Continuous Space Worm Algorithm QMC

This lecture will focus on the problem of measuring the expectation value of some operator $\hat{O}$ at finite temperature

i.e. the goal of any QMC is to measure

$$\langle \hat{O} \rangle = \frac{1}{Z} \mathrm{Tr}\left[e^{-\beta \hat{H}} \hat{O} \right]$$

where Z is the quantum partition function given by

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

In Monte-Carlo simulations, we are used to writing (1) as the sum over all possible system "configurations" x with weights $W(x)$:

$$\langle \hat{O} \rangle = \frac{\sum_x O(x) W(x)}{\sum_x W(x)} \qquad \sum_x \equiv \text{sum over all configurations.}$$

Classically the weight is just $W(x) \propto e^{-\beta E(x)}$, but in a quantum mechanical system where the potential & kinetic pieces of the Hamiltonian do not commute and things are more complicated.

Our task is thus to construct weights for a quantum configuration & a method to sample configurations. If we sample a list of configurations $l = 1, .., L$ according to their respective weights then

$$\langle \hat{O} \rangle = \langle \hat{O}(x) \rangle_W = \frac{1}{L} \sum_{l=1}^{L} O(x_l) \quad \text{as} \quad L \to \infty$$

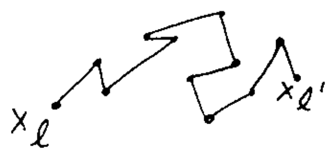
This list of configurations is a <u>Markov Chain</u> and must satisfy three criteria.

QMC CONTD.

1. EACH CONFIGURATION X_ℓ DEPENDS ONLY ON $X_{\ell-1}$, AND IS CHOSEN ACCORDING TO A POSITIVE PROBABILITY $P(X_{\ell-1} \rightarrow X_\ell)$

2. ANY TWO STATES X_ℓ & $X_{\ell'}$ MUST BE CONNECTED BY A FINITE SEQUENCE

$\Rightarrow$ "ERGODICITY"



CONFIGURATION SPACE

3. DETAILED BALANCE MUST BE SUSTAINED. $W(x)P(x \rightarrow y) = W(y)P(y \rightarrow x)$

CONSTRUCTING A QMC: DETERMINE THE NATURE OF YOUR CONFIGURATIONS X THEIR RESPECTIVE WEIGHTS & THE TRANSITION PROBABILITIES

FOR ALL FINITE-T QMC THIS IS DONE BY INVESTIGATING THE PARTITION FUNCTION:

$$Z = \mathrm{Tr}\, e^{-\beta \hat{H}} = \sum_\alpha \langle \alpha | e^{-\beta \hat{H}} | \alpha \rangle$$

I PATH-INTEGRAL QMC

(D.M. CEPERLEY, REV. MOD. PHYS. 67, 279 (1995))

LET US BEGIN BY TRYING TO DEVISE A QMC TO SIMULATE A COLLECTION OF N PARTICLES IN THE CONTINUUM. OUR HAMILTONIAN IS GIVEN BY:

$$\hat{H} = -\frac{\hbar^2}{2m} \sum_i \vec{\nabla}_i^2 + \sum_i \hat{V}_{ext}(\vec{r}_i) + \sum_{i<j} \hat{V}_{int}(\vec{r}_i - \vec{r}_j)$$

THE NATURAL BASIS STATES FOR THIS PROBLEM ARE THE POSITIONS OF ALL N PARTICLES AT ONE POINT IN TIME

$$|R\rangle = |\vec{r}_1, \ldots, \vec{r}_N\rangle$$

& $$\int \mathcal{D}R\, |R\rangle\langle R| = \mathbb{1}$$ $\Rightarrow$ PARTICLES HAVE TO BE SOMEWHERE.

QMC CONTD.

