$

Binning analysis

For binning much larger than τ_A we get effectively independent binned measurements

$\Rightarrow$ the naive error estimate converges to the correct value



Effective implementation need to store for each binning level (n):

$$\sum_i A_i^{(n)}, \qquad \sum_i \left(A_i^{(n)}\right)^2, \qquad \sum_{i=2^n+1}^{N} A_i$$

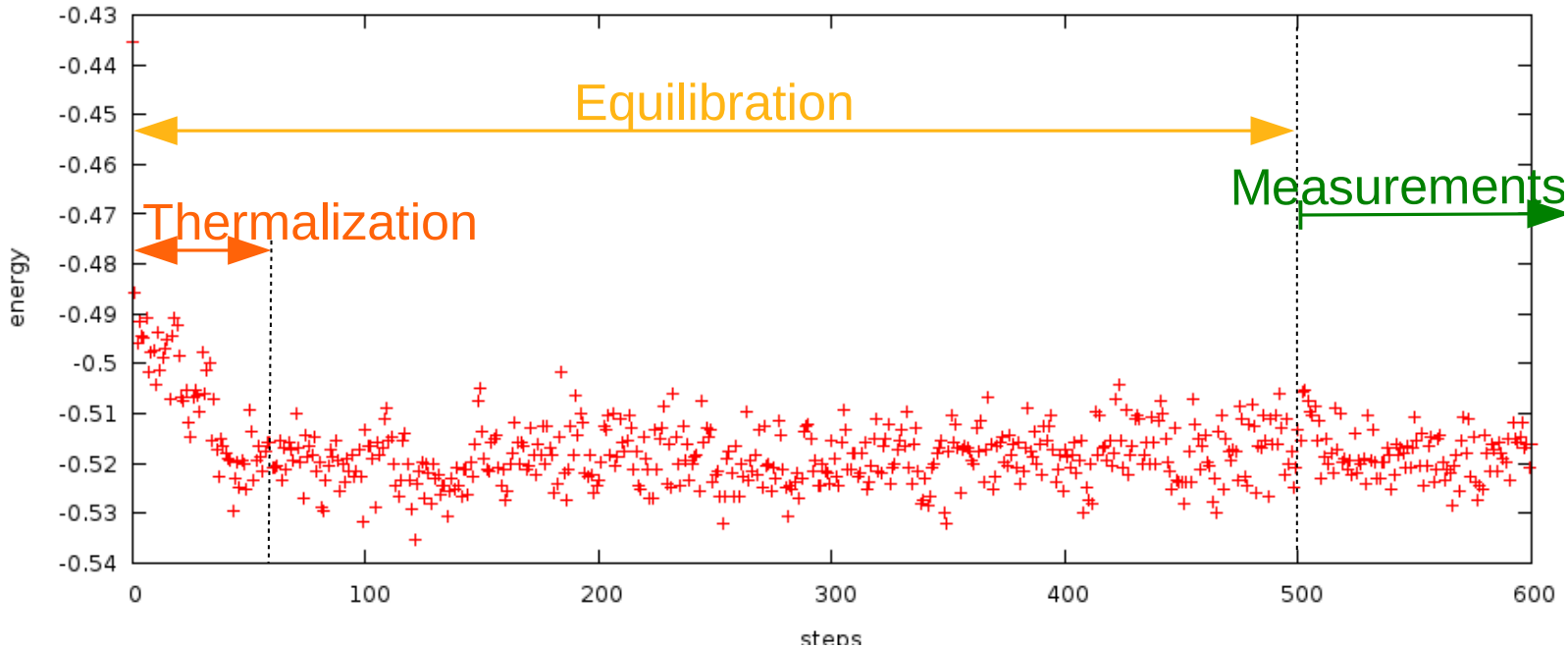
Implemented in library ALPS: `http://alps.comp-phys.org/`

Equilibration / Thermalization

The initial configuration is usually is a highly unprobable state $\rightarrow$ necessity to discard some initial ammount of configurations, till the random walk equilibrates

Thermalization time is the maximum of all autocorrelation times for all observables

