Short Takes 331

Toward QMC: Trace-determinant identities. Part 2

Toward finite-temperature Quantum Monte Carlo (QMC):

Trace-determinant identities. Part 2.

- In part 1 we showed that

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

grand-canonical trace

$$\hat{A} = \underset{\text{op.}}{\text{one-body}} = \sum_{ij} A_{ij}\, \hat{a}^\dagger_i \hat{a}_j$$

$$\mathrm{Tr}(\hat{O}) = \sum_{n_1 n_2 \dots} \langle n_1 n_2 \dots | \hat{O} | n_1 n_2 \dots \rangle \quad , \quad A_{ij} = \langle i | \hat{A} | j \rangle$$

occupation # of s.p. state 1

s.p. matrix elements of $\hat{A}$

- To show that

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

one uses BCH to prove that

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{Z}} \quad , \quad \text{where} \quad \hat{Z} = \sum_{ij} Z_{ij}\, \hat{a}^\dagger_i \hat{a}_j$$

and

$$Z_{ij} = \left[\ln\left[e^{A} e^{B}\right]\right]_{ij}$$

and then use the single-operator case above

- How to show this?

BCH claims

$$\hat{Z} = \hat{A} + \hat{B} + \frac{1}{2}[\hat{A}, \hat{B}] + \frac{1}{12}[\hat{A}, [\hat{A}, \hat{B}]] - \frac{1}{12}[\hat{B}, [\hat{A}, \hat{B}]] + \dots$$

where $[\hat{X}, \hat{Y}] = \hat{X}\hat{Y} - \hat{Y}\hat{X}$

Now, for fermions, we use anti-commutation relations, i.e. we must decompose the above further using

$$[\hat{U}, \hat{V}\hat{W}] = \hat{U}\hat{V}\hat{W} - \hat{V}\hat{W}\hat{U}$$
$$= \hat{U}\hat{V}\hat{W} + \hat{V}\hat{U}\hat{W} - \hat{V}\hat{U}\hat{W} - \hat{V}\hat{W}\hat{U}$$
$$= \{\hat{U}, \hat{V}\}\hat{W} - \hat{V}\{\hat{U}, \hat{W}\}$$

On the other hand, for bosons, we will use instead commutation relations

$$[\hat{U}, \hat{V}\hat{W}] = [\hat{U}, \hat{V}]\hat{W} + \hat{V}[\hat{U}, \hat{W}]$$

- These identities will help disentangle ops such as

$$[\hat{A}, \hat{B}] = \sum_{\substack{ij\\km}} A_{ij} B_{km} [\hat{a}_i^\dagger \hat{a}_j, \hat{a}_k^\dagger \hat{a}_m]$$

in both fermion and boson cases.

$$\{\hat{a}_i, \hat{a}_j^\dagger\} = \delta_{ij} \qquad\qquad [\hat{a}_i, \hat{a}_j] = \delta_{ij}$$

You end up showing that

$$\hat{Z} = \sum_{ij} Z_{ij}\, \hat{a}_i^\dagger \hat{a}_j \quad , \quad Z = A + B + \frac{1}{2}[A,B] + \dots$$
$$= \ln\left[e^A e^B\right]$$

- What about bosons?

Same line of proof, but something crucial changes...

$$\mathrm{Tr}\left[e^{\hat{A}}\right] = \mathrm{Tr}\left[\prod_k e^{D_k \hat{b}_k^\dagger \hat{b}_k}\right] \quad , \qquad \hat{b}_k^\dagger \hat{b}_k \text{ eigenvalues } n_k = 0, 1, 2, \dots \infty$$

$$= \sum_{n_1, n_2 \dots} \langle n_1 n_2 \dots | \prod_k e^{D_k \hat{b}_k^\dagger \hat{b}_k} | n_1 n_2 \dots \rangle$$

$$= \sum_{n_1=0}^{\infty} e^{D_1 n_1} \cdot \sum_{n_2=0}^{\infty} e^{D_2 n_2} \dots$$

$$= \left(1 - e^{D_1}\right)^{-1} \left(1 - e^{D_2}\right)^{-1} \dots \qquad = \prod_k \left(1 - e^{D_k}\right)^{-1}$$

$$= \det{}^{-1}\left(1 - e^{A}\right)$$

Then,

$$\mathrm{Tr}\left[e^{\hat{A}} e^{\hat{B}} \dots\right] = \det{}^{-1}\left(1 - e^{A} e^{B} \dots\right)$$