Quantum Monte Carlo

Introduction

The World-Line Algorithm

The Determinant Algorithm

The Impurity Algorithm

The “sign” Problem & Constraint Path

…

What is Quantum Monte Carlo (QMC)?

- **Solving quantum mechanical problems by using Monte Carlo methods.**
- QMC has been successfully applied to various interesting quantum systems.
- Compare to classical system, QMC is still under developing. There exists some technical problems, especially for fermions.
- Some QMC methods: **world-line, Green's function, variation, determinant, etc.**

Quantum Monte Carlo Simulations

- Characteristics:
  - Treat correlations exactly
  - "Exact" solutions on finite (bigger) lattices, 12×12, 16×16, 20×20, …
  - Check on approximations
- Issues:
  - Finite size scaling
  - Stability: low temperatures, larger U, etc
  - "Negative" sign problem -> Constrained Path Monte Carlo (CPMC)

Quantum Monte Carlo Overview

- QMC are the Monte Carlo method (ways to do integration/summation) applied to quantum systems.
- The formalism overhead for quantum applications is higher than that for classical applications (operator to number; D to D+1).
- There exists no single best QMC method.

Quantum Monte Carlo Overview

- It is usually based on **Path Integral** formalism to transfer D-dimensional **quantum operator** →

  D+1-dimensional **classical variables**.

- One evaluates matrix elements directly or uses **HS (alike)** transformation to transfer many-body problem into a one-body (non-interacting) problem.
- Trace over quantum degrees are exactly performed (QM expectations, Wick's theorem, etc.).
- Evaluate physical quantities (multi-dimensional integrals, classical) by the MC method.

Main QMC Methods

- **Lattice**
  - T = 0 AF (Projector)
    - VMC
    - GFMC
  - T ≠0 AF (Determinant)
    - World-Line
- **Continuum**
  - DMC (Projector)
  - VMC
  - GFMC
  - Path Integral

Main QMC Methods

- AF – Auxiliary Field. This is the heart of most QMC methods for lattice models.
- DMC – Diffusion MC. An AF method in disguise. It is extensively used & very useful.
- VMC – Variational MC. It is used more for continuum problems than for lattice.
- GFMC – Green's Function MC. It is used infrequently because computational overhead.
- World-Line – The path integral in a discrete basis.

Mathematics

- Commutation relations
- Trotter Decomposition
- Linear algebra: matrix manipulations, eigenvalue analysis, singular value decomposition, etc.
- Integration, e.g., Gaussian integral
- Random number generation

Technical Issues

- HS-like Transformations
- Time domain algorithm: impurity, etc.
- Rate of configurations change ($\Delta\tau$, local minimum, critical slowing down, etc.)
- Numerical stability
- Bit operation
- Hybridization with Molecular Dynamics
- Parallelization
- “negative” sign!

Introduction to World-Line QMC Algorithm

- General Framework
- Quantum Anharmonic Oscillator
- One-dimensional Extended Hubbard Model
- *Parallelization, etc.*
- *Example Code on CM-200*

World-Line QMC Framework

- It is based on the ***Path Integral*** formalism
- It is mainly used to compute finite-temperature properties. Zero-temperature properties are approached by taking $\beta \to \infty$
- Expectation value of an operator A

  $$\langle A \rangle = (\mathrm{Tr}\, A\, e^{-\beta H})/Z$$

  where $Z = \mathrm{Tr}\, e^{-\beta H}$, $H = T + V$
- Evaluate these expectation values (multi-dimensional integrals) by the MC method.

Two Useful Mathematical Facts

- Factorizibility of exponentials

$$e^{-\beta H} = (e^{-\Delta\tau H})^L = e^{-\Delta\tau H}\, e^{-\Delta\tau H} \ldots e^{-\Delta\tau H}$$

where $L\Delta\tau = \beta$

- Cyclic property of a trace

$$\begin{aligned} \mathrm{Tr}\, A\, e^{-\beta H} &= \mathrm{Tr}\, A\, e^{-L\Delta\tau H} \\ &= \mathrm{Tr}\, e^{-\Delta\tau H} A\, e^{-(L-1)\Delta\tau H} \\ &= \mathrm{Tr}\, e^{-2\Delta\tau H} A\, e^{-(L-2)\Delta\tau H} \\ &= \text{etc.} \end{aligned}$$

Formal Development

Let $\{|s\rangle\}$ be some complete set of states:

$$\langle s|s'\rangle = \delta(s - s') \text{ and } \int ds\ |s\rangle\langle s| = 1$$

$$\mathrm{Tr}\left(Ae^{-\beta H}\right) = \int ds_1 \langle s_1 \mid Ae^{-\beta H} \mid s_1\rangle$$

$$= \int ds_1 \langle s_1 \mid Ae^{-\Delta\tau H} e^{-\Delta\tau H} \cdots e^{-\Delta\tau H} \mid s_1\rangle$$

$$= \int ds_1 ds_2 \cdots ds_L \langle s_1 \mid Ae^{-\Delta\tau H} \mid s_2\rangle\langle s_2 \mid e^{-\Delta\tau H} \mid s_3\rangle \cdots \langle s_L \mid e^{-\Delta\tau H} \mid s_1\rangle$$

$$= \int \left(\prod_{l=1}^{L} ds_l\right) \frac{\langle s_1 \mid Ae^{-\Delta\tau H} \mid s_2\rangle}{\langle s_1 \mid e^{-\Delta\tau H} \mid s_2\rangle} \prod_{l=1}^{L} \langle s_l \mid e^{-\Delta\tau H} \mid s_{l+1}\rangle$$

$$= \int \prod_{l=1}^{L} ds_l A(s_1, s_2) P(s_1, s_2, \ldots, s_L) Z \qquad S_{L+1} = S_1$$

where $P(s_1, s_2, \ldots, s_L) = \frac{1}{Z} \prod_{l=1}^{L} \langle s_l \mid e^{-\Delta\tau H} \mid s_{l+1}\rangle$

Application of the MC Method

1. Regard different $\{|s_l\rangle\}$ as occurring at different "time" steps
2. At each time step l
   - Propose $|s_l\rangle \rightarrow |s'_l\rangle$
   - Accept or reject each proposed move, for example, according to

$$P(s_l \rightarrow s'_l) = \min\left[1, \frac{P(s_1,\ldots,s_l+\delta s_l,\ldots,s_L)}{P(s_1,\ldots,s_l,\ldots,s_L)}\right]$$

$$= \min\left[1, \frac{\langle s_{l-1}|e^{-\Delta\tau H}|s'_l\rangle}{\langle s_{l-1}|e^{-\Delta\tau H}|s_l\rangle}\right]$$

   - For each observable of interest, compute and record

$$A(s_{l-1}, s_l) = \frac{\langle s_{l-1}|Ae^{-\Delta\tau H}|s_l\rangle}{\langle s_{l-1}|e^{-\Delta\tau H}|s_l\rangle}$$

3. Go back to step 2 and repeat until sufficient statistics are accumulated.
4. Compute final averages, estimate statistical error, and quit.

