Pedagogical Intro to QMC

- Basic idea: given $\mathcal{H}$, gives $\int \underbrace{e^{-\beta\hat{\mathcal{H}}}}_{\rho(\{R\},\{R'\})} \overbrace{\hat{C}(\{R\})}^{\text{correlation function}}$

- Types of QMC:

	continuum	lattice
metropolis	path integral Monte Carlo (PIMC)	Continuous time
	Repetation	WORM
	Variational Monte Carlo (VMC)	Worldline
		Diagramatical
Pater Method	diffusion Monte Carlo (DMC)	
	auxillary field quantum Monte Carlo (AFQMC)	

- Metropolis Algorithm
  - Consider $\dfrac{\int \rho(x) f(x)}{\int \rho(x)} = \langle f \rangle.$ $\quad [\rho(x) \geq 0]$

  Imagine all $\{x\}$ forms a network of states (e.g., in Ising, $\{x\} = \{\uparrow\downarrow\downarrow\uparrow\cdots\}$, and connection's between state differ by one spin).

  Then, algorithm: (1) start with x_1

  (2) with $T(x\to y)$ choose neighbor y.

  (3) accept move by probability $\dfrac{T(y\to x)}{T(x\to y)}\dfrac{P(y)}{P(x)}$

  (4) Sample at some frequency.

- Concretely, consider $\dfrac{1}{Z}\int \langle R|e^{-\beta H}|R\rangle\, Q(R)\, dR = \langle Q\rangle$

$$\langle R|e^{-\beta\mathcal{H}}|R\rangle = \langle R|\, e^{-\tau\mathcal{H}} \underset{|R'\rangle\langle R'|}{\uparrow} e^{-\tau\mathcal{H}} \underset{|R''\rangle\langle R''|}{\uparrow} \cdots e^{-\tau\mathcal{H}}|R\rangle$$

Now, $e^{-\tau(\hat{T}+\hat{V})} \approx e^{-\tau\hat{T}} e^{-\tau\hat{V} + O(\tau^2)}$

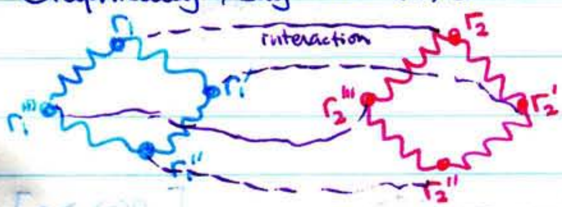
$$\langle R| e^{-\tau(\hat{T}+\hat{V})} |R'\rangle \approx \underbrace{\langle R| e^{-\tau\hat{T}} |R''\rangle}_{e^{-(R-R'')^2/4\tau}} \underbrace{\langle R''| e^{-\tau\hat{V}} |R'\rangle}_{e^{-\tau V(R')}}$$

Conceptually, by going to small τ, we enter high temperature limit where we know how to approximate

Then, the object we need is:

$$\langle Q\rangle = \frac{1}{Z}\int dR\,dR' \cdots dR^{(n)} \overbrace{\boxed{e^{-V(R)}\, e^{-V(R')}\, e^{-V(R'')}\, \underbrace{e^{-\frac{(R-R')^2}{4\tau}}}_{\text{spring cost between 2 pts.}}\, e^{-\frac{(R'-R'')^2}{4\tau}} \cdots}}^{\rho(R,R',\ldots)}$$

Graphically, say $R = (r_1, r_2)$

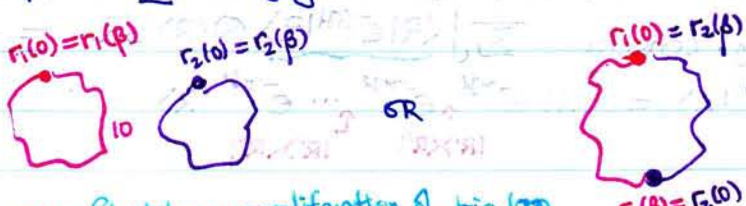


Our configurations are thus polymer loops

(If we care about the full density matrix $\langle R| e^{-\beta H} |R'\rangle$, then we just replace closed polymer with open polymer)

For bosons, we need:

$$\langle Q\rangle = \frac{1}{Z}\sum_\pi \int \rho(\pi(R), R', R'', \ldots)\, Q(R)$$



Remark: superfluidity ~ proliferation of big loop

For fermion,

$$\langle Q \rangle = \frac{1}{Z} \sum_\pi \int (-1)^\pi \rho(\pi(R), R', R'', \ldots) Q(R)$$

So now, schematically, we need $\dfrac{\int \rho(x) f(x) (-1)^\pi}{\int \rho(x) (-1)^\pi} = \dfrac{A}{B}$

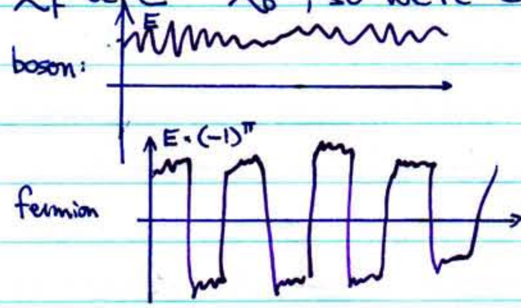
where $\begin{cases} A = \dfrac{\sum_\pi \int (-1)^\pi \rho(x) f(x)}{\sum_\pi \int \rho(x)} \\ B = \dfrac{\sum_\pi \int (-1)^\pi \rho(x)}{\sum_\pi \int \rho(x)} \end{cases}$

Problem (sign problem) in 4 ways:

(1) bosons tend to condense but fermion doesn't. In trying to do a fermion problem via boson, it takes long time to get out an answer.

(2) Mathematically, $Z_F \propto e^{-\beta N} Z_B$, so we're dividing $0/0$.

(3) Graphically

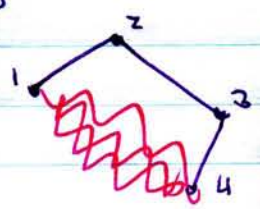


To handle sign problem, if we know analytically some regions of +'s & −'s in phase space cancel, then we only need to handle the remaining pieces $\Longrightarrow$ less variance.

Suppose we have $R_1, R_2, \ldots, R_6$. Define:

$$F[R_1, \ldots, R_4] = \sum_\pi \int (-1)^\pi \rho(R_1, \ldots, R_6) Q(R) \, dR_5 \, dR_6$$

We'll only keep $\{R_1, \ldots, R_4\}$ s.t.



$\neq 0$

Do similar for $F[R_1, R_2]$, ...

$F(R,R')$ turns out to be many-body density matrix $\rho^A(R,R')$
We just guess $\rho^A_{trial}(R,R')$ to extract zero patches.
This also satisfy variational principle (i.e. always overestimate)