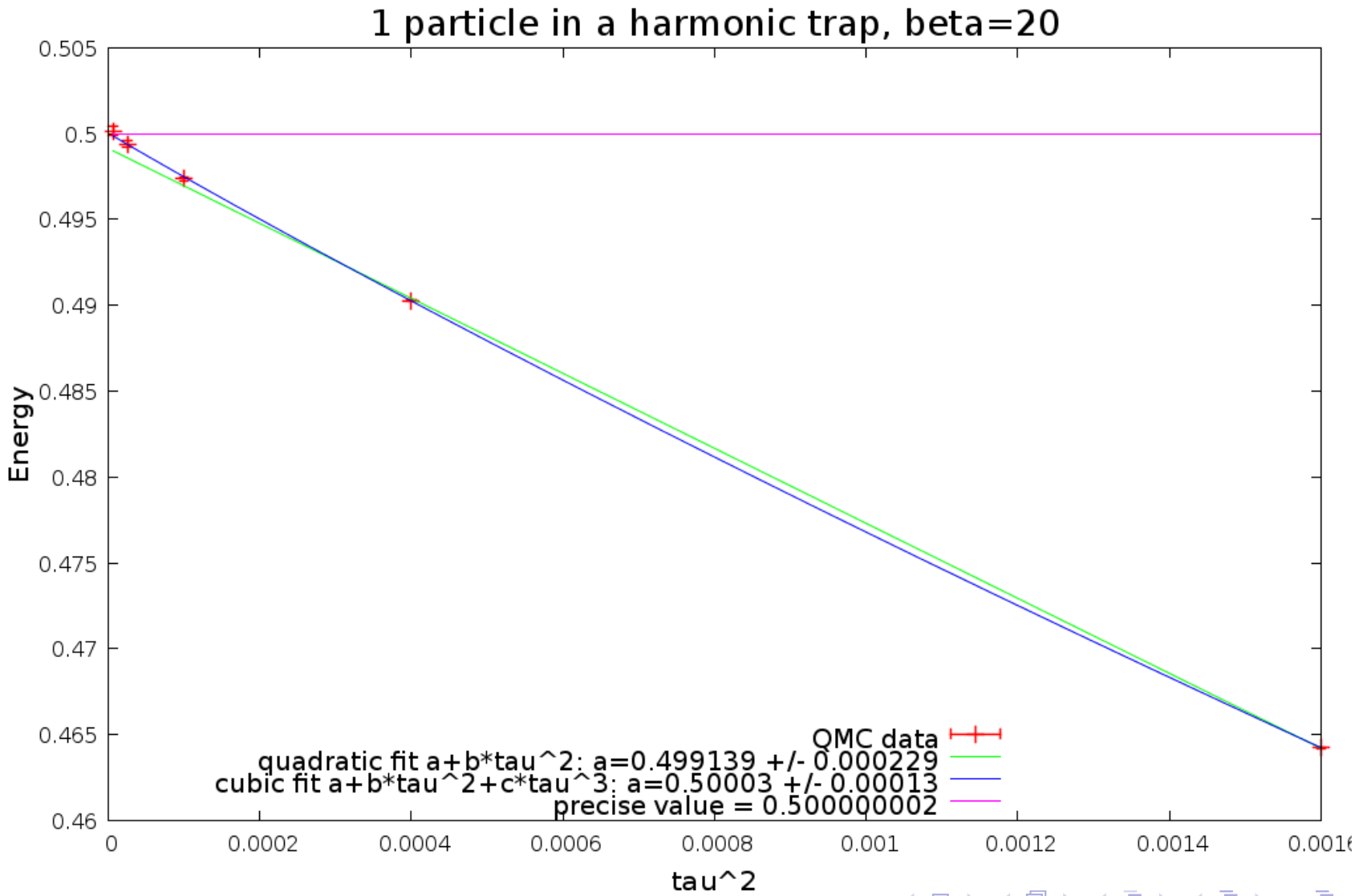
It is recommended to equilibrate the system for at least $10\times$ the thermalization time before starting measurements