Quantum Anharmonic Oscillator

- In this example there is only one quantum particle moving in a 1D continuum.
- Hamiltonian

$$\hat{H} = \hat{T} + \hat{V}$$

$$\hat{T} = \frac{\hat{p}^2}{2m}, \quad \hat{V} = V(\hat{x}) = \frac{1}{2} m\omega^2 x^2 + \lambda(x^2 - f^2)^2$$

- Typically, $\{|s\rangle\} = \{|x\rangle\}$, the eigenstates of the position operator

$$\hat{x}\,|\,x\rangle = x\,|\,x\rangle$$

$$V(\hat{x})\,|\,x\rangle = V(x)\,|\,x\rangle$$

Trotter Approximation

- Factorization of exponentials

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

- Symmetric Factorization of exponentials

$$e^{-\Delta\tau\,(\mathrm{A}+\mathrm{B})} = e^{-\Delta\tau\,\mathrm{A}/2}\, e^{-\Delta\tau\,\mathrm{B}}\, e^{-\Delta\tau\,\mathrm{A}/2}$$

$$+ \mathrm{O}([\mathrm{A},\mathrm{B}]\Delta\tau^{3})$$

Matrix Element Evaluation

- The key matrix element

$$\langle x_{l-1} | e^{-\Delta\tau \hat{H}} | x_l \rangle \approx \langle x_{l-1} | e^{-\Delta\tau \hat{T}} e^{-\Delta\tau \hat{V}} | x_l \rangle$$

$$= \langle x_{l-1} | e^{-\Delta\tau \hat{T}} | x_l \rangle e^{-\Delta\tau \hat{V}(x_l)}$$

$$\langle x_{l-1} | e^{-\Delta\tau T} | x_l \rangle = \langle x_{l-1} | e^{-\Delta\tau p^2/2m} | x_l \rangle$$

$$= \int dp \langle x_{l-1} | e^{-\Delta\tau p^2/2m} | p \rangle \langle p | x_l \rangle$$

where $|p\rangle$ is an eigenstate of the momentum operator

$$\langle x|p\rangle = e^{ipx}$$

- Accordingly $\langle x_{l-1} | e^{-\Delta\tau \hat{T}} | x_l \rangle = \int dp\, e^{-\Delta\tau\, p^2/2m} e^{ip(x_{l-1}-x_l)}$

$$= \sqrt{\frac{2m\pi}{\Delta\tau}} e^{\frac{1}{2}m\Delta\tau[(x_l - x_{l-1})/\Delta\tau]^2}$$

The Path Integral

- When all the pieces are assembled, an imaginary-time Feynman path integral appears

$$\langle A \rangle = \frac{\int \boldsymbol{Dx} A e^{-\Delta\tau S}}{\int \boldsymbol{Dx} e^{-\Delta\tau S}} \sim \frac{\int \boldsymbol{Dx} A e^{-d\tau S}}{\int \boldsymbol{Dx} e^{-d\tau S}} \quad \text{where } \boldsymbol{Dx} = \prod_l \boldsymbol{dx}_l$$

(The overall constants divide out of expectation values.)

$$S = \tfrac{1}{2} m\omega^2 \sum_l x_l^2 + \lambda \sum_l (x_l^2 - f^2)^2 + \frac{m}{2(\Delta\tau)^2} \sum_l (x_l - x_{l+1})^2$$

$$= \sum_l V(x_l) + \tfrac{1}{2} m \sum_l \left(\frac{x_l - x_{l+1}}{\Delta\tau} \right)^2$$

- The integration has the interpretation of a sum over all possible paths.

Physical Interpretation

- The single particle **quantum** problem has been transformed into a L particle **classical** problem.
- Each classical particle moves in the potential $V(x)$ and interacts with its neighbor through a harmonic potential whose force constant is $m/(\Delta\tau)^2$.
- Since $x_1 = x_{L+1}$, because of the periodicity in imaginary-time imposed by the trace, the particle chain forms a loop (**world-line**).

Important Points

- Choice of $\{|s_l\rangle\}$

  The states are usually chosen so that either T or V is easily diagonalized.

- Value of $\langle s_{l-1}|e^{-\Delta\tau H}|s_l\rangle$

  If $\Delta\tau$ is small, one can use the Trotter approximation as follow (assume $\{|s_l\rangle\}$ diagonalized V)

$$\begin{aligned}\langle s_{l-1}|e^{-\Delta\tau H}|s_l\rangle &\approx \langle s_{l-1}|e^{-\Delta\tau T}e^{-\Delta\tau V}|s_l\rangle \\ &= \int ds\, \langle s_{l-1}|e^{-\Delta\tau T}|s\rangle \langle s|\, e^{-\Delta\tau V}|s_l\rangle \\ &= \int ds\, \langle s_{l-1}|e^{-\Delta\tau T}|s\rangle\, e^{-\Delta\tau V(s_l)}\, \delta(s-s_l) \\ &= \langle s_{l-1}|e^{-\Delta\tau T}|s_l\rangle\, e^{-\Delta\tau V(s_l)}\end{aligned}$$

  The remaining matrix element is evaluated by some "standard" means.

Important Points

- Positivity of $P(s_1, s_2, \ldots, s_L)$

  In fact it is almost never always positive for fermions in two and higher dimensions and frustrated quantum spin systems.

