two examples of quantum-classic mapping

Jian Wang

Physics and Astronomy, UCLA

(Dated: April 17, 2018)

Abstract

This tutorial talks about how to map a quantum model to its classical counterpart, which is the first step for any quantum Monte Carlo simulation. Examples are given for 0d and 1d Ising models.

Another question is, how to relate the thermo and dynamic observables between them.

THE MAPPING

We start with an equilibrium state quantum problem $\hat{H}$ at temperature β. Our first goal is to find way to compute the partition function of this quantum system. By Trotter decomposition, we divide the problem into N sections. Usually N is choosen to be very large, so that the transfer matrix T can be approximated in first order as $T \approx 1 - \frac{\beta}{N}\hat{H} + O(\frac{\beta E}{N})^2$

$$Z = \mathrm{Tr}[(e^{-\beta\hat{H}})] = \mathrm{Tr}[(e^{-\frac{\beta}{N}\hat{H}})^N] = \mathrm{Tr}[T^N] \tag{1}$$

There is a duality about the transfer matrix T. On one hand, it is an operator $\hat{T}$ represented in the same Hilbert space as $\hat{H}$; on the other hand, it is a matrix with element $T_{mn} = \langle m|\hat{T}|n\rangle$. The idea of quantum-to-classical mapping, is to treat the transfer matrix as the exponential of classical Lagrangian in a step time.

$$[e^{-\frac{\beta}{N}\hat{H}}]_{mn} = T_{mn} = e^{L_{mn}} \tag{2}$$

It is very tricky in the above representation. Although I label L_{mn}, we shouldn't think of L_{mn} as a matrix. They are classical field configuration at successive time.

$$\begin{aligned} |m\rangle &\to n(\tau) \\ |n\rangle &\to n(\tau+1) \\ L_{mn} &\to L(n(\tau), n(\tau+1))\Delta\tau \end{aligned} \tag{3}$$

And if we treat the summation over duplicated Hilbert space $\{|n\rangle\}^N$ as a functional summation over all configuration of $n(\tau)$, and this is the essential quantum-classical mapping identity:

$$\sum_{\{|n\rangle\}^N} \langle n_1|T|\cdots|T|n_\tau\rangle\langle n_\tau|T|n_{\tau+1}\rangle\langle n_{\tau+1}|\cdots|T|n_1\rangle = \sum_{\text{all configuration } n(\tau)} e^{S[n(\tau)]} \tag{4}$$

where $S[n(\tau)] = \sum_{\tau=1}^{N} L(n(\tau), n(\tau+1))\Delta\tau$

- $L(n(\tau), n(\tau+1))\Delta\tau$ is a discrete version. In continues models, the analogy is time derivatives.

- We shouldn't care too much about exact Lagrangian expression, and they are not unique depends on how you design the Trotter cuts. The action $S = \sum L(n(\tau), n(\tau+1))\Delta\tau$ is more important to us, since our goal is just re-sum $Z_{quantum} = Z_{classical}$. Another reason is, some problem like spin-boson system, there is no local format of Lagrangian, the action involves double time integral.

- Hilbert dimension number → numbers of classical field configuration at given time slice τ. For Spin, Fermion problems, it is discrete in nature, the classical field configuration is also discrete. For Boson problem, it is real number field.

Next, I'm going to show some example of mapping. The models might be exactly solved, which is even better for us to test the result of quantum Monte Carlo.

single spin

The single spin Hamiltonian

$$H = -\Delta\sigma^x \tag{5}$$

The Hilbert space dimension is two, therefore the transfer matrix can be written and calculated explicitly:

$$T = e^{-\frac{\beta H}{N}} = e^{\frac{\beta\Delta}{N}\sigma^x} = \begin{pmatrix} \cosh(\beta\Delta/N) & \sinh(\beta\Delta/N) \\ \sinh(\beta\Delta/N) & \cosh(\beta\Delta/N) \end{pmatrix} \tag{6}$$

Corresponding to the Hilbert space dimension 2, the classical variable takes two values $\mu = \pm 1$. Assuming the classic action is:

$$S = -\sum_{\tau=1}^{N} \left(J\mu_\tau\mu_{\tau+1} + K \right) \tag{7}$$

The transfer matrix in classical parameter is $T_{\mu_\tau,\mu_{\tau+1}} = e^{L_{\mu_\tau\mu_{\tau+1}}}$

$$T = \begin{bmatrix} e^{-J} & e^{+J} \\ e^{+J} & e^{-J} \end{bmatrix} e^{K} \tag{8}$$