Discretization errors

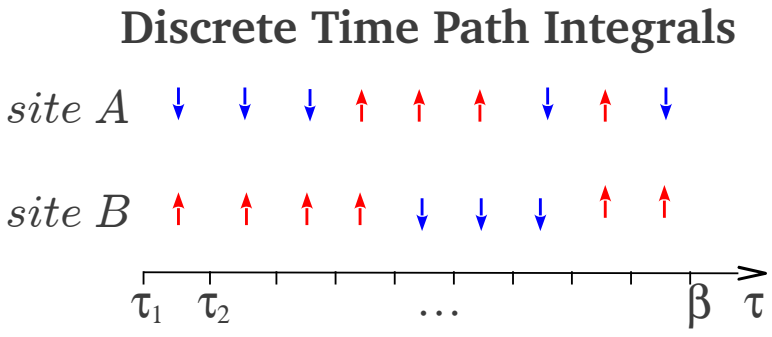
Due to finite $\tau = \frac{\beta}{M}$

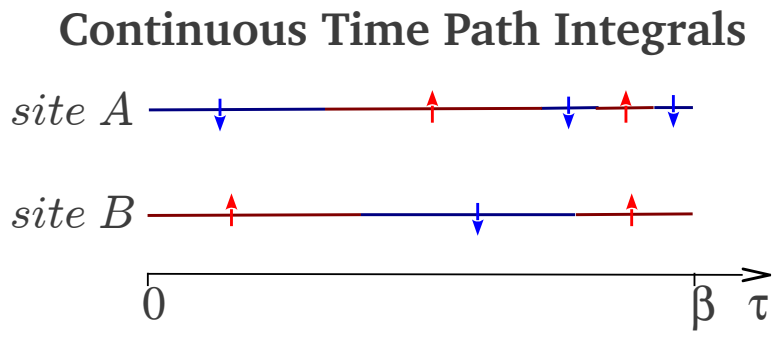
$\rightarrow$ precise results need extrapolation in M



Continuous-time formulation

For lattice models: continuous-time formulation to overcome the discretization error due to τ





Practical notes

Monte Carlo simulations can be easily and effectively parallelized, as there is essentially no communication needed during the random walk

- Initialization
- Equilibration (with different random seeds on different cores!)
- Random walk + measurements
- Gathering and storage of results

Simulation of fermions

Problem: $\pi(\mathbf{X})$ might be negative $\Rightarrow$ no probabilistic interpretation possible!
Trick: do the sampling according to $|\pi(\mathbf{X})|$

$$\bar{A} = \frac{\frac{1}{N!}\sum_P \int \mathrm{d}\mathbf{X}\, \pi(\mathbf{X}, P) A(\mathbf{X}, \mathbf{P})}{\frac{1}{N!}\sum_P \int \mathrm{d}\mathbf{X}\, \pi(\mathbf{X}, P)} = \frac{\langle A(\mathbf{X}, P) \cdot \mathrm{sign}(P)\rangle_{|\pi(\mathbf{X})|}}{\langle \mathrm{sign}(P)\rangle_{|\pi(\mathbf{X})|}}$$

Q: But does it **work well**?!

Complexity

Dimension of configuration space $\propto N$ (# of particles)
$\Rightarrow$ (# of configurations) scales exponentially with N

Monte Carlo approach, for any desired accuracy: **polynomial** in N (if the autocorrelation time does not increases faster than polynomial)

For fermions: $A = \frac{\sum_c A(c)p(c)}{\sum_c p(c)} = \frac{\langle A \cdot \mathrm{sign} \rangle_{|p(c)|}}{\langle \mathrm{sign} \rangle_{|p(c)|}}$

$$\Rightarrow \qquad \langle \mathrm{sign} \rangle_{|p(c)|} = \frac{Z}{Z'} = \exp\left(-\beta N (f - f') \right)$$

Z', f' ... correspond to the auxiliary system with weights $|p(c)|$

$$\Rightarrow \qquad \frac{\Delta \mathrm{sign}}{\langle \mathrm{sign} \rangle} \propto \frac{\sqrt{\left(\langle \mathrm{sign}^2 \rangle - \langle \mathrm{sign} \rangle^2 \right) / M}}{\langle \mathrm{sign} \rangle} \approx \frac{e^{\beta N (f - f')}}{\sqrt{M}}$$

Note: it is a problem of knowing a suitable representation.

