Pedagogical Intro to QMC

- Basic idea: given $H$, gives $\int e^{-\beta H} \hat{c}(FR) \hat{c}^\dagger(FR) dF dR$.

- Types of QMC:
  - **Continuum**
    - Path integral Monte Carlo (PIMC)
    - Metropolis
    - Variational Monte Carlo (VMC)
    - Diffusion Monte Carlo (DMC)
  - **Lattice**
    - Continuous-time WORM
    - Worldline
    - Diagrammatical
    - Auxiliary field quantum Monte Carlo (AFQMC)

- Metropolis Algorithm
  - Consider $\frac{\text{Spec} f_{\text{new}}}{\text{Spec} f_{\text{old}}} = \langle f \rangle$. $\rho(\omega) \geq 0$.

  Imagine all $\mathbb{R}^3$ forms a network of states (e.g., in Ising, $\{x\} = \{\uparrow, \downarrow\} \ldots$), and connections between states differ by one spin.

  Then, algorithm: (1) start with $x_0$,
  (2) with $T(x \to y)$ choose neighboring $y$.
  (3) accept move by probability $\frac{T(y \to x)}{T(x \to y)} P(y)$.
  (4) Sample at some frequency.

- Concretely, consider $\frac{1}{\mathbb{Z}} \int \langle R_1 e^{\beta h} | R \rangle Q(R) dR = \langle \alpha \rangle$.

  $\langle R_1 e^{\beta h} | R \rangle = \langle R_1 e^{x_1 h} e^{x_2 h} \ldots e^{x_n h} | R \rangle$.
Now, $e^{-\tau (\hat{F} + \hat{V})} \approx e^{-\tau \hat{F}} e^{-\tau \hat{V} + O(\tau^2)}$

$$\langle R | e^{-\tau (\hat{F} + \hat{V})} | R' \rangle \approx \frac{\langle R | e^{-\tau \hat{F}} | R' \rangle \langle R' | e^{-\tau \hat{V}} | R' \rangle}{e^{-(R-R')^2 / 4\tau}}$$

Conceptually, by going to small $\tau$, we enter high temperature limit where we know how to approximate

Then, the object we need is:

$$\langle Q \rangle = \frac{1}{Z} \int dR dR' \cdots dR^{(n)} e^{-V(R)} e^{-V(R')} \cdots e^{-\frac{(R-R')^2}{4\tau} \cdots \frac{(R-R')^2}{4\tau}}$$

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

Our configurations are thus polymer loops

$$\{ X_i \} \{ X_2 \}$$

(If we care about the full density matrix $\langle R | e^{-\sum \hat{F}^2} | R' \rangle$, then we just replace closed polymer with open polymer)

For bosons, we need:

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

Remark: superfluidity ~ proliferation of big loop
For fermion, 

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

So now, schematically, we need 

$$
\frac{\int_{\rho_{\text{even}}} (-1)^n}{\int_{\rho} (-1)^n} = \frac{A}{B}
$$

where 

$$
A = \frac{\sum_n (-1)^n \rho_{\text{even}}}{\sum_n \rho} \\
B = \frac{\sum_n (-1)^n \rho_{\text{odd}}}{\sum_n \rho}
$$

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 an answer.

2. Mathematically, \( Z_\text{F} \propto e^{-N} \) so we're dividing \(-N\)...

3. Graphically

To handle sign problem, if we know analytically some regions \( b \) +'s & -'s in phase space cancel, then we only need to handle the remaining pieces \( \Rightarrow \) less variance.

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

$$
F[R_1, \ldots, R_6] = \sum \int (-1)^n \rho(R_1, \ldots, R_6) Q(R) \, dR_1 \, dR_2
$$

We'll only keep \( \{R_1, \ldots, R_6\} \) s.t. \( z \neq 0 \)

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 $\rho^A(R,R')$ to extract zero patches. This also satisfy variational principle (i.e. always overestimate).