Comparing Equation (6) and (8), we got our exact mapping relations:

$$\tanh(\beta\Delta/N) = e^{2J} \tag{9a}$$

$$\sinh(\beta\Delta/N) = e^{J+K} \tag{9b}$$

spin chain

Also known as transverse field Ising model, it is exactly solvable.

$$H = -\Delta_1 \sum_{i=1}^{L} \sigma_i^z \sigma_{i+1}^z - \Delta_0 \sum_{i=1}^{L} \sigma_i^x \tag{10}$$

Notice that, the Hilbert space is 2^L dimensional. At first glance, it is impossible to written down T and compare directly. However, T is sparse matrix. Most of the matrix elements are zero, because crazy changes of field configuration in short time will be penalized.

We choose the classical field $\mu_{i,\tau} = \pm 1$, which corresponds to the eigenvectors of σ_i^z. Each time step, we further divide the transfer matrix into two parts.

$$T = e^{\frac{\beta\Delta_1}{N}\sum_{i=1}^{L}\sigma_i^z\sigma_{i+1}^z + \frac{\beta\Delta_0}{N}\sum_{i=1}^{L}\sigma_i^x} = T_1 T_0 + O(\frac{\beta\Delta_1}{N} + \frac{\beta\Delta_0}{N})^2 \tag{11}$$

The matrix is $2^L \times 2^L$: the complete basis set of $|n(\tau)\rangle, |m\rangle, |n(\tau+1)\rangle$ all take the eigenbasis of σ_i^z, is 2^L dimensional, which is **same as numbers of classical field configuration** $n_i(\tau)$ at given time.

$$\langle n(\tau)|T|n(\tau+1)\rangle \approx \sum_m \langle n(\tau)|T_1|m\rangle\langle m|T_0|n(\tau+1)\rangle \tag{12}$$

In this representation, $\langle n(\tau)|T_1|m\rangle$ is diagonal. The $\mu_{i,\tau}$ corresponds the quantum number of state $|n(\tau)\rangle$, $\quad \hat{\sigma}_i^z|n(\tau)\rangle = \mu_{i,\tau}|n(\tau)\rangle$

$$\langle n(\tau)|T_1|m\rangle = e^{\frac{\beta\Delta_1}{N}\sum_{i=1}^{L}\mu_{i,\tau}\mu_{i+1,\tau}}\delta_{n(\tau),m} \tag{13}$$

to solve $\langle m|T_0|n(\tau+1)\rangle$, we find that the interaction is decoupled in different spins' Hilbert space. In each subspace, the problem is already solved in Equation 6.

$$\langle m|T_0|n(\tau+1)\rangle = \prod_{i=1}^{L}\langle m_i|e^{\frac{\beta h}{N}\sigma_i^x}|n_i(\tau+1)\rangle = \prod_{i=1}^{L} e^{-(J_0 m_{i,\tau}\mu_{i,\tau+1}+K)} \tag{14}$$

where $J_0 = \frac{1}{2}\ln(\tanh(\beta\Delta_0/N))$

Combine T_1 and T_0, we have:

$$T = e^{L(\tau)} := e^{-\sum_{i=1}^{L}\left(J_1\mu_{i,\tau}\mu_{i+1,\tau}+J_0\mu_{i,\tau}\mu_{i,\tau+1}+K\right)} \tag{15}$$

Multiply all the time slices, we got our classical action

$$S = -\sum_{\tau=1}^{N}\sum_{i=1}^{L}\left(J_1\mu_{i,\tau}\mu_{i+1,\tau} + J_0\mu_{i,\tau}\mu_{\tau+1} + K\right) \tag{16}$$

The mapping is given by:

$$\tanh(\beta\Delta_0/N) = e^{2J_0} \tag{17a}$$

$$\sinh(\beta\Delta_0/N) = e^{J_0+K} \tag{17b}$$

$$\beta\Delta_1/N = J_1 \tag{17c}$$

high dimensional quantum Ising with transverse field

In the last section, I made some effort to make the notation looks beautiful. These includes to write subindex systematically as $\Delta_0, \Delta_1, J_0, J_1, T_0, T_1$.