Ref.:

M. Troyer and U.-J. Wiese: Phys. Rev. Lett. **94**, 170201 (2005).

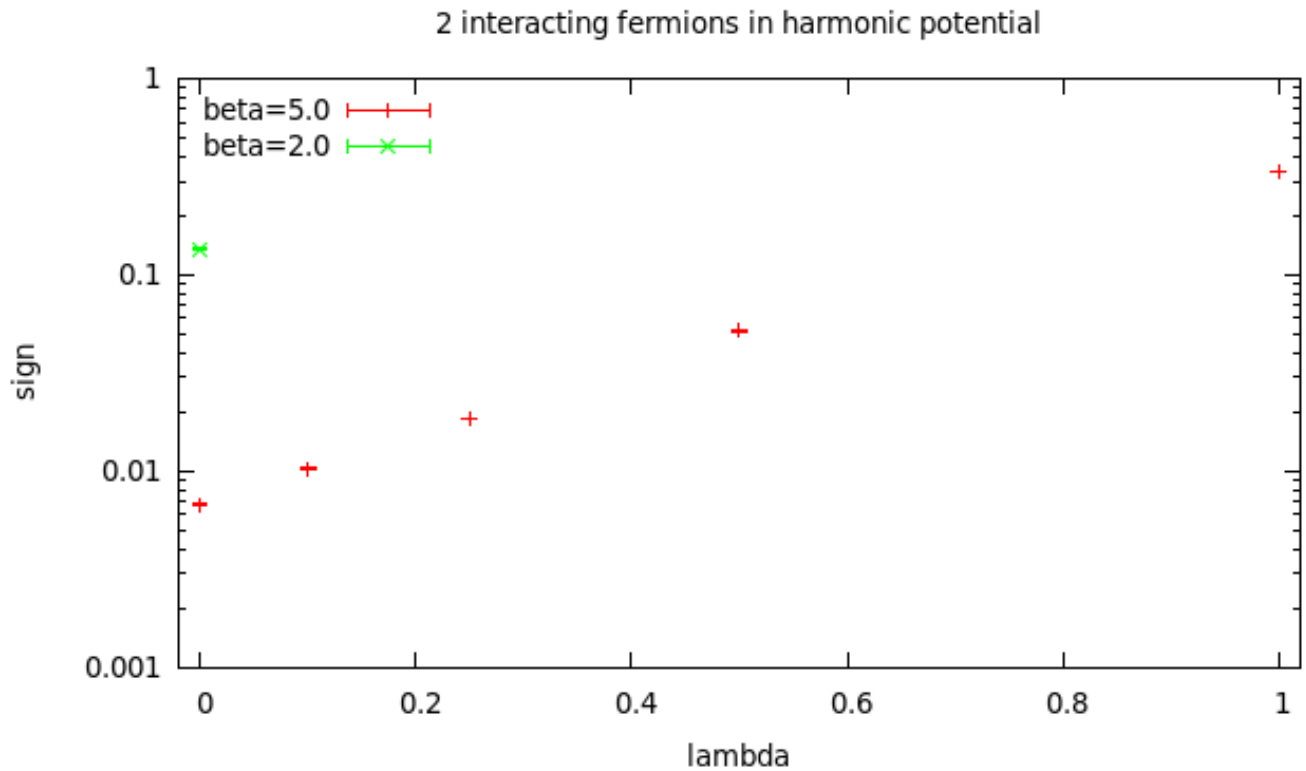
Sign problem illustration

Task: 2 interacting fermions in harmonic potential

$$\hat{\mathrm{H}} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2}m\omega^2 x_1^2 + \frac{1}{2}m\omega^2 x_2^2 - \lambda\,|x_1 - x_2| \qquad (2)$$

($\hbar = 1$, $\omega = 1$, $m = 1$, $k_B = 1$)

Method: PIMC as described so far, using coordinate basis.



Effective simulation of fermions

Hard due to the **sign problem**

Hubbard model:

$$\hat{\mathrm{H}} - \mu\hat{N} = \underbrace{-t \sum_{\langle i,j\rangle,\sigma} \left(\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma}\right) - \sum_{i,\sigma} \mu_{\sigma}\hat{n}_{i\sigma}}_{\hat{\mathrm{H}}_0} + \underbrace{U \sum_{i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}}_{\hat{\mathrm{H}}_U}$$

Few sign-free cases of the Hubbard model (if treated wisely):

- non-interacting fermions ($U = 0$)
- attracting fermions ($U < 0$) in absence of magnetic field ($\mu_{\uparrow} = \mu_{\downarrow}$)
- repulsive fermions ($U > 0$) on a bipartite lattice at half-filling ($\mu_{\sigma} = U/2$)

Note: here we work in grandcanonical ensemble (μVT)