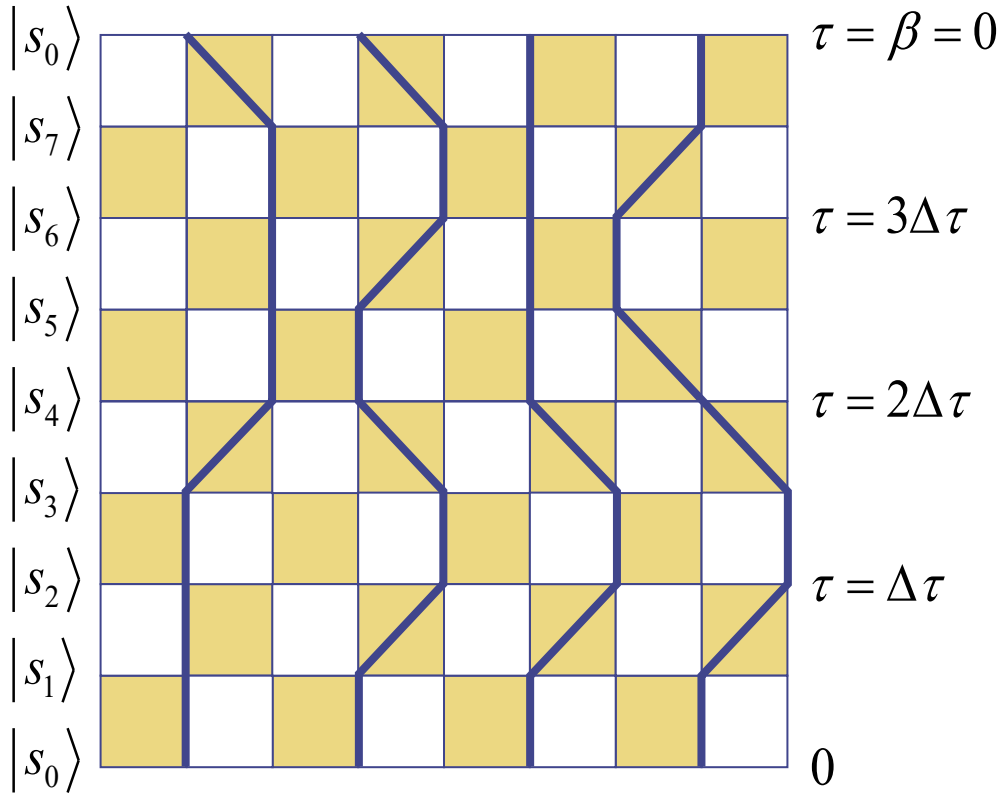
- Model dependent, e.g., XXZ model.

Physical Interpretation

- The ***d***-dimensional many particle quantum problem has been transformed into a ***d*+1**-dimensional classical problem.
- This could be regarded as an **Ising model** with complicated couplings (matrix elements) and the summation (Monte Carlo) is over all possible configuration (paths).
- Due to the periodicity in imaginary-time imposed by the trace, $s_0 = s_{2L}$, the ‘‘particle’’ travels in a loop, i.e., the ***world-line***.

Checkboards and World-lines

$$Z = \sum_{\mathrm{S}} \prod_{\substack{\text{shaded} \\ \text{squares}}} \left\langle s' \left| \hat{U} \right| s \right\rangle .$$



$$Z = \mathrm{Tr}\{e^{-\beta H}\}$$

$$= \sum_{s_0 \cdots s_{L-1}} \left\langle s_0 \left| e^{-\Delta\tau H} \right| s_{L-1} \right\rangle \cdots \left\langle s_2 \left| e^{-\Delta\tau H} \right| s_1 \right\rangle \left\langle s_1 \left| e^{-\Delta\tau H} \right| s_0 \right\rangle$$

$$= \sum_{s_0 \cdots s_{2L-1}} \left\langle s_0 \left| U_2 \right| s_{2L-1} \right\rangle \cdots \left\langle s_3 \left| U_1 \right| s_2 \right\rangle \left\langle s_2 \left| U_2 \right| s_1 \right\rangle \left\langle s_1 \left| U_1 \right| s_0 \right\rangle$$

where $H = H_1 + H_2, \quad U_{1(2)} \equiv e^{-\Delta\tau H_{1(2)}}, \quad \Delta\tau \equiv \beta / L .$

World-Line QMC Algorithm

- Applications
- Path Integral Decomposition of the Partition Function
- Checkboard and World-line
- Propagation Matrix Elements
- Monte Carlo Simulation
- Statistics of WLQMC
- Parallelization of WLQMC

World-Line QMC Applications

- Hubbard-like (e-e) models
- Peierls-Hubbard (e-p) models
- Short-range interactions
- Mostly one dimension
- Non-frustrated spin models (2-, 3-D)

:

:

1-D Extended Hubbard Model

$$H = -t \sum_{i=1,\sigma=\uparrow\downarrow}^{N} \left(c_{i,\sigma}^{\dagger} c_{i+1,\sigma} + H.c \right) + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow} + V \sum_{i=1}^{N} n_i n_{i+1}$$

$$= H_1 \left(i : \text{odd} \right) + H_2 \left(i : \text{even} \right)$$

where $n_{i\sigma} = c_{i,\sigma}^{\dagger} c_{i,\sigma}$ and $n_i = n_{i\uparrow} + n_{i\downarrow}$.

All terms in $H_{1(2)}$ commute with each other.

Parameter:

Coulomb interactions: U, V, ($t = 1$).

Band filling: $\rho \equiv N_e/N$.

XXZ Model Hamiltonian

$$H = \sum_{\langle i,j \rangle} J_x \left(S_i^x S_j^x + S_i^y S_j^y \right) + J_z S_i^z S_j^z = \sum_{\langle i,j \rangle} \frac{J_x}{2} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) + J_z S_i^z S_j^z$$

$$\left(\hat{B}_{i,i+1} \qquad \hat{V}_{i,i+1} \right)$$

where $\langle i, j \rangle$: Nearest-Neighbor Pair

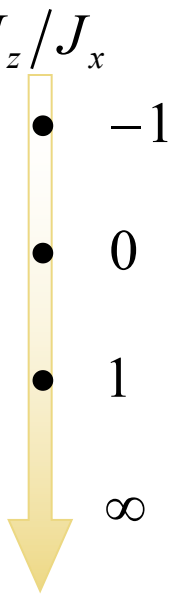
S_i^α : Spin Operator on Site i

FMH Model : $J_z = -J_x$

XY Model : $J_z = 0$

AMH Model : $J_z = J_x \equiv J > 0$

Ising Model : $J_x = 0$



Functional Integral Decomposition

The partition function $Z = \mathrm{Tr}\, e^{-\beta\hat{H}}$, could be rewritten as a discrete form by dividing the imaginary time interval $0 \le \tau < \beta$ into L slices of width $\Delta\tau = \beta/L$ and inserting complete sets of states at each time-slice:

$$Z = \sum_{s_0 \cdots s_{L-1}} \left\langle s_0 \left| e^{-\Delta\tau\hat{H}} \right| s_{L-1} \right\rangle \cdots \left\langle s_2 \left| e^{-\Delta\tau\hat{H}} \right| s_1 \right\rangle \left\langle s_1 \left| e^{-\Delta\tau\hat{H}} \right| s_0 \right\rangle$$

