

Path Integral Monte Carlo II

Brief reminder: density matrix fulfills product property and can be approximated using the Trotter decomposition ($\Delta\tau = \beta/M$):

$$e^{-\beta\hat{H}} = \left(e^{-\Delta\tau\hat{H}} \right)^M \approx \left(e^{-\Delta\tau\hat{T}} e^{-\Delta\tau\hat{V}} \right)^M$$

In the limit of $\sqrt{\lambda\Delta\tau} \ll L$ one obtains:

$$\rho(\vec{R}_0, \vec{R}_M; \beta) = \int d\vec{R}_1 \int d\vec{R}_2 \dots \int d\vec{R}_{M-1} (4\pi\lambda\Delta\tau)^{-3NM/2} \exp \left[- \sum_{m=1}^M \left(\frac{(\vec{R}_{m-1} - \vec{R}_m)^2}{4\lambda\Delta\tau} + \Delta\tau V(\vec{R}_m) \right) \right] \geq 0$$

primitive approximation for density matrix

More explicitly: position-dependent part of Z for pair interactions $V(\vec{R}_m) = \sum_{i=1}^N \sum_{j=i+1}^N v(\vec{r}_i(\tau_m) - \vec{r}_j(\tau_m))$

is $\int d\vec{R}_1 \int d\vec{R}_2 \dots \int d\vec{R}_m e^{-\beta\tilde{V}(\{\vec{R}\})}$

with

$$\tilde{V}(\{R\}) = \sum_{i=1}^N \sum_{j=1+i}^N \frac{1}{M} \sum_{m=1}^M v(\vec{r}_i(\tau_m) - \vec{r}_j(\tau_m)) \\ + \sum_{i=1}^N \underbrace{\frac{M}{4\lambda\beta^2}}_{k/2} \sum_{m=1}^M (\vec{r}_i(\tau_{m-1}) - \vec{r}_i(\tau_m))^2$$

Fractal nature

In the case of a smooth imaginary-time path

$$\vec{r}(\tau) \text{ we would expect } |\vec{r}(\tau_i) - \vec{r}(\tau_j)|^2 \leq v_{\max}^2 |\tau_i - \tau_j|^2$$

however, in limit $V \rightarrow 0$ we get

$$\langle |\vec{r}_i(\tau_m) - \vec{r}_i(\tau_{m-1})|^2 \rangle = 3(2\lambda\Delta\tau)$$

\rightarrow in the limit $\Delta\tau \rightarrow 0$, each polymer acquires infinite length! (smoothing + shading)

Role of temperature

In the polymer model, the finite size of each polymer is an entropic effect: for fixed spring constant k , the size would vanish for $T \rightarrow 0$.

However: for fixed M , $k \propto T^2 \Rightarrow |\vec{r}_i(\tau_{m-1}) - \vec{r}_i(\tau_m)|^2 \propto T^{-1} \rightarrow \infty$

for fixed τ : $k \propto T \Rightarrow |\vec{r}_i(\tau_{m-1}) - \vec{r}_i(\tau_m)|^2 \propto T^0 \rightarrow \text{const}$
and $M \rightarrow \infty$!

in both cases: polymer diameter $\propto \sqrt{\lambda\beta} \rightarrow \infty$

Connection to Feynman-Kac path integral

For simplicity, write only for Z (analogous for ρ):

$$Z = \left\langle (4\pi\lambda\Delta\tau)^{-3NM/2} \prod_{m=1}^M e^{-\frac{|\vec{R}_{m-1} - \vec{R}_m|^2}{4\lambda\Delta\tau}} e^{-\Delta\tau V(\vec{R}_m)} \right\rangle_{\text{uniform}}$$

$$= Z_{\text{free}} \left\langle \prod_{m=1}^M e^{-\Delta\tau V(\vec{R}_m)} \right\rangle_{\text{free}} \leftarrow \begin{array}{l} \{\vec{R}_m\} \text{ generated} \\ \text{according to} \\ Z \text{ for } V=0 \end{array}$$

$$= Z_{\text{free}} \left\langle \exp\left[-\sum_{m=1}^M \Delta\tau V(\vec{R}_m)\right] \right\rangle_{\text{free}}$$

$$\xrightarrow{M \rightarrow \infty} Z_{\text{free}} \left\langle \exp\left[-\int_0^\beta V(\vec{R}(\tau)) d\tau\right] \right\rangle_{\text{free}}$$

$$e^{-\beta(F - F_{\text{free}})} = \frac{Z}{Z_{\text{free}}} = \left\langle \exp\left[-\int_0^\beta V(\vec{R}(\tau)) d\tau\right] \right\rangle_{\text{free}}$$

Monte Carlo sampling of the partition function

Not possible: naive simple sampling (take all $\vec{r}_i(\tau_m)$ as independent random variables in L^3)

