Short Takes 331

Toward QMC: Trace-determinant identities

Toward finite-temperature Quantum Monte Carlo (QMC):

Trace-determinant identities. Part 1.

So far...

$$\mathcal{Z} = \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right] \quad , \quad \hat{H} = \hat{T} + \hat{V}$$

$$e^{-\beta\hat{H}} = \left[e^{-\tau\hat{H}}\right]^{N_\tau} \quad , \quad \beta = \tau N_\tau$$

$$e^{-\tau\hat{H}} = e^{-\tau\hat{T}}\, e^{-\tau\hat{V}} \quad , \quad (T-S) \qquad \text{ep. 1}$$

$$e^{-\tau\hat{V}} = \int \mathcal{D}\sigma \; e^{-\tau\hat{V}[\sigma]} \quad , \quad (H-S) \qquad \text{ep. 2}$$

Last time I used but did not prove that...

$$\mathrm{Tr}\left[e^{\hat{A}}e^{\hat{B}}e^{\hat{C}}\ldots\right] = \det\left(\mathbb{1} + e^{A}e^{B}e^{C}\ldots\right) ,$$

$\hat{A}, \hat{B}, \hat{C}, \ldots$ are one-body ops. (fermionic)

$A, B, C, \ldots$ are the single-particle reps of $\hat{A}, \hat{B}, \hat{C}, \ldots$, respectively

$\{ |i\rangle ,\ i = 0, 1, \ldots \ ;\ \text{s.p. states} \}$

A is a matrix of elements

$$A_{ij} = \langle i | \hat{A} | j \rangle$$

Proof

1. $\mathrm{Tr}\left[e^{\hat{A}}\right] = \det\left(\mathbb{1} + e^{A}\right)$

$$\hat{A} = \text{one-body op} \underset{\text{by def.}}{=} \sum_{ij} \langle i | \hat{A} | j \rangle\, \hat{a}^\dagger_i \hat{a}_j = \sum_{ij} A_{ij}\, \hat{a}^\dagger_i \hat{a}_j$$

Here, $\{\hat{a}_i, \hat{a}^\dagger_j\} = \delta_{ij}$ (fermions)

Diagonalize A:

$A = U^\dagger D U$, D diagonal , U unitary

$$\Rightarrow \hat{A} = \sum_{ij} (U^\dagger D U)_{ij} \, \hat{a}^\dagger_i \hat{a}_j \qquad D = \begin{pmatrix} D_1 & & \\ & D_2 & \\ & & \ddots \end{pmatrix}$$

$$= \sum_{ijk} \hat{a}^\dagger_i U^\dagger_{ik} D_k U_{kj} \hat{a}_j$$

$$= \sum_k \hat{b}^\dagger_k D_k \hat{b}_k \quad , \quad b_k = \sum_j U_{kj} \hat{a}_j$$

$$b^\dagger_k = \sum_j a^\dagger_j U^\dagger_{jk}$$

With this result,

$$e^{\hat{A}} = \prod_k e^{D_k \hat{b}^\dagger_k \hat{b}_k}$$

$$= \prod_k \left[1 + (e^{D_k} - 1) \hat{b}^\dagger_k \hat{b}_k\right] , \quad \text{because} \quad \left(\hat{b}^\dagger_k \hat{b}_k\right)^2 = \hat{b}^\dagger_k \hat{b}_k$$

Note: • for any op $\hat{O}$ s.t. $\hat{O}^2 = \hat{O}$,
$e^{c\hat{O}} = 1 + (e^c - 1) . \hat{O}$

• the eigenvalues of $\hat{O}$ can only be 0 or 1. ← fermions!

Then, $$\mathrm{Tr}\left[e^{\hat{A}}\right] = \sum_{k_1 k_2 \dots} \langle k_1 | \langle k_2 | \dots \prod_k \left[1 + (e^{D_k} - 1) \hat{b}^\dagger_k \hat{b}_k\right] \dots | k_2 \rangle | k_1 \rangle$$

$$= (1 + e^{D_1})(1 + e^{D_2}) \dots$$

$$= \det\left(\mathbb{1} + e^D\right) = \det\left(\mathbb{1} + e^A\right).$$

2. $e^{\hat{A}} e^{\hat{B}}$??

→ Use Baker-Campbell-Hausdorff to turn...

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{Z}}$$, then apply part 1 to $e^{\hat{Z}}$

Turns out $\hat{Z} = \sum_{ij} \underbrace{\left(\ln\left[e^{A} e^{B}\right]\right)_{ij}}_{Z_{ij}} \hat{a}_i^{+} \hat{a}_j$