Write $\hat{\boldsymbol{H}}$ as the sum of two easily diagonalizable pieces, $\hat{\boldsymbol{H}} = \hat{\boldsymbol{H}}_1 + \hat{\boldsymbol{H}}_2$,

$$\hat{H}_1 = \sum_{i \text{ odd}} -t\hat{B}_{i,i+1} + \hat{V}_{i,i+1},$$

$$\hat{H}_2 = \sum_{i \text{ even}} -t\hat{B}_{i,i+1} + \hat{V}_{i,i+1},$$

where $\hat{B}_{i,i+1} = c^{\dagger}_{i,\sigma} c_{i+1,\sigma} + \text{h.c.}$

$$\hat{V}_{i,i+1} = V n_i n_{i+1} + \frac{1}{2} U \left(n_{i\uparrow} n_{i\downarrow} + n_{i+1\uparrow} n_{i+1\downarrow} \right).$$

Trotter approximation: $e^{-\Delta\tau\hat{H}} = e^{-\Delta\tau\hat{H}_2/2} e^{-\Delta\tau\hat{H}_1} e^{-\Delta\tau\hat{H}_2/2} + O\left(\Delta\tau^3\right)$

We obtain,

$$Z = \sum_{s_0 \cdots s_{2L-1}} \left\langle s_0 \left| e^{-\Delta\tau \hat{H}_2} \right| s_{2L-1} \right\rangle \cdots \left\langle s_3 \left| e^{-\Delta\tau \hat{H}_1} \right| s_2 \right\rangle \left\langle s_2 \left| e^{-\Delta\tau \hat{H}_2} \right| s_1 \right\rangle \left\langle s_1 \left| e^{-\Delta\tau \hat{H}_1} \right| s_0 \right\rangle$$

$$= \sum_{s_0 \cdots s_{2L-1}} \left\langle s_0 \left| \hat{U}_2 \right| s_{2L-1} \right\rangle \cdots \left\langle s_3 \left| \hat{U}_1 \right| s_2 \right\rangle \left\langle s_2 \left| \hat{U}_2 \right| s_1 \right\rangle \left\langle s_1 \left| \hat{U}_1 \right| s_0 \right\rangle$$

where $\hat{U}_i = e^{-\Delta\tau \hat{H}_i}$.

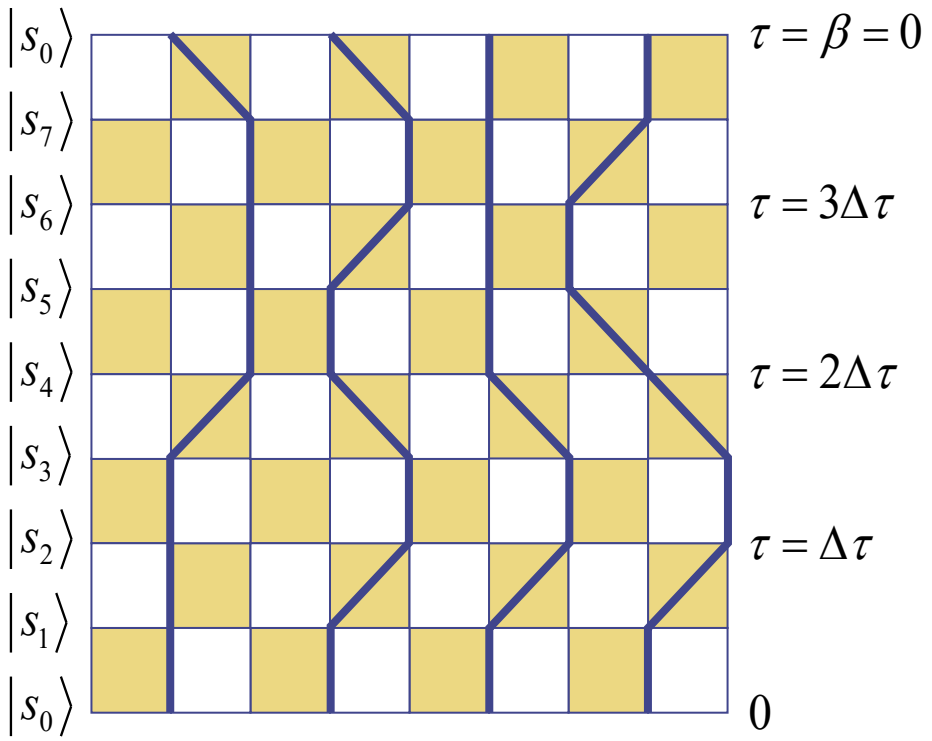
With the choice of $\hat{H}_{\binom{1}{2}}$, the individual evolution terms $\hat{U}_n = e^{-\Delta\tau \hat{H}_n}$ may be rewritten as

$$e^{-\Delta\tau \hat{H}_{\binom{1}{2}}} = \prod_{i\binom{odd}{even}} e^{-\Delta\tau \frac{1}{2} \hat{V}_{i,i+1}} e^{\Delta\tau t \hat{B}_{i,i+1}} e^{-\Delta\tau \frac{1}{2} \hat{V}_{i,i+1}} + O\left(\Delta\tau^3\right)$$

$$\left\langle s_{\alpha+1} \left| e^{-\Delta\tau \hat{H}_{\binom{1}{2}}} \right| s_\alpha \right\rangle = \prod_{i\binom{odd}{even}} \left\langle s_{\alpha+1} \left| e^{-\Delta\tau \frac{1}{2} \hat{V}_{i,i+1}} e^{\Delta\tau t \hat{B}_{i,i+1}} e^{-\Delta\tau \frac{1}{2} \hat{V}_{i,i+1}} \right| s_\alpha \right\rangle$$