THE PARTITION FUNCTION IS THEN GIVEN BY:

$$Z = \mathrm{Tr}\, e^{-\beta \hat{H}} = \int d\vec{r}_1 \cdots \int d\vec{r}_N \langle \vec{r}_1, \ldots, \vec{r}_N | e^{-\beta \hat{H}} | \vec{r}_1, \ldots, \vec{r}_N \rangle$$

$$= \int \mathcal{D}R \langle R | e^{-\beta \hat{H}} | R \rangle$$

IT WILL BE USEFUL TO WRITE THINGS IN TERMS OF THE DENSITY MATRIX IN THE POSITION BASIS:

$$\rho(R, R', \beta) \equiv \langle R | e^{-\beta \hat{H}} | R' \rangle$$

IT CAN BE SHOWN THAT IN THIS REPRESENTATION ALL MATRIX ELEMENTS OF $\hat{\rho}$ ARE REAL & POSITIVE.

NOW, IF WE WRITE $\hat{H} = \hat{T} + \hat{V}$ WE KNOW THAT SINCE $[\hat{T}, \hat{V}] \neq 0$ WE CANNOT WRITE $\hat{\rho} = e^{-\beta \hat{H}} \neq e^{-\beta \hat{T}} e^{-\beta \hat{V}}$!

THE CORRECTIONS (DUE TO BAKER-CAMPBELL-HAUSDORFF) ARE OF ORDER (β) SO AT LOW T $(\beta \gg 1)$ WE MAKE <u>HUGE</u> ERRORS.

HOWEVER WE NOTE THAT OBVIOUSLY THE HAMILTONIAN COMMUTES WITH ITSELF.

$$\text{i.e.} \quad e^{-(\beta/2 + \beta/2)\hat{H}} = e^{-\frac{\beta}{2}\hat{H}} e^{-\frac{\beta}{2}\hat{H}}$$

SO THE DENSITY MATRIX SATISFIES A CONVOLUTION RELATION:

$$\rho(R, R; \beta) = \int \mathcal{D}R' \, \underbrace{\rho(R, R'; \beta/2) \, \rho(R', R; \beta/2)}_{\text{HIGHER TEMPERATURE}}$$

QMC CONTD.

∴ RETURNING TO OUR EXPRESSION FOR THE PARTITION FUNCTION, WE CAN PERFORM THIS CONVOLUTION M TIMES WHERE $M \in \mathbb{Z} \gg 1$

$$Z = \int \mathcal{D}R \langle R | e^{-\beta \hat{H}} | R \rangle = \int \mathcal{D}R_0 \cdots \int \mathcal{D}R_{M-1} \langle R_0 | e^{-\frac{\beta}{M}\hat{H}} | R_1 \rangle \cdots \langle R_{M-1} | e^{-\frac{\beta}{M}\hat{H}} | R_0 \rangle$$

& LET US DEFINE $\Delta\tau = \frac{\beta}{M} \ll 1$.

LET US LOOK MORE CLOSELY AT A SINGLE TERM IN THIS PRODUCT EXPANSION

$$\langle R_{\ell-1} | e^{-\Delta\tau \hat{H}} | R_\ell \rangle = \langle R_{\ell-1} | \hat{U}(-i\hbar\Delta\tau) | R_\ell \rangle$$

WHERE $\hat{\mathcal{U}}(t) = e^{-\frac{i t}{\hbar}\hat{H}}$ IS THE USUAL TIME-EVOLUTION OPERATOR OF QUANTUM MECHANICS. I.e. EACH FACTOR EVOLVES THE STATE OF THE SYSTEM BY A DISCRETE STEP IN "IMAGINARY TIME"

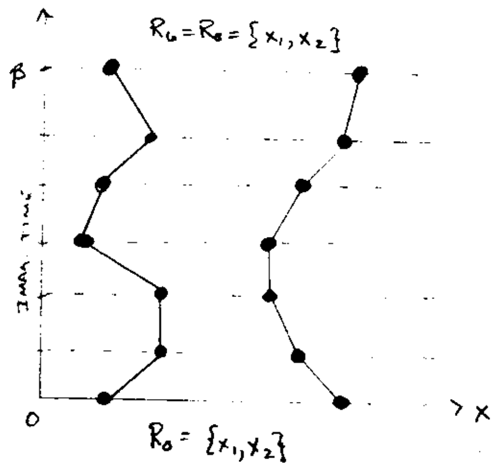
WE THUS HAVE A NEW INTERPRETATION OF OUR PARTITION FUNCTION IN TERMS OF "CONFIGURATIONS", I.e. WE SUM OVER ALL POSSIBLE IMAGINARY TIME TRAJECTORIES OF PARTICLES WHICH BEGIN AND END AT THE SAME POSITION. THIS IS JUST A RE-STATEMENT OF THE DISCRETE PATH INTEGRAL PICTURE OF FEYNMAN.

