Short Takes 331

Toward QMC: Hubbard-Stratonovich transformation

Toward finite-temperature Quantum Monte Carlo (QMC):

The Hubbard-Stratonovich transformation.

- Last time

$$\mathcal{Z} = \mathrm{tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right] \longrightarrow e^{-\beta\hat{H}}$$ is the important object.

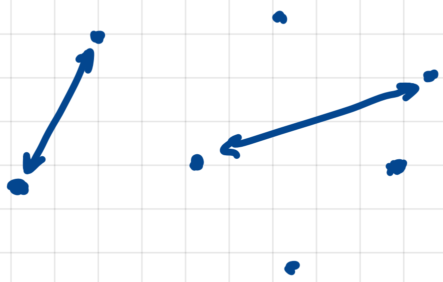
$$e^{-\beta\hat{H}} \longrightarrow e^{-\tau\hat{H}}$$ via Trotter-Suzuki factorization.

$$\beta = \tau N_\tau$$

$$e^{-\tau\hat{H}} \to e^{-\tau\hat{T}}\, \underline{e^{-\tau\hat{V}}}$$

- The main reason the problem is hard is the interaction factor.

$e^{-\tau\hat{V}}$, $\hat{V}$ is a two- (or higher-) body operator



- It would all be much easier if both $\hat{T}$ and $\hat{V}$ were one-body operators. Then, $\hat{H} = \hat{T} + \hat{V}$ can be fully calculated in the single-particle basis and

$$[\hat{H}]_{ij} = \langle i|\hat{H}|j\rangle = H_{ij}$$

$\{|i\rangle,\ i = 0, 1, 2, \dots\}$

one-body rep of $\hat{H}$

Then, $$\mathcal{Z} = \det\left(\mathbb{1} + e^{\beta\mu} e^{-\beta H}\right)$$

more on this later!

- The Hubbard-Stratonovich transformation allows us to write...

$$e^{-\tau \hat{V}} = \int \mathcal{D}\sigma \; e^{-\tau \hat{V}[\sigma]}$$

two-body op. (or higher!)

one-body op. ; transf-dependent!

field integral $\mathcal{D}\sigma = \prod_x d\sigma(x)$

There are many ways to implement this transf., but they are all (or most) based on Gaussian integration:

$$e^{A^2} = \int dx \; e^{-x^2 + 2Ax} ,$$

where A^2 plays the role of $\hat{V}$ and x plays the role of σ.

- Armed with this result,

$$\mathcal{Z} = \mathrm{Tr}\left[e^{-\tau(\hat{T}-\mu\hat{N})} e^{-\tau\hat{V}} e^{-\tau(\hat{T}-\mu\hat{N})} e^{-\tau\hat{V}} \cdots \right]$$

$$= \int \mathcal{D}\sigma \; \mathrm{Tr}\Big[\underbrace{e^{-\tau(\hat{T}-\mu\hat{N})} e^{-\tau\hat{V}[\sigma]} e^{-\tau(\hat{T}-\mu\hat{N})} e^{-\tau\hat{V}[\sigma]} \cdots}_{\hat{\mathcal{U}}[\sigma]} \Big]$$

$$= \int \mathcal{D}\sigma \; \det\left(\mathbb{1} + \mathcal{U}[\sigma]\right)$$

more about this step next time!

$\mathcal{U}$: single-particle rep of $\hat{\mathcal{U}}$.

Note $\hat{\mathcal{U}}$ is a product of exp of one-body ops.