Checkboard and World-lines

$$Z = \sum_{\mathrm{S}} \prod_{\substack{\text{shaded} \\ \text{squares}}} \left\langle s' \left| \hat{U} \right| s \right\rangle .$$



$$Z = \mathrm{Tr}\{e^{-\beta H}\}$$

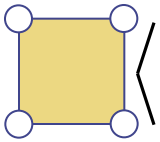
$$= \sum_{s_0 \cdots s_{L-1}} \left\langle s_0 \left| e^{-\Delta\tau H} \right| s_{L-1} \right\rangle \cdots \left\langle s_2 \left| e^{-\Delta\tau H} \right| s_1 \right\rangle \left\langle s_1 \left| e^{-\Delta\tau H} \right| s_0 \right\rangle$$

$$= \sum_{s_0 \cdots s_{2L-1}} \left\langle s_0 \left| U_2 \right| s_{2L-1} \right\rangle \cdots \left\langle s_3 \left| U_1 \right| s_2 \right\rangle \left\langle s_2 \left| U_2 \right| s_1 \right\rangle \left\langle s_1 \left| U_1 \right| s_0 \right\rangle$$

where $H = H_1 + H_2$, $\quad U_{1(2)} \equiv e^{-\Delta\tau H_{1(2)}}$, $\quad \Delta\tau \equiv \beta / L$.

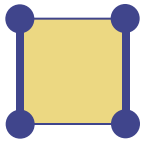
Propagation Matrix Elements

The matrix elements $\left\langle s_{\alpha+1} \left| e^{-\Delta\tau \hat{H}_n} \right| s_\alpha \right\rangle$ may factor into the product of two-site evolution matrix elements, $(\mathbf{U} = \mathbf{0})$



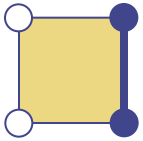
$\left\langle 00 \left| \hat{U} \right| 00 \right\rangle = 1$

$0000_2 = 0$



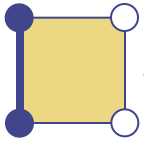
$\left\langle 11 \left| \hat{U} \right| 11 \right\rangle = e^{-\Delta\tau V}$

$1111_2 = 15$



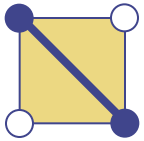
$\left\langle 01 \left| \hat{U} \right| 01 \right\rangle = \cosh(t\Delta\tau)$

$0110_2 = 6$



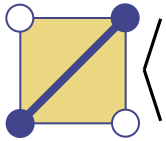
$\left\langle 10 \left| \hat{U} \right| 10 \right\rangle = \cosh(t\Delta\tau)$

$1001_2 = 9$



$\left\langle 01 \left| \hat{U} \right| 10 \right\rangle = \sinh(t\Delta\tau)$

$1010_2 = 10$



$\left\langle 10 \left| \hat{U} \right| 01 \right\rangle = \sinh(t\Delta\tau)$

$0101_2 = 5$

Monte Carlo Simulations

- Boltzmann Weight

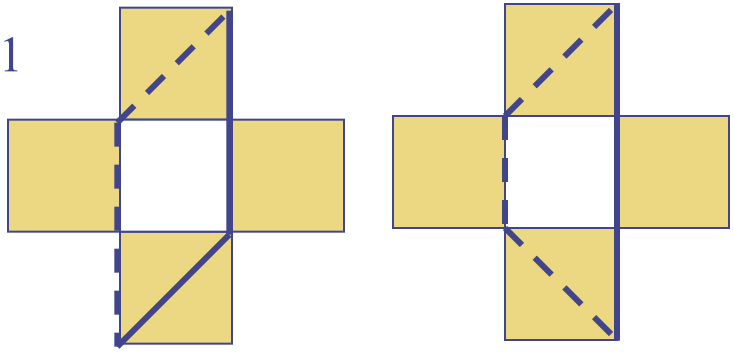
$$P(\mathrm{S}) = \left\langle s_1 \left| \hat{U}_2 \right| s_{2L} \right\rangle \cdots \left\langle s_3 \left| \hat{U}_2 \right| s_2 \right\rangle \left\langle s_4 \left| \hat{U}_1 \right| s_1 \right\rangle / Z$$

where $P(\mathrm{S})$ is the probability for configuration S.