EQUIVALENTLY, THIS IS THE QUANTUM-CLASSICAL MAPPING, THAT WE CAN THINK OF A d-DIMENSIONAL QUANTUM SYSTEM AS A $(d+1)$-DIMENSIONAL CLASSICAL SYSTEM WITH WEIRD PERIODIC BOUNDARY CONDITIONS IN ONE OF THE DIMENSIONS.

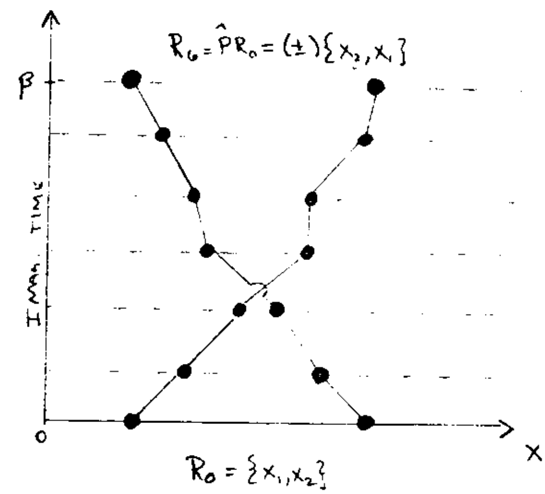
QMC CONTD.

WHAT DOES THIS MEAN FOR OUR CONFIGURATIONS?

CONSIDER THE CASE WHERE: $d = 1$, $N = 2$, $M = 6$



HOWEVER, FOR IDENTICAL PARTICLES, A PERFECTLY GOOD STATE IS:



THERE IS ANOTHER WAY TO THINK ABOUT PARTICLE IMAGINARY TIME TRAJECTORIES OR WORLDLINES DUE TO DAVID CHANDLER. WE CAN THINK OF THEM AS CLASSICAL RING POLYMERS.

D. CHANDLER & P.G. WOLYNES, J. CHEM. PHYS. 74, 4078 (1981).

THINGS TO NOTE IN THIS PICTURE:

1. A CLASSICAL PARTICLE WOULD CONSIST OF A POLYMER OF ZERO RADIUS.
2. THE "SIZE" OF A POLYMER IS RELATED TO ITS THERMAL DE BROGLIE WAVELENGTH: $\lambda_{dB} = \sqrt{\frac{2\pi\hbar^2}{mk_BT}}$
3. FOR A FINITE SIZE SYSTEM WITH PBC, WORLDLINES CAN "WIND" AROUND THE CELL. THE # OF TIMES THE DO THIS IS CALLED THE WINDING NUMBER, IT IS A TOPOLOGICALLY PROTECTED VARIABLE WHOSE DISTRIBUTION IS RELATED TO THE SUPERFLUID DENSITY.

QMC CONTD.

OK, NOW WE KNOW ABOUT CONFIGURATIONS BUT WHAT ABOUT THE WEIGHTS. LET US CONSIDER ONE OF THE TRANSITION AMPLITUDES:

$$\rho(R_{\ell-1}, R_\ell, \Delta\tau) = \langle R_{\ell-1}| e^{-\Delta\tau(\hat{T}+\hat{V})} |R_\ell\rangle$$

BECAUSE $\Delta\tau$ IS SMALL, WE CAN MAKE A PRIMITIVE APPROXIMATION, I.E.

$$e^{-\Delta\tau(\hat{T}+V)} = e^{-\Delta\tau\hat{T}} e^{-\Delta\tau\hat{V}} + O(\Delta\tau)$$

WE CAN OF COURSE KEEP HIGHER ORDER TERMS USING BETTER FACTORIZATION SCHEMES & IN PRACTICE WE EMPLOY A GENERALIZED SUZUKI FACTORIZATION WHICH IS ACCURATE TO ORDER $\Delta\tau^4$! [S.A. CHIN, PHYS. LETT. A 226, 344 (1997)]

$$\hat{\mathcal{U}} = \hat{V} + \alpha\tau^2 [\hat{V}, [\hat{T}, \hat{V}]]$$

FOR THE PURPOSES OF THIS LECTURE WE WILL MAKE THE "PRIMITIVE APPROXIMATION"

