Fermion Sign Problem in Physics

Abhirup Mukherjee

A general problem in statistical mechanics is to compute thermal averages of quantities. Given the W microstates $\{|j\rangle\}$ and the energy values $\{E_j\}$ associated with them, the thermal average of a quantity $\hat{A}$ is defined as

$$\left\langle \hat{A} \right\rangle = \frac{\sum_{j=1}^{W} \hat{A}_j f_j}{\sum_j f_j} \tag{0.1}$$

$f_j, j = 1, 2, ..., W$ is the probability of reaching the microstate $|j\rangle$. For system with N particles, the number of microstates will go as 2^N, so it becomes impractical to evaluate such a summation (or integral, in the case of a continuous spectrum) naively. Classical Monte-Carlo chooses a smaller set of microstates $\{|i\rangle\}$, according to the distribution f, and then approximates the average as

$$\left\langle \hat{A} \right\rangle \approx \frac{1}{w} \sum_{i=1}^{w} \hat{A}_i \tag{0.2}$$

where w is the number of chosen states, out of the W total microstates.

A quantum mechanical system described by a Hamiltonian $\mathcal{H}$ will have a similar expression for expectation values.

$$\left\langle \hat{A} \right\rangle = \frac{1}{\text{Trace}\left[e^{-\beta\mathcal{H}}\right]} \text{Trace}\left[\hat{A}e^{-\beta\mathcal{H}}\right] = \frac{1}{Z} \text{Trace}\left[\hat{A}e^{-\beta\mathcal{H}}\right] \tag{0.3}$$

W here stands for the dimension of the Hilbert space this problem lives in, and j labels some complete basis in this space. To use Monte-Carlo, we need to put the partition function Z into a "classical form".

$$\begin{aligned}
&\sum_{j=1}^{W} \langle j| e^{-\beta\mathcal{H}} |j\rangle \\
&= \sum_{n=0}^{\infty} \sum_{j=1}^{W} \frac{1}{n!} (-\beta)^n \langle j| \mathcal{H}^n |j\rangle \\
&= \sum_{n=0}^{\infty} \sum_{j=1}^{W} \sum_{j_1,j_2,...j_{n-1}=1}^{W} \frac{1}{n!} (-\beta)^n \langle j| \mathcal{H} |j_1\rangle \langle j_1| \mathcal{H} |j_2\rangle \langle j_2| \mathcal{H} |j_3\rangle ... \langle j_{n-1}| \mathcal{H} |j\rangle \\
&= \sum_{n=0}^{\infty} \sum_{j,j_1,j_2,...j_{n-1}=1}^{W} \frac{1}{n!} (-\beta)^n \mathcal{H}_{j,j_1} \mathcal{H}_{j_1,j_2} ... \mathcal{H}_{j_{n-1},j}
\end{aligned} \tag{0.4}$$

The sums over j_i are all sums over all the microstates. If we consider the global summation $\sum_{j,j_1,j_2,...j_{n-1}=1}^{W}$, the string $j, j_1, j_2, ...j_{n-1}$ in a particular term of the summation denotes a set of n microstates of the system. For example, if we are in a two-state problem, a possible term of the summation would like $1, 1, 0, 1, 0, 0, 0, 1$. The number of states in the string is decided by the index n. The collective summation

$$\sum_{n=0}^{\infty} \sum_{j,j_1,j_2,...j_{n-1}=1}^{W} \tag{0.5}$$

is thus a summation over such strings of varying lengths. We denote such a string by s. The partition function can then be written as

$$Z = \sum_{s} f_s \tag{0.6}$$

where $s \equiv j, j_1, j_2, ...j_{n-1}, \forall\ j_i \in [1, W]$ and $\forall\ n \in [0, \infty]$, and

$$f_s = \frac{1}{n!} (-\beta)^n \mathcal{H}_{j,j_1} \mathcal{H}_{j_1,j_2} ... \mathcal{H}_{j_{n-1},j} \tag{0.7}$$

In the form eq. 0.6, the quantum-mechanical trace resembles the classical partition function. The numerator of the expectation value can also be written in a similar fashion:

$$\begin{aligned} \text{Trace}\left[\hat{A}e^{-\beta\mathcal{H}}\right] &= \sum_{j=1}^{W} \langle j| \hat{A}e^{-\beta\mathcal{H}} |j\rangle \\ &= \sum_{n=0}^{\infty} \sum_{j,j_1,j_2,...j_n=1}^{W} \frac{1}{n!} (-\beta)^n A_{jj_1} \mathcal{H}_{j_1 j_2} \mathcal{H}_{j_2 j_3} ... \mathcal{H}_{j_n j} \\ &= \sum_{s} A_s f_s \end{aligned} \tag{0.8}$$