- Possible Move

$$s \equiv n_{i,l} + n_{i,l+1} - n_{i+1,l} - n_{i+1,l+1}$$

$$= \pm 2$$



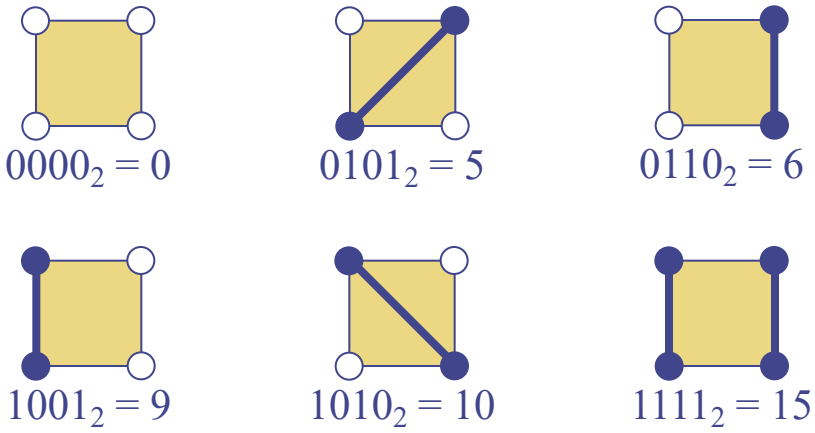
- Ratio of Change

$$R = [\tanh(\Delta\tau\, t)]^{sx} [\cosh(\Delta\tau\, t)]^{sy}$$

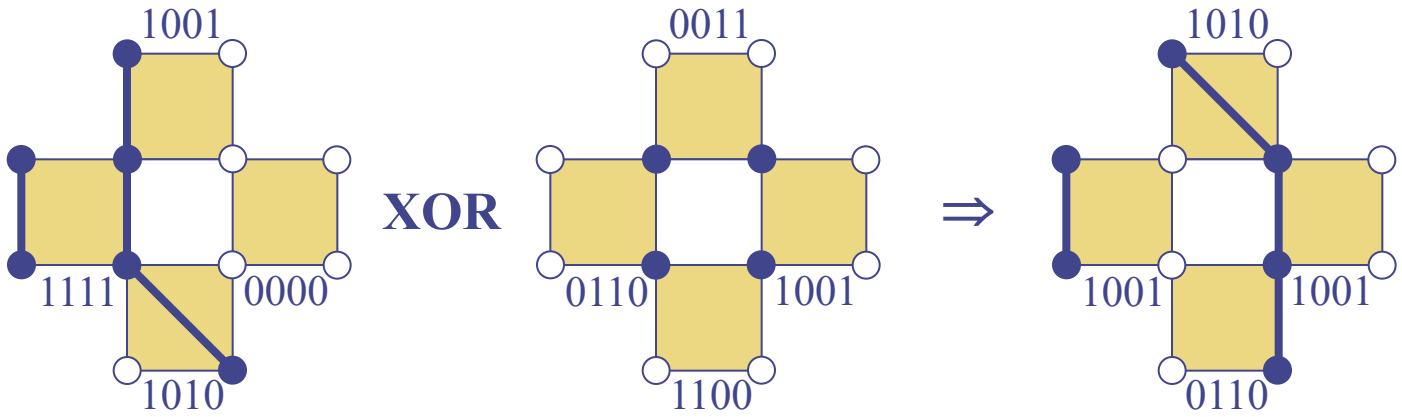
$$x = 1 - n_{i+1,l-1} - n_{i+1,l+2}$$

$$y = n_{i-1,l} - n_{i+2,l}$$

Plaquette Representation and Bits Operation



16 binary numbers



Correlation Functions and Measurements

- Local Operator

$$CDW(i,j) = \left\langle \left(\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}\right)\left(\hat{n}_{j\uparrow} + \hat{n}_{j\downarrow}\right)\right\rangle$$

$$= \frac{1}{2LM}\sum_{m=1}^{M}\sum_{l=1}^{2L}\sum_{k=1}^{N} n(i+k,l)\,n(j+k,l)$$

- Non-local Operator

$g(i-j,\tau) = \left\langle c_i(\tau)\, c_j^{\dagger}(0)\right\rangle$. One has to disconnect world lines.

- 2-Site Operator

$$\hat{B} = \hat{B}_1 + \hat{B}_2$$

$$\left\langle \hat{B}(n)\right\rangle = \mathrm{Tr}\left(\hat{U}_1\hat{U}_2\right)^{L-n}\hat{B}\left(\hat{U}_1\hat{U}_2\right)^{n} / Z$$

$$= \mathrm{Tr}\, P(\mathrm{S})\left(\frac{\left\langle s_{2n+1}\left|\hat{U}_1\hat{B}_1\right|s_{2n}\right\rangle}{\left\langle s_{2n+1}\left|\hat{U}_1\right|s_{2n}\right\rangle} + \frac{\left\langle s_{2n}\left|\hat{U}_2\hat{B}_2\right|s_{2n-1}\right\rangle}{\left\langle s_{2n}\left|\hat{U}_2\right|s_{2n-1}\right\rangle}\right).$$

Statistics of WLQMC

- MC Steps

  Fast

- Measurements

  Slow (non-local)

- Reach Equilibrium

  Slow

- Local Minimum for Large U, V

  Special treatment.

Comments - Technical Issues

- Choice of the size of $\Delta\tau$
  - Empirically determined so the systematic error is smaller than the acceptable statistical error.
  - If made too small, unacceptably large auto-correlation times result.
  - New methods (continuous time methods) eliminate the Trotter approximation but that is not their principal advantage.
- Measurement of unequal time Green's functions such as $G_{ij}(\tau>0) = \langle x_i(\tau)\, x_j(0)\rangle$ is impractical.
  - Measurements of this type of quantity is the main advantage of the continuous time methods.

Comments - General Issues

- Three-dimensional simulations are almost never done because of the small systems sizes possible with currently available computer time allocations.
- The World-Line (Path Integral) method is very useful for 1,2D bosonic and quantum spin systems.
- These methods are not very useful for frustrated quantum spin systems.
  - The lack of positivity of matrix elements prevent the sampling probability from always being positive.
  - This, as other QMC sign problems, leads to variances in computed results increasing exponentially with increasing system size and decreasing temperature.

For electron and electron-phonon systems, use is limited to 1D

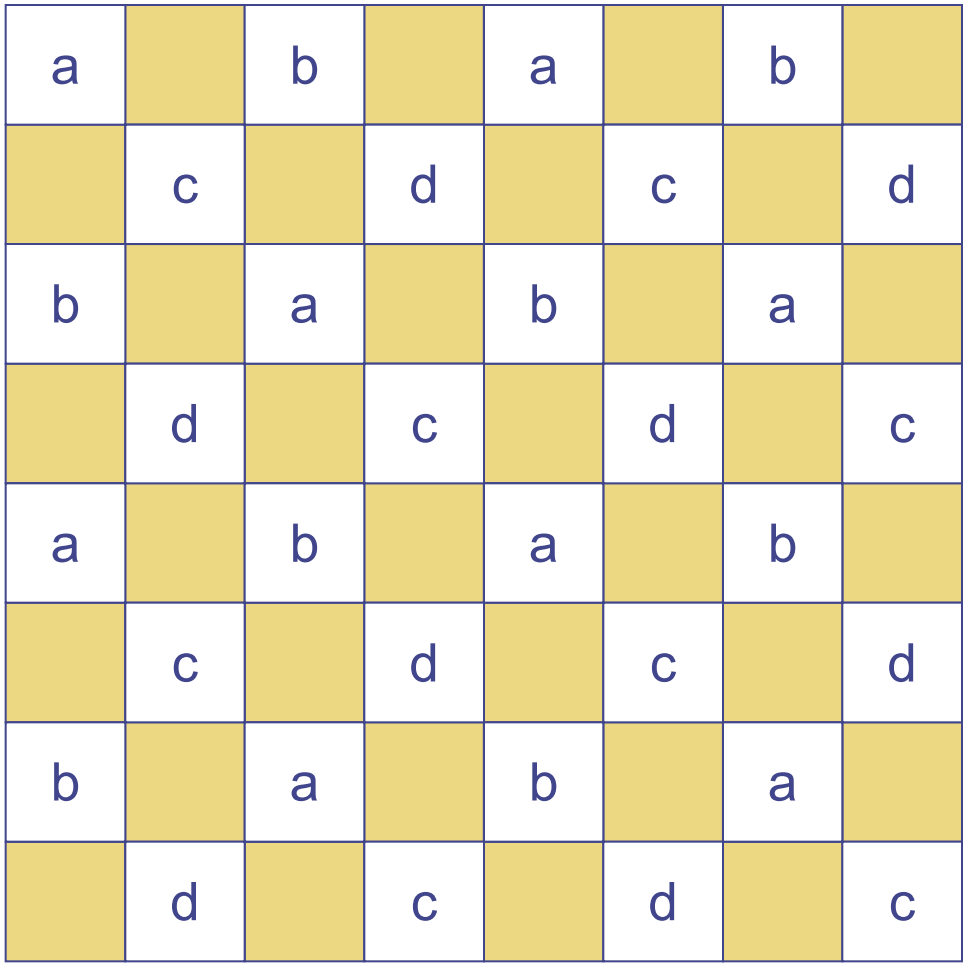
- In 2D, the fermion sign problem can be horrendous.
  - It requires sampling from probabilities which are not always positive.
  - It is caused by exchanging an odd number of electrons.
- Simulations of fermions with spin use two checkerboards, one for up and one for down spin.
  - With the electron occupancies on one spin are fixed, one samples the occupancies of the other spin, then vice versa.
- Simulation of electron-phonon systems use the **world-line** method for the electron part and the path integral method for the phonon part.
  - With the electron occupancies fixed, one samples the lattice displacements and then vice versa.