NOW,

$$\rho(R_{-1}, R; \Delta\tau) \approx \int \mathcal{D}R' \langle R_{\ell-1}| e^{-\Delta\tau\hat{T}} |R'\rangle\langle R'| e^{-\Delta\tau\hat{V}} |R_\ell\rangle$$

& PROVIDED THE POTENTIAL IS IMAGINARY TIME INDEPENDENT

$$\langle R'| e^{-\Delta\tau\hat{V}} |R_\ell\rangle = e^{-\Delta\tau V(R_\ell)} \delta(R' - R_\ell)$$

SO

$$\rho(R_{\ell-1}, R_\ell; \Delta\tau) = \langle R_{\ell-1}| e^{-\Delta\tau\hat{T}} |R_\ell\rangle e^{-\Delta\tau V(R_\ell)}$$

THE KINETIC PART IS A BIT MORE DIFFICULT. LET US WRITE OUR POSITION STATE IN THE FOURIER BASIS

$$|R_\ell\rangle = |\vec{r}_{1\ell}, \ldots, \vec{r}_{N\ell}\rangle = \prod_{i=1}^{N} \int \frac{d^d p_{i\ell}}{(2\pi)^d} e^{i\sum_{i=1}^{N} \vec{p}_{i\ell}\cdot\vec{r}_{i\ell}} |\vec{p}_{1\ell}, \ldots, \vec{p}_{N\ell}\rangle$$

QMC CONTD.

$$\lambda = \frac{\hbar^2}{2m}$$

$$\langle R_{\ell-1}| e^{-\lambda\Delta\tau \sum_{i=1}^{N} \hat{\vec{\nabla}}_i^2} |R_\ell\rangle$$

$$= \prod_{i=1}^{N} \int \frac{d^d p_{i\ell}}{(2\pi)^d} \int \frac{d^d k_{i\ell-1}}{(2\pi)^d} e^{-i\sum_{i=1}^{N} \vec{k}_{\ell-1}\cdot\vec{r}_{i\ell-1}} e^{i\sum_{i=1}^{N} \vec{p}_{i\ell}\cdot\vec{r}_{i\ell}} \langle \vec{k}_{1\ell-1},\ldots,\vec{k}_{N\ell-1}| e^{-\lambda\Delta\tau\sum_{i=1}^{N}\hat{\vec{\nabla}}_i^2} |\vec{p}_{1\ell},\ldots,\vec{p}_{N\ell}\rangle$$

$$= \prod_{i=1}^{N} \int \frac{d^d p_i}{(2\pi)^d} e^{-\lambda\Delta\tau\sum_{i=1}^{N} p_{i\ell}^2 + i\sum_{i=1}^{N} \vec{p}_{i\ell}\cdot(\vec{r}_{i\ell}-\vec{r}_{i\ell-1})}$$

$$= \prod_{i=1}^{N}\prod_{\mu=1}^{d} \left\{ \int \frac{dp_{i\ell}^{\mu}}{(2\pi)} \exp\left[-\lambda\Delta\tau (p_{i\ell}^{\mu})^2 + i\, p_{i\ell}^{\mu}(r_{i\ell}^{\mu} - r_{i\ell-1}^{\mu})\right]\right\}$$

THIS IS A SIMPLE GAUSSIAN INTEGRAL THAT GIVES:

$$\langle R_{\ell-1}| e^{-\Delta\tau\hat{T}} |R_\ell\rangle = \prod_{i=1}^{N}\prod_{\mu=1}^{d}\left\{ \frac{1}{(4\pi\lambda\Delta\tau)^{1/2}} \exp\left[-\frac{1}{4\lambda\Delta\tau}(r_{i\ell}^{\mu}-r_{i\ell-1}^{\mu})^2\right]\right\}$$

$$= (4\pi\lambda\Delta\tau)^{-\frac{Nd}{2}} e^{-\frac{1}{4\lambda\Delta\tau}|\vec{r}_{i\ell}-\vec{r}_{i\ell-1}|^2}$$