It turned out that, this careful treatment is very useful to generalize the problem into high dimensions. If we have a $d-$dimensional lattice $L_1 \times L_2 \times \cdots L_d$, there are anisotropy Ising interactions $\Delta_d, \cdots, \Delta_2, \Delta_1$ and a global transverse field Δ_0. The Hamiltonian, not formally written, but I think you know it:

$$H = -\Delta_d \sum_{i=1}^{L_d} \sigma^z_{i_d}\sigma^z_{i_d+1} - \cdots \Delta_2 \sum_{i=1}^{L_2} \sigma^z_{i_2}\sigma^z_{i_2+1} - \Delta_1 \sum_{i=1}^{L_1} \sigma^z_{i_1}\sigma^z_{i_1+1} - \Delta_0 \sum_{i}^{\text{all sites}} \sigma^x_i \tag{18}$$

can be mapped to a classical problem with extra dimension in τ

$$S = -\sum_{\text{nearest neighbour}}^{N\times L_1\times L_2\times\cdots L_d} \left(J_d\mu_i\mu_j + \cdots + J_2\mu_i\mu_j + J_1\mu_i\mu_j + J_0\mu_i\mu_j + K\right) \tag{19}$$

The mapping:

$$\tanh(\beta\Delta_0/N) = e^{2J_0} \tag{20a}$$

$$\sinh(\beta\Delta_0/N) = e^{J_0+K} \tag{20b}$$

$$\beta\Delta_1/N = J_1 \tag{20c}$$

$$\cdots$$

$$\beta\Delta_d/N = J_d \tag{20d}$$

The proof is same as the spin chain. Now, the transfer matrix is has $(d+1)$ terms, $T = T_d \cdots T_2 T_1 T_0$, where T_0 is not diagonal, others are diagonal.

STATISTICAL QUANTITIES

With the quantum-classical mapping done, and provide we have an efficient sampling algorithm, we can calculate any physical quantities via (naively, ignoring fancy statistical tools)

$$\langle A\rangle = \mathrm{Tr}[Ae^{-\beta H}]/Z = \frac{1}{\mathrm{STEPS}}\sum_{n=1}^{\mathrm{STEPS}} A_n \tag{21}$$

The physical quantity series $A_1, A_2, \cdots, A_n, \cdots$ comes from the Monte Carlo sampling series of the field configuration $\Phi_1, \Phi_2, \cdots, \Phi_n, \cdots$.

In this chapter, I will try to solve such a problem: *for given quantum operator $\hat{A}$, how can we construct a quantity from the classical field $A = A(\Phi)$?*

In the language of functional integral, the problem is stated as: *what functional should we use?*

$$\frac{\int D\Phi A(\Phi) e^{S[\Phi]}}{\int D\Phi e^{S[\Phi]}} \tag{22}$$

$$\mathrm{Tr}[Ae^{-\beta H}] = \sum_{\{|n\rangle\}^{N+1}} \langle n_0|A|n_1\rangle\langle n_1|T|\cdots|T|n_\tau\rangle\langle n_\tau|T|n_{\tau+1}\rangle\langle n_{\tau+1}|\cdots|T|n_0\rangle \tag{23}$$

If A is diagonal in the basis $\langle n_0|A|n_1\rangle = A(n_0)\delta_{n_0,n_1}$, then we just use $A(n_0)$ as the form of functional. Notice that $A(n_0)$ only uses $\tau = 0$ time slice, not the full field configuration $\Phi = n(\tau)$, this might be a huge waste of data.

If A is not diagonal, I don't know.

I believe, this is a great subject in statistical data analysis.

Magnetization, susceptibility, energy, heat capacity, free energy and entropy

One should first understand the physics, and utilize the summation rules, then design the Monte Carlo analysis.

Suddenly, I don't know how to do this in MC.

Should complete this later.

DYNAMICS

Can the dynamics of quantum ensemble can be all captured by the density matrix in Schrdinger picture? I think so. Because the evolution of each state is known.(Don't mix with Heisenberg picture, it is a constant there $\rho_H = e^{-\beta H}$)

$$\rho_S(t) \tag{24}$$

Back to some practical problem, we want to calculate $\langle A(t)B(0)\rangle$. Using Heisenberg representation, we get the result:

$$\mathrm{Tr}\big[e^{\beta H}e^{iHt}Ae^{-iHt}B\big]/Z \tag{25}$$

We can't use Monte Carlo to sample it. But if we try imaginary time:

$$t \to i\tau \tag{26}$$

We are then able to solve $\langle A(i\tau)B(0)\rangle$. Proof:

Suppose, A and B are diagonal in the basis. $\mathrm{Tr}\big[e^{\beta H}e^{-H\tau}Ae^{+H\tau}B\big] = \mathrm{Tr}[T^{N-s}AT^sB]$, which is the classical variable correlation of A_0B_s.