The Metropolis algorithm is not always the most efficient Monte Carlo algorithm

- For lattice system with a small number of discrete states per plaquette $$P(s \to s') = \frac{R}{1+R}$$ where R is the ratio of the after and before probabilities, is often more efficient.
- For quantum spins and some electron problems, **loop/cluster algorithms** can be three or more orders of magnitude more efficient.
- For boson (phonon) systems the hybrid Monte Carlo method is much more efficient (see below).

Parallelisation of WLQMC

- Parallel Machines: Origin 2000, PC Cluster, etc
- Four independent sub-lattices.



Other QMC Methods

- The principle is the same: change quantum problem into classical problem via path integral, quantum D dimensions => classical $D+1$ dimensions.
- Operator => numeric number by evaluating it in a selected basis $\{|s_l\rangle\}$. Choice of $\{|s_l\rangle\}$?
- Express all measurements in a matrix form.
- Perform Monte Carlo integration (sampling) to evaluate relevant summations.
- For boson & spin systems, straightforward, while for fermion, there is "sign" problem.

The Peierls-Hubbard Model

$$H = H_{\text{electron}} + H_{\text{phonon}} + H_{\text{electron-phonon}}$$

$$H_{\text{electron}} = -t \sum_{\langle i,j\rangle,\sigma} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + H.c \right) + \sum_i U_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle i,j\rangle} n_i n_j + \sum_{i\sigma} \varepsilon_i n_{i\sigma} + \sum_i (-1)^i h_s \left(n_{i\uparrow} - n_{i\downarrow} \right)$$

$$H_{\text{phonon}} = \sum_i \left(\frac{p_i^2}{2m} + \frac{1}{2} K_1 q_i^2 + \frac{1}{4} g_1 q_i^4 \right) + \sum_i \frac{P_i^2}{2M} + \sum_{\langle i,j\rangle} \left(\frac{1}{2} K_2 u_{ij}^2 + \frac{1}{4} g_2 u_{ij}^4 \right)$$

$$H_{\text{electron-phonon}} = \lambda_1 \sum_{i\sigma} q_i n_{i\sigma} + \lambda_2 \sum_{\langle i,j\rangle,\sigma} u_{ij} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + H.c \right)$$

where $n_i = n_{i\uparrow} + n_{i\downarrow}$

u_{ij} = Relative Lattice Displacement on Bond $\langle i, j \rangle$

q_i = Optical Phonon

SSH, Holstein (Dimerization, Soliton, etc).

Adiabatic Approximation (Double well)

Monte Carlo Simulations

$$
\begin{aligned}
Z &= \mathrm{Tr}\left(e^{-\beta H}\right) \\
&= \int \prod_{i,l} \mathrm{d}q_{il}\mathrm{d}u_{il}\, \exp\left[-s'\left(q_{il};u_{il}\right)\right] \\
&\times \mathrm{Tr} \prod_{l=1}^{L} \left\{ \exp\left[\Delta\tau \sum_{i\mathrm{even},\sigma} t_{i,i+1}^{(l)} \left(c_{i\sigma}^{\dagger} c_{i+1\sigma} + H.c\right) - \lambda_1 q_{il} n_{il\sigma} \right] \right. \\
&\qquad \left. \exp\left[\Delta\tau \sum_{i\mathrm{odd},\sigma} t_{i,i+1}^{(l)} \left(c_{i\sigma}^{\dagger} c_{i+1\sigma} + H.c\right) - \lambda_1 q_{il} n_{il\sigma} \right] \right\}
\end{aligned}
$$

where

$$\beta = \Delta\tau L$$

$$t_{i,i+1}^{(l)} = t - \lambda_2 \left(u_{i+1,l} - u_{il}\right)$$

$$
\begin{aligned}
s'\left(q_{il};u_{il}\right) &= \frac{m_1}{2\Delta\tau}\left(q_{i,l+1} - q_{il}\right)^2 + \frac{\Delta\tau}{2} m_1 \omega_1^2 q_{il}^2 + \frac{\Delta\tau}{4} g_1 q_{il}^4 \\
&+ \frac{m_2}{2\Delta\tau}\left(u_{i,l+1} - u_{il}\right)^2 + \frac{\Delta\tau}{2} m_2 \omega_2^2 \left(u_{i+1,l} - u_{il}\right)^2 + \frac{\Delta\tau}{4} g_2 \left(u_{i+1,l} - u_{il}\right)^4
\end{aligned}
$$

$$e^{\Delta\tau\left(H_1+H_2\right)} \simeq e^{\Delta\tau H_1} e^{\Delta\tau H_2} e^{\Delta\tau^2 [H_1,H_2]}$$

Notation

- Use electron occupation number as basis

  $n_{il\sigma}$ (operator) $\rightarrow$ $n_{il\sigma}$ (c-number)