PUTTING EVERYTHING TOGETHER WE HAVE THE FULL EXPRESSION FOR THE PARTITION FUNCTION:

$$Z = \frac{1}{N!}\sum_{P}(\pm 1)^P (4\pi\lambda\Delta\tau)^{-\frac{NdM}{2}} \prod_{i=1}^{N}\prod_{\alpha=0}^{M-1} \int d\vec{r}_{i\alpha} \exp\left\{-\sum_{\alpha=0}^{M-1}\sum_{i=1}^{N}\left[\frac{|\vec{r}_{i\alpha}-\vec{r}_{i\alpha+1}|^2}{4\lambda\Delta\tau} + \Delta\tau\sum_{j=1}^{N} V(\vec{r}_{i\alpha}-\vec{r}_{j\alpha})\right]\right\}$$

PERMUTATION SIGN IS +1 : BOSONS

-1 : FERMIONS

KINETIC BETWEEN SLICES

POTENTIAL AT SAME SLICE.

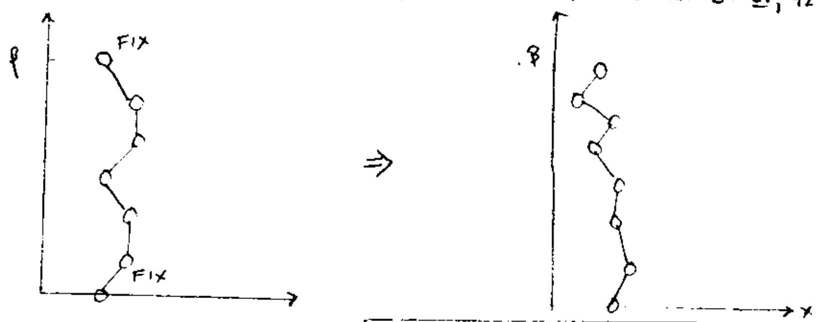
THIS EXPRESSION FOR THE PARTITION FUNCTION IS ESSENTIALLY JUST A VERY HIGH DIMENSIONAL INTEGRAL WHICH METROPOLIS SAMPLING IS VERY WELL SUITED TO SOLVE EFFICIENTLY.

QMC CONT'D.

WE CAN GENERATE CONFIGURATIONS ACCORDING TO THE KINETIC PIECE (P) AND WEIGHT THEM ACCORDING TO THE POTENTIAL PIECE (W).

TYPES OF MOVES:

1. STAGING [M. SPRIK, M. L. KLEIN & D. CHANDLER. PHYS. REV. B. 31, 4234 (1985)]

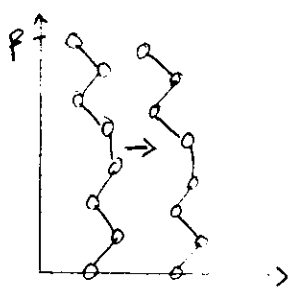


$$P_{STAGING} = e^{-\Delta\tau[\mathcal{U}(y)-\mathcal{U}(x)]}$$

★ BECAUSE THE FREE DENSITY MATRIX IS GAUSSIAN, WE CAN SAMPLE THE KINETIC PIECE EXACTLY (WEIGHT = 1) ONLY HAVE TO MEASURE CHANGE IN POTENTIAL ENERGY

$$\rho_K(\vec{r},\vec{r}\,';\Delta\tau) = (4\pi\lambda\tau)^{-d/2}\, e^{-\frac{|\vec{r}-\vec{r}\,'|^2}{4\lambda\tau}}$$