QMC as time-dependent pertubation theory

Interaction representation ($\hat{H}_U = \hat{H}_{\rm int}$): $\hat{A}^I(t) = e^{\tau \hat{H}_0} \hat{A} e^{-\tau \hat{H}_0}$

$$
\begin{aligned}
Z &= \mathrm{Tr}\left(e^{-\beta \hat{H}}\right) = \mathrm{Tr}\left(e^{-\mathcal{T}_\tau \left(\beta \hat{H}_0 + \int_0^\beta \mathrm{d}\tau\, \hat{H}_{\rm int}(\tau)\right)}\right) \\
&= \mathrm{Tr}\left(\mathcal{T}_\tau e^{-\beta \hat{H}_0} e^{-\int_0^\beta \mathrm{d}\tau\, \hat{H}_{\rm int}(\tau)}\right) \\
&= \mathrm{Tr}\left(\mathcal{T}_\tau e^{-\beta \hat{H}_0} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \int_0^\beta \mathrm{d}\tau_1 \ldots \int_0^\beta \mathrm{d}\tau_k\, \hat{H}_{\rm int}(\tau_1) \ldots \hat{H}_{\rm int}(\tau_k)\right) \\
&= Z_0 \sum_{k=0}^{\infty} (-1)^k \int_0^\beta \mathrm{d}\tau_k \int_0^{\tau_k} \mathrm{d}\tau_{k-1} \ldots \int_0^{\tau_2} \mathrm{d}\tau_1 \left\langle \hat{H}_{\rm int}(\tau_k) \ldots \hat{H}_{\rm int}(\tau_1) \right\rangle_0
\end{aligned}
$$

with $\langle \ldots \rangle_0 \equiv \frac{1}{Z_0} \mathrm{Tr}\left(\mathcal{T}_\tau e^{-\beta \hat{H}_0} [\ldots]\right)$;
ordering $0 < \tau_1 < \tau_2 < \ldots < \tau_k < \beta$ in last line

Note: $Z_0 \left\langle \hat{H}_{\rm int}(\tau_k) \ldots \hat{H}_{\rm int}(\tau_1) \right\rangle_0 =$

$$
\mathrm{Tr}\left(e^{-(\beta-\tau_k)\hat{H}_0}\, \hat{H}_{\rm int}\, e^{-(\tau_k-\tau_{k-1})\hat{H}_0} \ldots e^{-(\tau_2-\tau_1)\hat{H}_0}\, \hat{H}_{\rm int}\, e^{-(\tau_1-0)\hat{H}_0}\right)
$$

Perturbative expansion of the partition function

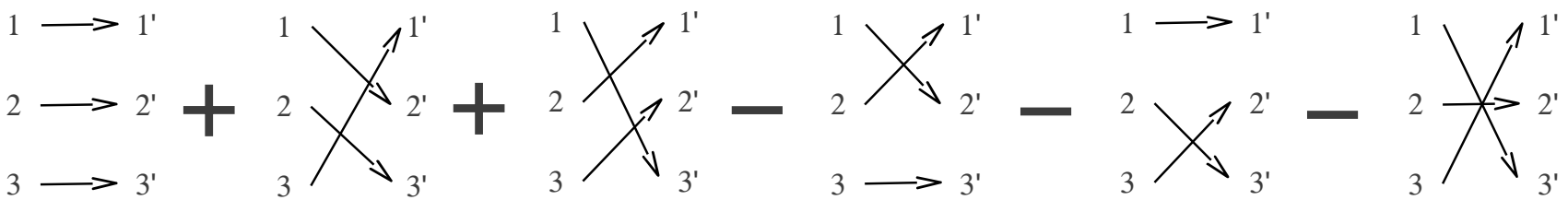
For $\hat{\mathrm{H}}_{\mathrm{int}} = \hat{\mathrm{H}}_U = U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$:

$$
\begin{aligned}
Z/Z_0 &= \sum_{k=0}^{\infty} \frac{(-U)^k}{k!} \sum_{i_1,\ldots,i_k} \int_0^\beta \mathrm{d}\tau_1 \ldots \int_0^\beta \mathrm{d}\tau_k \times \\
&\qquad \times \left\langle T_\tau n_{i_1\uparrow}(\tau_1) n_{i_1\downarrow}(\tau_1) \ldots n_{i_n\uparrow}(\tau_k) n_{i_n\downarrow}(\tau_k) \right\rangle_0 \\
&= 1 + \frac{(-U)}{1!} \sum_i \int_0^\beta \mathrm{d}\tau_1 \, \left\langle n_{i\uparrow}(\tau_1) n_{i\downarrow}(\tau_1) \right\rangle_0 \\
&\quad + \frac{(-U)^2}{2!} \sum_{i,j} \int_0^\beta \mathrm{d}\tau_1 \int_0^\beta \mathrm{d}\tau_2 \, \left\langle T_\tau n_{i\uparrow}(\tau_1) n_{i\downarrow}(\tau_1) n_{j\uparrow}(\tau_2) n_{j\downarrow}(\tau_2) \right\rangle_0 \\
&\quad + \ldots
\end{aligned}
$$

Wick's theorem for finite temperature

Wick's theorem schematic for 3 noninteracting particles:

$$\left\langle T_\tau c_1(\tau_1)c_2(\tau_2)c_3(\tau_3)c_{3'}^\dagger(\tau_{3'})c_{2'}^\dagger(\tau_{2'})c_{1'}^\dagger(\tau_{1'})\right\rangle_0 =$$



In general:

$$\left\langle T_\tau c_1(\tau_1)c_2(\tau_2)\dots c_{2'}^\dagger(\tau_{2'})c_{1'}^\dagger(\tau_{1'})\right\rangle_0 =$$

$$= \sum_{\text{permutations } p} (-1)^p \prod_r \underbrace{\left\langle T_\tau c_r(\tau_r)c_{p_r}^\dagger(\tau_{p_r})\right\rangle_0}_{\text{single-particle noninteracting Green's function}}$$

$\rightarrow$ structure of a **determinant**

Updates in continuous-time framework

$$Z = \sum_{k=0}^{\infty} \sum_{i_1,\ldots,i_k} \int_0^\beta \mathrm{d}\tau_1 \ldots \int_{\tau_{k-1}}^\beta \mathrm{d}\tau_k \overbrace{(-U)^k \det D_\downarrow(\mathbf{X}) \det D_\uparrow(\mathbf{X})}^{w(k, i_1, \tau_1, \ldots, i_k, \tau_k)}$$

Sampling over configurations $\mathbf{X} \equiv (k, i_1, \tau_1, \ldots, i_k, \tau_k)$

Time ordering assumed: $\tau_1 \leq \tau_2 \leq \ldots \leq \tau_k$

Weight: $w(k, i_1, \tau_1, \ldots, i_k, \tau_k)\mathrm{d}\tau_1 \ldots \mathrm{d}\tau_k$

Insertion update: $(k \to k+1)$ $\quad T_{\text{insertion}} = \frac{\mathrm{d}\tau}{N_{\text{sites}}\beta}$

Removal update: $(k+1 \to k)$ $\quad T_{\text{removal}} = \frac{1}{k+1}$

Acceptance rate:

$$A_{\text{insertion}} = \min\left(1, \frac{w(k+1, \ldots)}{w(k, \ldots)\mathrm{d}\tau} \frac{N_{\text{sites}}\beta}{k+1}\right)$$

$\to$ **infinitesimals cancel**

Note: $\langle \text{perturbation order} \rangle \propto \beta U$

Bipartite lattice treatment

$$\hat{\mathrm{H}} - \mu\hat{N} = -t \sum_{\langle i,j\rangle,\sigma} \left(\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma} \right) - \sum_{i,\sigma} \mu_\sigma \hat{n}_{i\sigma} + U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

Assumptions:

- bipartite lattice with sublattices A, B ($i \equiv (\mathbf{r}\alpha,\ \alpha = A, B)$
- nearest-neighbor hoppings only (precisely: A$\leftrightarrow$B only)

