Lecture 4: Analytical Continuation

In the last class, we showed that Feynman path integrals provide an appealing and computationally tractable strategy for evaluating quantum Boltzmann statistical quantities, which stem from the canonical partition function,

$$Q = \sum_{\nu} e^{-\beta E_\nu}, \tag{1}$$

in terms for a classical configuration integral of an isomorphic ring-polymer system

$$Q = \lim_{n\to\infty} \left(\frac{m\omega_n}{2\pi\hbar}\right)^{n/2} \int dx_1 \ldots \int dx_n e^{-\beta U_{\mathrm{eff}}(\mathbf{x})} \tag{2}$$

where

$$U_{\mathrm{eff}}(\mathbf{x}) = \frac{1}{n}\sum_{j=1}^{n} \frac{1}{2} m\omega_n^2 (x_j - x_{j+1})^2 + \frac{1}{n}\sum_{j=1}^{n} V(x_j) \tag{3}$$

and $V(x)$ is the potential energy function for the system.

In the current class, we recognize that that correlation functions evaluated on the imaginary-time axis can be analytically continued onto the real-time axis, thus providing an avenue for (numerically tractable) quantum statistical results to be used for the evaluation of (numerically intractable) exact quantum dynamics properties.

A. Time correlation functions on the imaginary- and real-time axes

Thus far, we have considered “imaginary-time" path integrals, involving matrix elements of the form

$$\langle x| e^{-\beta \hat{H}} |x'\rangle. \tag{4}$$

Allowing β to be an imaginary number $\beta = it/\hbar$, we see that this matrix element becomes the familiar quantum mechanical time-evolution matrix element

$$\langle x| e^{-it\hat{H}/\hbar} |x'\rangle. \tag{5}$$

As this suggests, there are profound connections between information on the real-time and imaginary-time axes of quantum mechanical TCFs.

Consider the quantum TCF for the autocorrelation of operator $\hat{A}$, in the standard form:

$$C(t) = \frac{1}{Q}\mathrm{Tr}\left[e^{-\beta\hat{H}}\hat{A}e^{it\hat{H}/\hbar}\hat{A}e^{-it\hat{H}/\hbar}\right] = \langle A(0)A(t)\rangle. \tag{6}$$

Now, allowing time to be complex:

$$C(t+i\lambda\hbar) = \langle A(0)A(t+i\lambda\hbar)\rangle = \frac{1}{Q}\mathrm{Tr}\left[e^{-(\beta-\lambda)\hat{H}}\hat{A}e^{-\lambda\hat{H}}e^{it\hat{H}/\hbar}\hat{A}e^{-it\hat{H}/\hbar}\right] \tag{7}$$

where we see the splitting of the Boltzmann operator across the time-zero evaluation of the operator, which is familiar from the Kubo-transform. For a Hamiltonian with energy spectrum that is bounded from below (but not necessarily above) note that this splitting only makes sense for $\lambda \in [0,\beta]$, such that the TCF in Eq. ?? is an analytical function only in the range $\lambda \in [0,\beta], t \in (-\infty,\infty)$.

B. Evaluation of an imaginary-time correlation function

Assuming that $\hat{A}(\hat{x})$ is a function of position, we now consider numerical evaluation of the TCF on the imaginary-time axis,

$$C(i\lambda\hbar) = \frac{1}{Q}\mathrm{Tr}\left[e^{-(\beta-\lambda)\hat{H}}\hat{A}e^{-\lambda\hat{H}}\hat{A}\right], \qquad \lambda \in [0,\beta]. \tag{8}$$

Discretizing $\lambda_j = \beta_m j, j = 1,\ldots,n$, where $\beta_n = \beta/n$, we have

$$C(i\lambda_j\hbar) = \frac{1}{Q}\mathrm{Tr}\left[e^{-\beta_n(n-j)\hat{H}}\hat{A}e^{-\beta_n j\hat{H}}\hat{A}\right], \tag{9}$$

and introducing resolutions of the identities and performing the Trotter approximation, we obtain

$$C(i\lambda_j\hbar) = \frac{1}{Q}\int dx_1\ldots\int dx_n \prod_{k=1}^{j}\langle x_k|e^{-\beta_n\hat{H}}|x_{k+1}\rangle A(x_j)\prod_{l=j+1}^{n}\langle x_l|e^{-\beta_n\hat{H}}|x_{l+1}\rangle A(x_1) \tag{10}$$

$$= \frac{1}{Q}\left(\frac{m\omega_n}{2\pi\hbar}\right)^{n/2}\int dx_1\ldots\int dx_n e^{-\beta U_{\mathrm{eff}}(\mathbf{x})}A(x_1)A(x_j) \tag{11}$$

