Short Takes 331

Toward QMC: Generating field configurations

Toward finite-temperature Quantum Monte Carlo (QMC):

Generating field configurations

Last time...

$$\langle \hat{X}[\sigma] \rangle = \int \mathcal{D}\sigma \, P[\sigma] \, X[\sigma] \quad , \qquad P[\sigma] = \frac{\det M[\sigma]}{\mathcal{Z}}$$

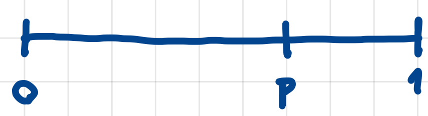
$$\rightarrow \frac{1}{N_{samples}} \cdot \sum_{k=1}^{N_{samples}} X[\sigma_k]$$

samples: $\{ \sigma_k \, , \; k = 1, 2, \dots, N_{samples} \}$

- How do we generate these samples?

  → Metropolis algorithm

  - Pick a starting config σ_0 (e.g. random)
  - Make a change $\Delta\sigma$
  - Calculate $$p = \frac{P[\sigma_0 + \Delta\sigma]}{P[\sigma_0]}$$
  - Decide:
    - if $p \geq 1 \rightarrow$ keep $\sigma_1 = \sigma_0 + \Delta\sigma$
    - if $p < 1 \rightarrow \begin{cases} \text{keep } \sigma_1 = \sigma_0 + \Delta\sigma \text{ with probability } p \\ \text{or} \\ \text{reject and set } \sigma_1 = \sigma_0 \end{cases}$



  - Return to step 2.

This process generates a Markov chain.

If we wait long enough and sample snapshots along the way (allowing enough time in between samples), the resulting set $\{\sigma_k\}$ will be distributed according to $P[\sigma]$.

→ Thermalization

→ Decorrelation

Both can be especially slow close to phase transitions.

- Bigger problem: the "sign" problem.

  - What if $P[\sigma]$ does not have a definite sign?

    Then it is not a well-defined probability.

    Could we use $|P[\sigma]|$?

$$\int D\sigma \frac{\operatorname{Det} M[\sigma]}{Z} X[\sigma] = \frac{\int D\sigma \, |\operatorname{Det} M[\sigma]| \, X[\sigma] \, . \, e^{i\varphi[\sigma]}}{\int D\sigma \, |\operatorname{Det} M[\sigma]| \, e^{i\varphi[\sigma]}} \cdot \frac{\int D\sigma \, |\operatorname{Det} M[\sigma]|}{\int D\sigma \, |\operatorname{Det} M[\sigma]|}$$

$$= \frac{\langle\langle X[\sigma] e^{i\varphi[\sigma]} \rangle\rangle_{|P|} \longrightarrow 0}{\langle\langle e^{i\varphi[\sigma]} \rangle\rangle_{|P|} \longrightarrow 0} \quad !!$$

This problem is everywhere (CM, finite-μ QCD, QC, ...)

Lots of literature & attempts to solve it!