Particle-hole transformation on flavor $\downarrow$:

$$\hat{c}_{\mathbf{r}A\uparrow} = \tilde{c}_{\mathbf{r}A\uparrow}, \qquad \hat{c}_{\mathbf{r}B\uparrow} = \tilde{c}_{\mathbf{r}B\uparrow}, \qquad \hat{c}_{\mathbf{r}A\downarrow} = \tilde{c}^\dagger_{\mathbf{r}A\downarrow}, \qquad \hat{c}_{\mathbf{r}B\downarrow} = -\tilde{c}^\dagger_{\mathbf{r}B\downarrow}$$

$$\Rightarrow \hat{n}_{i\uparrow} = \tilde{n}_{i\uparrow}, \qquad \hat{n}_{i\downarrow} = 1 - \tilde{n}_{i\downarrow},$$

$$\hat{c}^\dagger_{\mathbf{r}A\sigma}\hat{c}_{\mathbf{r}'B\sigma} + \hat{c}^\dagger_{\mathbf{r}'B\sigma}\hat{c}_{\mathbf{r}A\sigma} = \tilde{c}^\dagger_{\mathbf{r}A\sigma}\tilde{c}_{\mathbf{r}'B\sigma} + \tilde{c}^\dagger_{\mathbf{r}'B\sigma}\tilde{c}_{\mathbf{r}A\sigma}$$

$$\hat{\mathrm{H}} - \mu\hat{N} = -t \sum_{\langle i,j\rangle,\sigma} \left(\tilde{c}^\dagger_{i\sigma}\tilde{c}_{j\sigma} + \tilde{c}^\dagger_{j\sigma}\tilde{c}_{i\sigma} \right) - (\mu_\uparrow - U)\tilde{n}_\uparrow + \mu_\downarrow \tilde{n}_\downarrow - U \sum_i \tilde{n}_{i\uparrow}\tilde{n}_{i\downarrow}$$

For $\mu_\uparrow = \mu_\downarrow = U/2$ we get flavor-symmetric model

Jackknife analysis (a special case of bootstrapping)

Usage: *For error estimate in the case of derived quantities*[4] *which have to be computed from the observables*

Data: *potentially cross-correlated binned (with binning* $\gg \tau_a, \tau_b$*) measurements* a_i, b_i $(1 \leq i \leq n \sim 100)$
Quantity of interest: $f(a, b)$

Jackknife procedure:

$$\text{mean} = f(\tilde{a}_0, \tilde{b}_0) - (n-1)\left[\frac{1}{n}\sum_{i=1}^{n} f(\tilde{a}_i, \tilde{b}_i) - f(\tilde{a}_0, \tilde{b}_0)\right],$$

$$\text{variance} = (n-1)\left[\frac{1}{n}\sum_{i=1}^{n} f(\tilde{a}_i, \tilde{b}_i)^2 - \left(\frac{1}{n}\sum_{i=1}^{n} f(\tilde{a}_i, \tilde{b}_i)\right)^2\right],$$

$$\text{with} \quad \begin{array}{ll} \tilde{x}_0 = \frac{1}{n}\sum_{j=1}^{n} x_j & \text{(simple mean)} \\ \tilde{x}_i = \frac{1}{n-1}\sum_{j\neq i} x_j & \text{(Jackknife bins)} \end{array}$$

Implemented in library ALPS: `http://alps.comp-phys.org/`

[4] For instance all physical measurements in the case of fermions

Boundary effects and finite size effects

Boundary effects **can be avoided** by using of periodic boundary condition.

Finite size effects:

- far from phase transitions they become small for systems much larger than the correlation length[5]
- close to the phase transitions: finite size scaling

[5] The correlation length might be in some cases of the order of 100 or more sites.

Stochastic series expansion

Taylor series for mapping of the quantum system onto the classical

$$
\begin{aligned}
Z &= \mathrm{Tr}\left(e^{-\beta\hat{\mathrm{H}}}\right) = \sum_{n=0}^{\infty}\frac{\beta^n}{n!}\mathrm{Tr}\left(\left(-\hat{\mathrm{H}}\right)^n\right) \\
&= 1+\sum_{n=1}^{\infty}\frac{\beta^n}{n!}\sum_{\{i_0,\ldots,i_{n-1}\}}\left\langle i_0\right|-\hat{\mathrm{H}}\left|i_1\right\rangle\left\langle i_1\right|-\hat{\mathrm{H}}\left|i_2\right\rangle\ldots\left\langle i_{n-1}\right|-\hat{\mathrm{H}}\left|i_0\right\rangle
\end{aligned}
$$