We thus see that correlation functions on the imaginary-time are straightforwardly obtained from purely statistical quantities and may thus be evaluated using either classical Monte Carlo or molecular dynamics sampling techniques. Intriguingly, using the analyticity of the TCF, it indicates that all real-time dynamics is in principle available from a purely classical calculation! We now investigate how this works in practice...

C. Relating real and imaginary time via analytical continuation

First, we perform a brief digression to establish that the TCF in the standard form ($C(t)$, Eq. ??) contains the same information as in the Kubo-transformed TCF that we have seen previously,

$$\tilde{C}(t) = \frac{1}{\beta Q}\int_0^{\beta} d\lambda \ \mathrm{Tr}\left[e^{-(\beta-\lambda)\hat{H}}\hat{A}e^{-\lambda\hat{H}}e^{it\hat{H}/\hbar}\hat{A}e^{-it\hat{H}/\hbar}\right] = \int_0^{\beta} d\lambda \ C(t+i\lambda\hbar). \tag{12}$$

To prove this, we consider the Fourier transform of $C(t+i\lambda\hbar)$,

$$P^{(\lambda)}(\omega) = \int_{-\infty}^{\infty} dt \ e^{-i\omega t}C(t+i\lambda\hbar) \tag{13}$$

$$= \frac{2\pi}{Q}\sum_{i,j}|A_{ij}|^2 e^{-\beta E_i-\lambda(E_j-E_i)}\delta(\omega-(E_j-E_i)/\hbar), \tag{14}$$

where we have expanded the trace and introduced a resolution of the identity in terms of the energy eigenstates of the system. It is thus easy to show (see homework) that

$$P^{(0)}(\omega) = \tilde{P}(\omega)\frac{\beta\hbar\omega}{1-e^{-\beta\hbar\omega}}, \tag{15}$$

where the LHS is the Fourier transform of the TCF in the standard form and the RHS is the Fourier transform of the Kubo-transformed TCF

$$\tilde{P}(\omega) = \frac{1}{\beta}\int_0^{\beta} d\lambda \ P^{(\lambda)}(\omega). \tag{16}$$

Eq. ?? indicates that the standard and Kubo-transformed versions of the TCF have the same information content.

Then, as shown in Ref. 1, the imaginary-time and real-time axes of the TCF can be related via

$$C(i\lambda\hbar) = \int_0^{\infty} g_+(\lambda,t)\tilde{C}(t)dt, \tag{17}$$

where $g_+(\lambda,t) = \mathrm{Re}[g(\lambda,t)]$ and

$$g(\lambda,t) = -\pi\left(2\beta\hbar\sinh^2\left(\frac{\pi t}{\beta\hbar} - i\frac{\pi\lambda}{\beta}\right)\right)^{-1} \tag{18}$$

is an easily evaluated function.

Note that Eq. ?? is a remarkable result that directly relates information on the imaginary-tine axis $C(i\lambda\hbar)$ to the *exact* real-time dynamics of the system (via $\tilde{C}(t)$). It would seem that all that we have to do is to evaluate $C(i\lambda\hbar)$ via classical statistical mechanical sampling methods, and then invert Eq. ?? to obtain the real-time dynamics. Unfortunately, this inversion is numerically ill-conditioned, such that very small numerical errors on the imaginary-time axes create very large numerical uncertainties on the real-time axis. As a result, numerical methods based on analytical continuation are primarily limited to the characterization of real-time dynamics

dynamics on short timescales (typically, $t \sim \beta\hbar$, for which the inversion can be stably performed), which limits the practical utility of the method. Therefore, we shall next turn our attention to methods that use imaginary-time path-integrals to *approximate* the real-time dynamics.

[1] Habershon, Braams, and Manolopoulos, *J. Chem. Phys.*, **127** (2007) 174108.