One goal of quantum Monte Carlo method is to extract real time information from the imaginary time correlation. This is called the analytic continuation problem. More often, people look at frequency domain, to extract information from Matsubara frequency $G(i\omega_n)$ data points to real frequency $G(\omega + 0^+)$. The foundation is the analytic Green function $G(z)$, it is analytic in the upper half complex plane. Next, I am going to demonstrate this, using the single spin as an example.

single spin dynamics

The dynamical operator is chosen to be the same $A = B = \sigma^z$. Our goal is to demonstrate such general identities:

$$G(z) = \int_{-\infty}^{+\infty} \frac{\rho(\omega)}{z - \omega} d\omega \tag{27a}$$

$$G^R(\omega) = G(\omega + 0^+) \tag{27b}$$

$$G^M(\omega_n) = G(i\omega_n) \tag{27c}$$

$$\rho(\omega) = -\frac{1}{\pi} \Im[G^R(\omega)] \tag{27d}$$

$$G^R(t) = -i\langle [A(t), B(0)] \rangle \Theta(t) \tag{27e}$$

$$G^M(\tau) = \langle \mathcal{T}[A(i\tau)B(0)] \rangle \tag{27f}$$

$$G^R(t) \leftrightarrow G^R(\omega) \tag{27g}$$

$$\tag{27h}$$

I was confused by this formalism for years, the $\frac{\text{physics intuition}}{\text{math complexicity}}$ ratio is very small! There are too many un-physical, un-observed quantities here, imaginary time, Matsubara frequencies. And quantum mechanics makes all these formalism even more mysteries.

I looked around to find some intuition, engineering friends taught me concepts like LTI system, s-domain, Z-transformation, I was amazed me a lot. The electric circuit problems in Chaikin & Lubinsky book is very helpful.

The quantum machine is a black box, which we don't need to understand from the outside user interface. When an interaction is turned on from the outside $H_I(t) = \lambda B f(t)$, we assume, the black box is a linear response system (in the weak interaction limit $\lambda \to 0$). The response of operator A is

$$\delta A(t) = \lambda \int \chi(t - t') f(t') dt' \tag{28}$$

Therefore, the essential function, which captures all the response information is $\chi(t - t')$. It is just $G^R(t)$, it doesn't depend on the way we give weak perturbation. **The linear response information all comes from the system correlation by itself. [fluctuation-dissipation theorem]**

How about energy?

When we choose $A = B$ to be the same operator. The interaction energy is known

immediately:

$$\text{energy}(t) = \lambda \delta A(t) \cdot f(t) \tag{29}$$

Some derivation shows that $\frac{d}{dt}\text{energy} \propto \omega\rho(\omega)$

my question is (1) stable sin and cosine function makes $H_I(t)$ sin, therefore energy is bounded (2) where does the energy goes?

$\frac{\rho(\omega)}{\rho(-\omega)} = e^{-\frac{\hbar\omega}{k_B T}}$ is the detailed balance, it is not the wrong in this context, should be the Fourier transfrom of $\langle A(t)B(0)\rangle$. **the system is in equilibrium. therefore, the quantum transitions show keeps a detailed balance.**

The result:

$$H = -\Delta\sigma^x \tag{30a}$$

$$\langle\sigma^z(t)\sigma^z(0)\rangle = \cos(2\Delta t) + i\tanh(\beta\Delta)\sin(2\Delta t) \tag{30b}$$

$$\langle\sigma^z(i\tau)\sigma^z(0)\rangle = \frac{\cosh\Delta(\beta - 2\tau)}{\cosh\beta\Delta} \tag{30c}$$

$$G^R(t) := -i\langle[\sigma^z(t), \sigma^z(0)]\rangle\Theta(t) = 2\tanh(\beta\Delta)\sin(2\Delta t)\Theta(t) \tag{30d}$$

$$G^R(\omega) = \tanh(\beta\Delta)\big(\frac{1}{\omega + 2\Delta + i\eta} - \frac{1}{\omega - 2\Delta + i\eta}\big) \tag{30e}$$

$$G^M(\omega_n) = \tanh(\beta\Delta)\big(\frac{1}{i\omega_n + 2\Delta} - \frac{1}{i\omega_n - 2\Delta}\big) \tag{30f}$$

$$G(z) = \tanh(\beta\Delta)\big(\frac{1}{z + 2\Delta} - \frac{1}{z - 2\Delta}\big) \tag{30g}$$

$$\rho(\omega) = \tanh(\beta\Delta)\big(-\delta(\omega + 2\Delta) + \delta(\omega - 2\Delta)\big) \tag{30h}$$

Before going, let's understand some of the physics. When $\beta\Delta \to 0$, we have $\tanh(\beta\Delta) = 1$, the temperature is much less than the energy scale, the system is have a Rabi oscillation $\langle\sigma^z(t)\sigma^z(0)\rangle = e^{i\omega_0 t}$, when no decay (for our simple model).