1) single-particle displacement moves (\sim classical atoms)

a) select particle i

b) draw displacement $\vec{\delta}$ from uniform distribution inside cube $[-\frac{\Delta}{2}, \frac{\Delta}{2}]^3$

c) propose move $\vec{r}_i(\tau_m) \rightarrow \vec{r}_i(\tau_m) + \vec{\delta}$ for all m

d) accept with probability $p = \min\{1, e^{-\beta \Delta V}\}$

• These moves are only useful for not too low T

• Δ is adjusted for acceptance probability of 25% - 75%

2) single-particle single-slice moves

a) select particle i and slice m

(i) classic rule

b) random displacement $\vec{\delta}$ uniformly from cube $[-\frac{\Delta}{2}, \frac{\Delta}{2}]^3$

c) propose move $\vec{r}_i(\tau_m) \rightarrow \vec{r}_i(\tau_m) + \vec{\delta}$ for single m

d) accept with prob. $p = \min\{1, e^{-\beta \Delta \tilde{V}}\}$

• now also kinetic contributions to $\Delta \tilde{V}$

• adjust $\Delta \approx \sqrt{2 \Delta T}$ to $\sim 50\%$ acceptance prob.

(ii) free-particle sampling

In general, the probability density for position vector \vec{R}_m at fixed \vec{R}_i for $i \neq m$ can be written as

$$P[\vec{R}_m] \propto \rho(\vec{R}_{m-1}, \vec{R}_m; \Delta\tau) \rho(\vec{R}_m, \vec{R}_{m+1}; \Delta\tau)$$

specifically for $\vec{V}=0$ we have

$$P[\vec{R}_m] \propto \exp\left[-\frac{|\vec{R}_{m-1} - \vec{R}_m|^2}{4\lambda\Delta\tau}\right] \exp\left[-\frac{|\vec{R}_m - \vec{R}_{m+1}|^2}{4\lambda\Delta\tau}\right]$$

$$\begin{aligned}(x-a)^2 + (x-b)^2 &= 2x^2 - 2x(a+b) + a^2 + b^2 \\ &= 2\left[x^2 - 2x\frac{a+b}{2} + \left(\frac{a+b}{2}\right)^2\right] + \frac{(a-b)^2}{2}\end{aligned}$$

$$\Rightarrow P[\vec{R}_m] \propto \exp\left[-\frac{|\vec{R}_m - \vec{R}_{av}|^2}{2\lambda\Delta\tau}\right]; \quad \vec{R}_{av} = \frac{\vec{R}_{m-1} + \vec{R}_{m+1}}{2}$$

in case of single-particle move:

$$P[r_i(\tau_m)] \propto \exp\left[-\frac{|\vec{r}_i(\tau_m) - \vec{r}_i^{av}|^2}{2\lambda\Delta\tau}\right]; \quad \vec{r}_i^{av} = \frac{\vec{r}_i(\tau_{m+1}) + \vec{r}_i(\tau_{m-1})}{2}$$

This can be sampled directly (diffusion step)

b) draw $\vec{\delta}$ from Gaussian distribution with width $\sqrt{\lambda\Delta\tau}$ (in each dimension)

c) propose move $\vec{r}_i(\tau_m) \rightarrow \frac{\vec{r}_i(\tau_{m-1}) + \vec{r}_i(\tau_{m+1})}{2} + \vec{\delta}$

d) accept with probability $\min\{1, e^{-\beta\Delta V}\}$

(this expression is valid for primitive approximation; generalize for better actions)

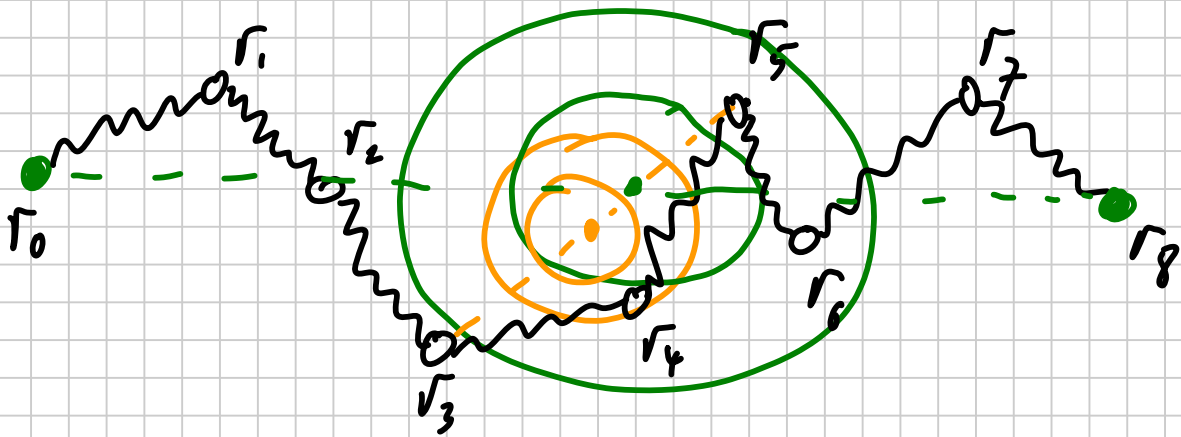
procedure analogous to diffusion Monte Carlo

$$|0\rangle = \lim_{\beta \rightarrow \infty} e^{-\beta \hat{H}} |\psi_0\rangle \approx \prod_{m=1}^M (e^{-\Delta\tau \hat{V}} e^{-\Delta\tau \hat{T}}) |\psi_0\rangle$$