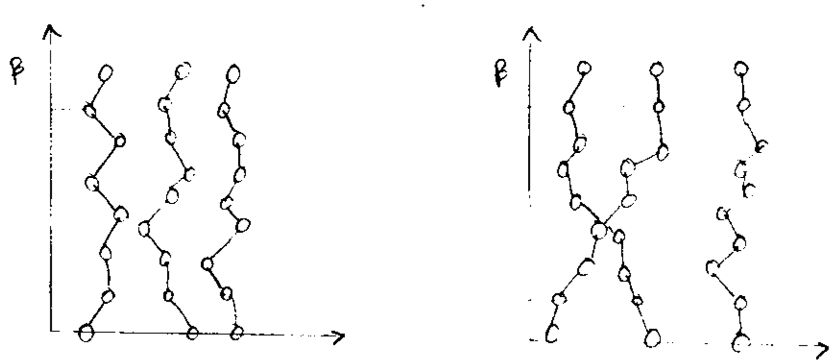
2. CENTER OF MASS



★ WE HAVE NOT AFFECTED THE KINETIC PIECE OF THE ACTION SO WE NEED ONLY WEIGHT WITH THE POTENTIAL ENERGY CHANGE.

$$P_{CoM} = e^{-\Delta\tau[\mathcal{U}(y)-\mathcal{U}(x)]}$$

3. PERMUTATION SAMPLING



+ 5 MORE PERMUTATIONS!

THIS IS THE MAJOR PROBLEM WITH CONVENTIONAL PIMC SINCE THE SAMPLING TABLE GROWS LIKE $N!$

HOWEVER THIS WAS STATE OF THE ART UNTIL 2006!

$$\boxed{N_{MAX} \sim 100}$$

QMC CONTD.

II THE WORM ALGORITHM

N. Prokf'ev, B. Svistunov & I. Tupitsyn, Phys. Lett 238, 253 (1998).
M. Boninsegni, N. Prokof'ev & B. Svistunov, Phys. Rev. E 74, 036701 (2006)

THIS ALGORITHM SOLVES 2 PROBLEMS AT ONCE.

1. ALLOWS US TO WORK IN THE GRAND CANONICAL ENSEMBLE
2. ALLOWS US TO SAMPLE TOPOLOGICALLY INEQUIVALENT WINDING SECTORS WITH ONLY LOCAL UPDATES.

THIS IS ACCOMPLISHED BY EXTENDING OUR CONFIGURATION SPACE TO INCLUDE "WORMS" WHICH ARE NON-PERIODIC WORLDLINES.

WE EXTEND OUR SIMULATION TO:
$$Z_W = \sum_{N=0}^{\infty} Z(N) e^{\beta\mu N} + Z'$$

CONVENTIONAL PIMC PARTITION FUNCTION AT FIXED N

WITH:
$$Z' = C \sum_{\alpha_h, \alpha_t} \int d\vec{r}_h \int d\vec{r}_t \; g(\vec{r}_h, \vec{r}_t, (\alpha_h - \alpha_t)\Delta\tau)$$

where g IS RELATED TO THE SINGLE-PARTICLE MATSUBARA GREEN FUNCTION

$$g(\vec{r}_1, \vec{r}_2; \tau_1, \tau_2) \sim \left\langle \hat{\mathcal{T}} \left\{ \hat{\psi}(\vec{r}_1, \tau_1), \hat{\psi}^{+}(\vec{r}_2, \tau_2) \right\} \right\rangle$$

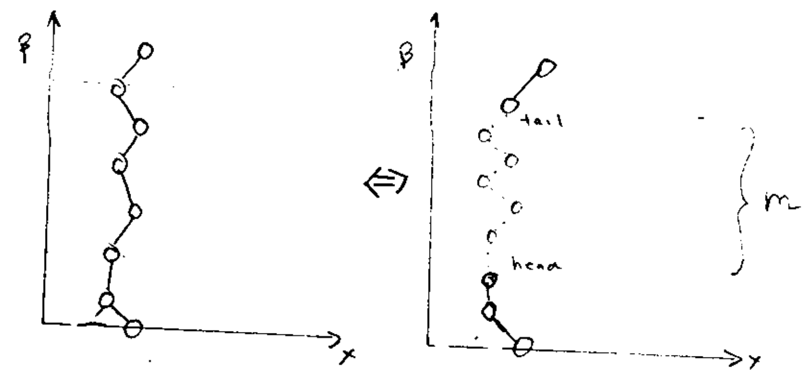
TIME ORDERING

INCLUDING THESE NEW CONFIGURATIONS IS RATHER SIMPLE BUT WE ONLY MEASURE PHYSICAL OBSERVABLES WHEN THEY ARE ABSENT!