In this simple problem, the spectrum doesn't depend on temperature.

Now let's talk about the analytic continuation problem:

$$G^M(\omega_n) \to \rho(\omega) \tag{31}$$

$$G^M(\omega_n) = \int_{-\infty}^{+\infty} \frac{\rho(\omega)}{i\omega_n - \omega} d\omega \tag{32}$$

Here are some tips:

1. choice of Matsubara frequency points

   Theoretically, the infinite numbers of Matsubara points $\omega_n = \frac{2\pi}{\beta}n$ where $n = 1, 2, 3, 4, \cdots$ will determines $\rho(\omega)$ uniquely.

   In practice, the Monte Carlo data, we have β and finite N, the Matsubara frequency is periodic in $\Omega = \frac{2\pi}{\beta}N = \frac{2\pi}{\Delta\tau}$, which corresponds to the imaginary time direction unit step time scale.

$$\omega_{n+N} \equiv \omega_n \equiv \omega_n + \Omega \tag{33}$$

   Initially, we should only take positive $\omega_n > 0$, since there is no poles in the upper half plane, and we can arrive at Equation (32). **But, now the periodicity makes it unclear that, which frequency is negative. Careful analysis shall be taken here.**

   Another point, we notice that, the function $\frac{1}{z+2\Delta} - \frac{1}{z-2\Delta}$ changes its value significantly with the range of $|z_2 - z_1| \sim \Delta$. If we design very bad Matsubara points set, for example: $|\omega_{n2} - \omega_{n1}| \ll \Delta$ or $|\omega_{n2} - \omega_{n1}| \gg \Delta$, there will be less information contained in the data, as uncertainty will destroy everything easily.

add plot

   Unfortunately, the energy scale Δ is unknown a prior in most problems, and it might also dependents on β, here is the rule:

$$\frac{2\pi}{\beta} \lesssim \text{Energy Scale Interested} \lesssim \frac{2\pi}{\beta}N \tag{34}$$

2. the symmetry and summation rules

   From this particular example, we see $\rho(\omega) = -\rho(-\omega)$ is an odd function. $\langle\sigma(i\tau)\sigma(0)\rangle$ is real and even centered at $\beta/2$. If we can utilize the property, the Kernel form can be modified to be better, the result will be more accurate.

   Physically, $\langle\sigma^z(t)\rangle$ is a real quantity, therefore, the linear response coefficient $\chi(t - t')$ should also be real (or pure imaginary, depends on the convention) . For any real

function $f(t)$, it s Fourier transform $F(\omega) = \int f(t)\cos(\omega t) + if(t)\sin(\omega t)dt$, The imaginary part of F must be odd.

Summation rule in frequency domain, is a **refection** of identity in real time, for fermion $\langle\{c^\dagger(0), c(0)\}\rangle \equiv 1$, for Bosons $\langle[\sigma^z(0), \sigma^z(0)]\rangle \equiv 0$.

In fermion case $\int_{-\infty}^{+\infty} \rho(\omega)d\omega = 1$; spin case $\int_{-\infty}^{+\infty} \rho(\omega)d\omega = 0$ which is already contained in the odd property.

With the odd symmetry in mind, we have

$$G^M(\omega_n) = \int_{-\infty}^{+\infty} \frac{i\omega_n + \omega}{-\omega_n^2 - \omega^2}\rho(\omega)d\omega = \int_0^{+\infty} \frac{2\omega}{-\omega_n^2 - \omega^2}\rho(\omega)d\omega \tag{35}$$

3. prior knowledge

$$\rho(\omega) \geq 0 \quad \text{for } \omega > 0 \tag{36}$$

This is the idea of maximum entropy method.

Here is a test for the Kernel in Equation (35), $\int_0^{+\infty} \frac{2\omega}{-\omega_n^2-\omega^2}\tanh(\beta\Delta)\delta(\omega - 2\Delta)d\omega = \frac{4\Delta}{-\omega_n^2-\Delta^2}$, successful, except the sign need to be checked throughout this paper.