\uparrow birth/death
 \uparrow diffusion of "walkers"
 \uparrow diffusion of "walkers"

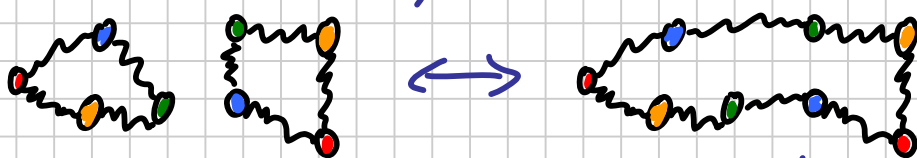
1) and 2) are in principle sufficient for distinguishable particles. However: single-slice moves inefficient for large M

2') Multilevel-sampling



On fine grid: \vec{r}_4 cannot move very far
 idea: • consider coarse grid with $\tilde{\Delta\tau} = 4\Delta\tau$ first
 • construct more iteratively
 • keep track of intermediate proposal prob.
 • correct everything in final acceptance rule

3) Exchange moves: for distinguishable particles, we must allow exchanges (discrete move - not possible in MD)



In practice: combine with multilevel moves.

Observables

• density, pair correlation function, structure factor: directly from $\{R_m\}$

• already the energy is nontrivial

(i) "direct" or "Hamiltonian" estimator:

$$E_H = \frac{\text{Tr}(\hat{H} e^{-\beta \hat{H}})}{\text{Tr}(e^{-\beta \hat{H}})} = \dots$$

(ii) thermodynamic estimator

$$E_T = -\frac{1}{Z} \frac{dZ}{d\beta}$$
$$= \frac{1}{n} \sum_{m=1}^n \left\langle \frac{3N}{2\Delta T} - \frac{|\bar{R}_m - \bar{R}_{m-1}|^2}{4\Delta T^2} + V(\bar{R}_m) \right\rangle$$

(iii) virial estimator

$$E_V = \left\langle \dots - \frac{1}{2} F^m \Delta_m \dots \right\rangle$$

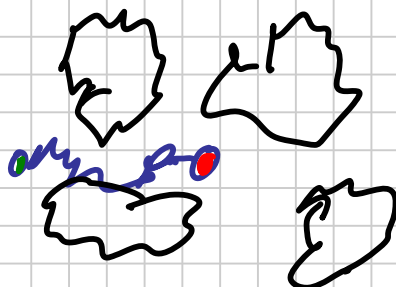
← deviation from center of mass

↑ generalized force

• condensate fraction

insert two free ends \vec{r}_0, \vec{r}_f
measure prob $(\vec{r}_0 - \vec{r}_f)$

no exchange:

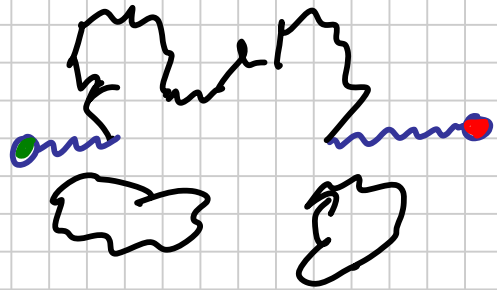


$$p \propto e^{-a|\vec{r}_0 - \vec{r}_f|^2}$$

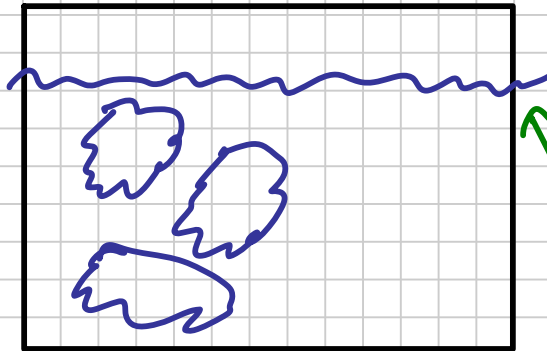
with exchange:

$$P \xrightarrow{T \rightarrow 0} \text{const.}$$

i.e. $\vec{k} = 0$



- superfluid density



↑ non zero winding number

Application to vacancies in solid ^4He
see slides