Short Takes 331

Toward QMC: Calculating thermal expectation values

Toward finite-temperature Quantum Monte Carlo (QMC):

Calculating expectation values

- So far...

$$\mathcal{Z} = \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right] = \int \mathcal{D}\sigma \, \det\left(\mathbb{1} + z\,\mathcal{U}[\sigma]\right)$$

TS, HS

$$z = e^{\beta\mu}$$

$$\mathcal{U}[\sigma] = T\,\mathcal{V}_1[\sigma]\,T\,\mathcal{V}_2[\sigma]\,T\,\mathcal{V}_3[\sigma]\,\dots\,T\,\mathcal{V}_{N_\tau}[\sigma]$$

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

contains all the parameters of the theory, except μ.

- Now, how do we calculate $\langle\hat{O}\rangle$?

Example: Particle number

$$\langle\hat{N}\rangle = \frac{1}{\mathcal{Z}} . \mathrm{Tr}\left[\hat{N}\, e^{-\beta(\hat{H}-\mu\hat{N})}\right]$$

$$= \frac{\partial \ln \mathcal{Z}}{\partial(\beta\mu)} \quad , \quad \beta\mu = \ln z$$

$$= \frac{1}{\mathcal{Z}} \int \mathcal{D}\sigma \, \underbrace{\frac{\partial}{\partial(\beta\mu)}\left[\det\left(\mathbb{1} + z\,\mathcal{U}[\sigma]\right)\right]}_{\shortparallel}$$

$$\det\left(\mathbb{1} + z\,\mathcal{U}[\sigma]\right) . \mathrm{Tr}\left[\left(\mathbb{1} + z\,\mathcal{U}[\sigma]\right)^{-1} z\,\mathcal{U}[\sigma]\right] \quad , \quad \frac{\partial z}{\partial \beta\mu} = z$$

Property:

$$\frac{\partial \det M}{\partial\lambda} = \det M . \frac{\partial\left(\mathrm{Tr}\ln M\right)}{\partial\lambda} = \det M . \mathrm{Tr}\left(M^{-1}\frac{\partial M}{\partial\lambda}\right)$$

$$\det M = \prod_k \lambda_k = \exp\left(\sum_\lambda \ln \lambda\right)$$
$$= \exp\left[\mathrm{Tr}(\ln M)\right]$$

$$= \left\langle\!\left\langle \mathrm{Tr}\left[(\mathbb{1} + z\,\mathcal{U}[\sigma])^{-1} \cdot z\,\mathcal{U}[\sigma]\right] \right\rangle\!\right\rangle_{P[\sigma]} ,$$

$$\langle\langle X \rangle\rangle = \int \mathcal{D}\sigma\, P[\sigma]\, X[\sigma] \quad , \qquad P[\sigma] = \frac{\det(\mathbb{1} + z\,\mathcal{U}[\sigma])}{\mathcal{Z}}$$

Our job:

- Generate σ-field configurations $\longrightarrow \{\sigma_k ,\ k = 1, \dots, N_{samples}\}$ distributed according to $P[\sigma]$.
  (the MC part!)

- Estimate $\langle \hat{N} \rangle$ by calculating the average $\bar{N}$:

$$\bar{N} = \frac{1}{N_{samples}} \cdot \sum_{k=1}^{N_{samples}} \mathrm{Tr}\left[(\mathbb{1} + z\,\mathcal{U}[\sigma])^{-1} \cdot z\,\mathcal{U}[\sigma]\right]$$

Another example: One-body density matrix

Here we look for

$$\langle \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}') \rangle \longrightarrow \left\langle\!\left\langle \left[(\mathbb{1} + z\,\mathcal{U}[\sigma])^{-1} z\,\mathcal{U}[\sigma]\right]_{\vec{r}'\vec{r}} \right\rangle\!\right\rangle_{P[\sigma]}$$

$$\bar{f}_{\vec{r},\vec{r}'} = \frac{1}{N_{samples}} \cdot \sum_{k=1}^{N_{samples}} \left[(\mathbb{1} + z\,\mathcal{U}[\sigma])^{-1} \cdot z\,\mathcal{U}[\sigma]\right]_{\vec{r}'\vec{r}}$$

Think about: How would you calculate $E = \langle \hat{H} \rangle$?