Simplifies for $\hat{\mathrm{H}} = -\sum_{\mathrm{b}}\hat{\mathrm{H}}_b$:

$$
Z = 1+\sum_{n=1}^{\infty}\frac{\beta^n}{n!}\sum_{\{i_0,\ldots,i_{n-1}\}}\sum_{b_1,\ldots,b_n}\left\langle i_0\right|\hat{\mathrm{H}}_{b_1}\left|i_1\right\rangle\left\langle i_1\right|\hat{\mathrm{H}}_{b_2}\left|i_2\right\rangle\ldots\left\langle i_{n-1}\right|\hat{\mathrm{H}}_{b_n}\left|i_0\right\rangle
$$

All the matrix elements of $\hat{\mathrm{H}}_b$ need to be positive, otherwise cancellation

- addition of positive constant to the diagonal terms
- for antiferromagnetic coupling: basis rotation on a sublattice (of a bipartite lattice)

Cluster updates

Local updates are inefficient:

- for large discretization M
- in the vicinity of the continuous phase transitions ($\rightarrow$ long correlation length $\rightarrow$ long autocorrelation times)

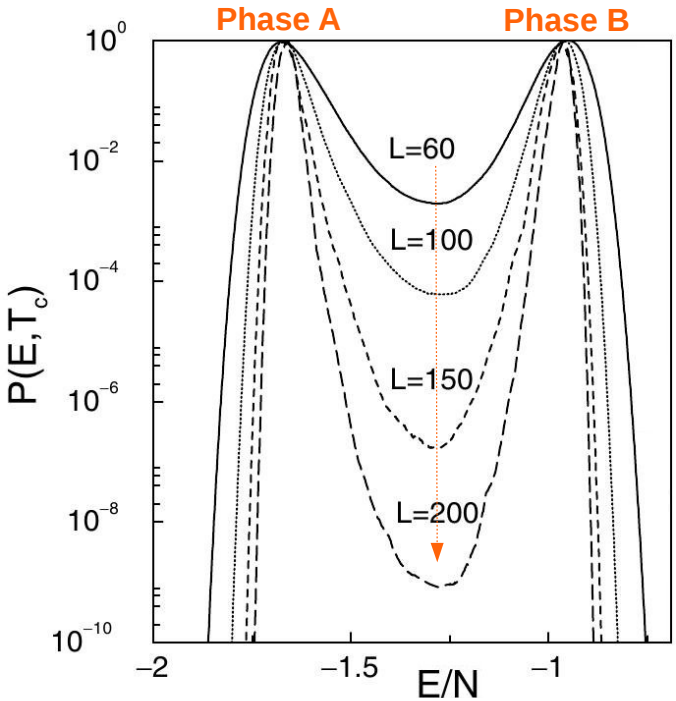
$\rightarrow$ large autocorrelations $\rightarrow$ reduction of number of effective measurements $\rightarrow$ larger statistical errors

$\rightarrow$ need for **global updates** (updating a full worldline, or several at once) to overcome the problem

Side effect:
Cluster updates enable usage of **improved estimators**

Critical slowing down

- "critical slowing down" in the case of continuous phase transitions and local updates
- true critical slowing down in case of phase transitions of 1^{st} order



Ref.:
F. Wang and D.P. Landau,
Phys. Rev. Lett. **86**, 2050 (2001).

$\rightarrow$ multicanonical ensemble (iteratively) aiming for flat histogram of energy,

$$Z = \sum_E \rho(E) e^{-\beta E}$$

Summary

- **Monte Carlo** measurement for intregrals/sums in high dimension
- random walk using the **Metropolis algorithm**
- **Suzuki–Trotter** formula for **mapping** of a quantum system onto a classical
- **sign problem** for fermions

Literature

- Lecture notes *Computational quantum physics* by M. Troyer (chapter 5, 9 and Monte Carlo notes) `http://www.itp.phys.ethz.ch/education/fs12/cqp`
- Introductory book *Quantum mechanics and path integrals* by R. P. Feynman and A. R. Hibbs (1965)
- N. Metropolis, *et al*: J. of Chem. Phys. **21**, 1087 (1953)
- *Selected topics from statistical physics* by V. Černý and M. Medo (chapters 3,4)
- *Continuous-time Monte Carlo methods for quantum impurity models* by E. Gull, *et al*: Rev. Mod. Phys. **83**, 349 (2011)
- on stochastic series expansion by R. Melko: `http://pitp.physics.ubc.ca/confs/sherbrooke2012/archives/Melko_SSEQMC.pdf`