EXCEPT FOR THE SWAP UPDATE, THESE ALL COME IN COMPLIMENTARY PAIRS WHICH AUTOMATICALLY SATISFY DETAILED BALANCE.

QMC CONTD.

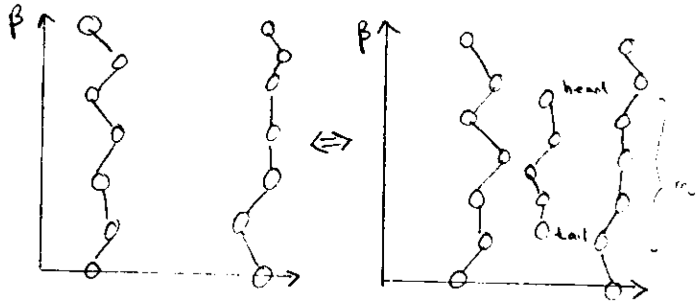
1. OPEN / CLOSE



$$P_{OPEN} = \frac{C \bar{M} N M e^{-\Delta\tau \Delta U - \mu m \Delta\tau}}{\rho_0(\vec{r}_h, \vec{r}_t, m\Delta\tau)}$$

$$P_{CLOSE} = \frac{\rho_0(\vec{r}_h, \vec{r}_t, m\Delta\tau) e^{-\Delta\tau \Delta U + \mu m \Delta\tau}}{C \bar{M} N M}$$

2. INSERT / REMOVE

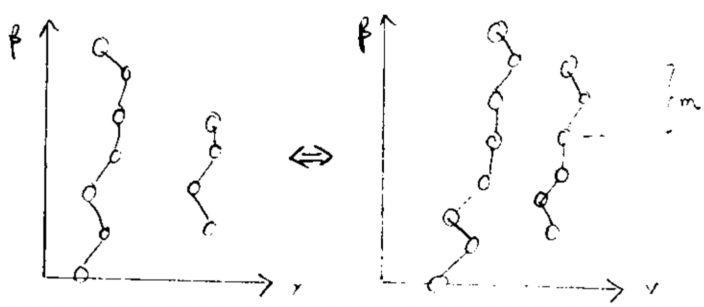


VOLUME

$$P_{INSERT} = C V M \bar{M} e^{-\Delta\tau \Delta U + \mu m \Delta\tau}$$

$$P_{REMOVE} = \frac{e^{-\Delta\tau \Delta U - \mu m \Delta\tau}}{C V M \bar{M}}$$

3. ADVANCE / RECEDE

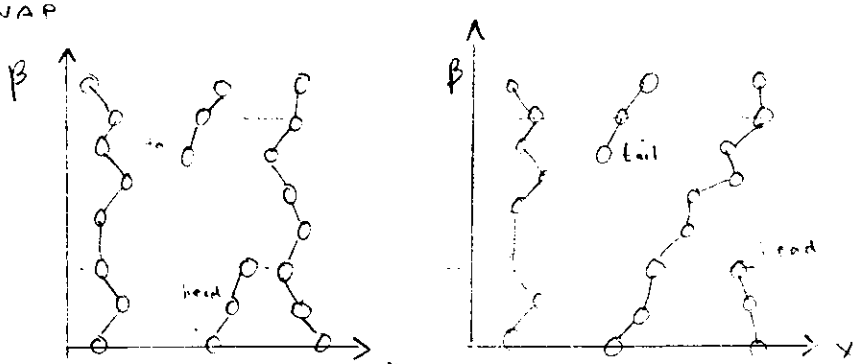


$$P_{ADVANCE} = e^{-\Delta\tau \Delta U + \mu m \Delta\tau}$$

$$P_{RECEDE} = e^{-\Delta\tau \Delta U - \mu m \Delta\tau}$$

★ CAN DO THIS FROM THE HEAD OR TAIL.

4. SWAP



★ WITH EVERY SWAP MOVE WE INCREASE THE LENGTH OF THE WORM BY M.

LONG WORMS CAN EXPLORE THE SPACE OF MANY-BODY PERMUTATIONS THROUGH SINGLE PARTICLE LOCAL UPDATES