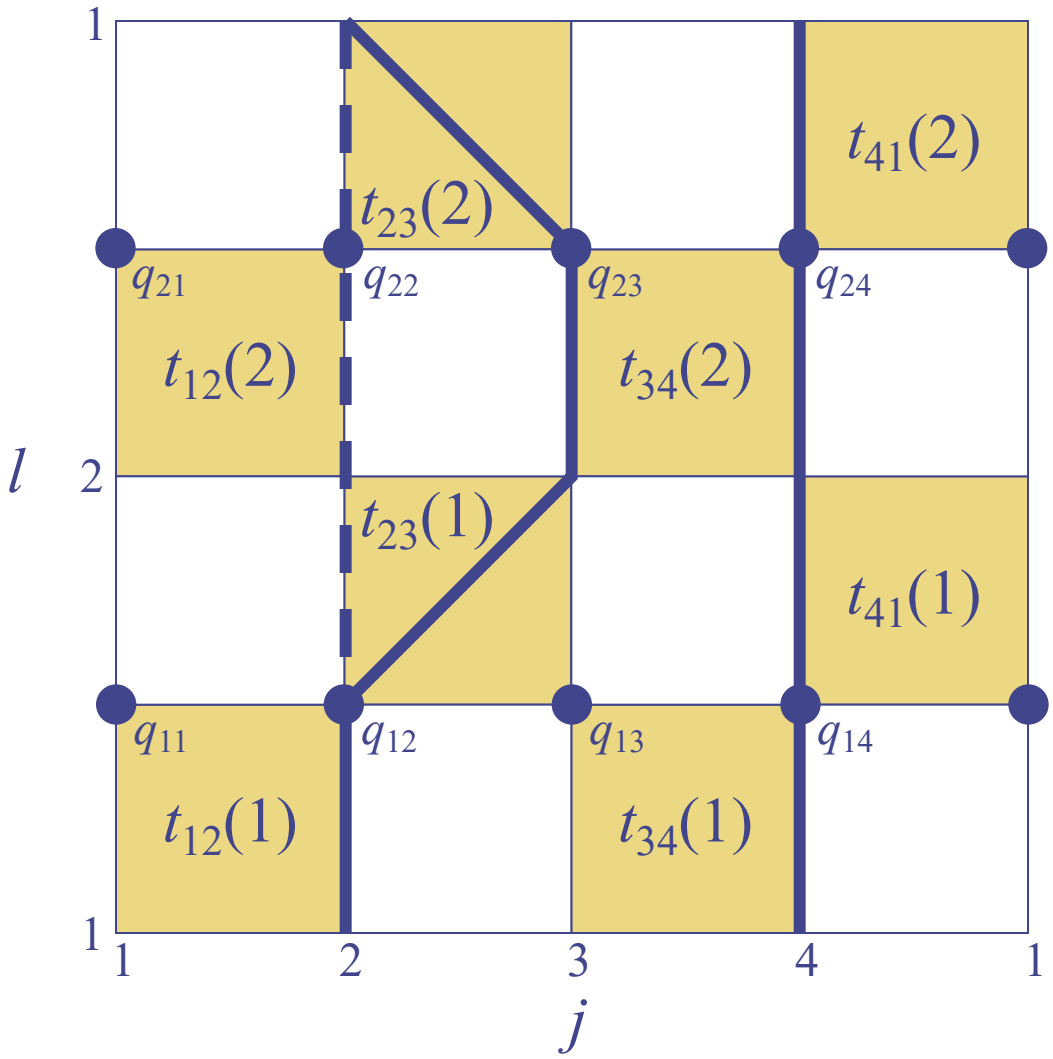
-  represents matrix elements
-  represent electron world line
- Change of configurations (Stochastic Process)
- Electron Part:

  local move (highly parallel)

  conservation rule, etc.

Checkboard Representation of Configuration



Methodology

- Electron Part: World-line Monte Carlo, which is local
  - Parallelizable (Vectorizable)
  - Much Fast
  - Larger system and lower Temperature
  - e.g. $N = 512$, $\beta = 128$, $U = 16$
- Phonon Part: Hybrid Monte Carlo
  - Reach equilibrium faster than Metropolies

Phonon Part

- Metropolis: $q_{il} \to q_{il} + \Delta r \qquad r \in [-1,1]$

  $u_{il} \to u_{il} + \Delta r' \qquad r' \in [-1,1]$

  compare $e^{\Delta s}$ with $r'' \in [0,1]$. (Slowly reach equilibrium).

- Hybrid Monte Carlo: Introduce fictitious momentum P_{il} and P_{il} conjugate to q_{il} and u_{il}, respectively.

$$
\begin{aligned}
s' \to s\left(\tilde{P}_{il}, q_{il}; P_{il}, u_{il}\right) \\
= \sum_{i,l}\Bigg[& \frac{\tilde{P}_{il}^2}{2M_1} + \frac{m_1}{2\Delta\tau}\left(q_{i,l+1} - q_{il}\right)^2 + \frac{\Delta\tau}{2} m_1 \omega_1^2 q_{il}^2 + \frac{\Delta\tau}{4} g_1 q_{il}^4 \\
& + \frac{P_{il}^2}{2M_2} + \frac{m_1}{2\Delta\tau}\left(u_{i,l+1} - u_{il}\right)^2 + \frac{\Delta\tau}{2} m_2 \omega_2^2 \left(u_{i+1,l} - u_{il}\right)^2 + \frac{\Delta\tau}{4} g_2 \left(u_{i+1,l} - u_{il}\right)^4 \\
& + \lambda_1 q_{il}\left(n_{i\uparrow} + n_{i\downarrow}\right) + \tilde{s}\left(u_{il}\right)\Bigg]
\end{aligned}
$$

Dynamic Equations

$$\tilde{P}_{il} \to \tilde{P}'_{il} = \tilde{P}_{il} + \left(-\frac{\partial s}{\partial q_{il}}\right) \mathrm{d}t$$

$$q_{il} \to q'_{il} = q_{il} + \left(\frac{\partial s}{\partial \tilde{P}_{il}}\right) \mathrm{d}t$$

$$P_{il} \to P'_{il} = P_{il} + \left(-\frac{\partial s}{\partial u_{il}}\right) \mathrm{d}t$$

$$u_{il} \to u'_{il} = u_{il} + \left(\frac{\partial s}{\partial P_{il}}\right) \mathrm{d}t$$

- Energy conservation $s(t_0) = s(t_1)$, sampling phase space move rapidly.
- Accumulate error after finite time interval t is taken care of by Metropolis algorithm $e^{\Delta s} V(r)$.
- Highly parallelizable (vectorization)