Quantum Mechanics

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1 Anharmonic Oscillator

1.1 Thermal paths and quantum statistical mechanics

Recall the partition function from statistical mechanics,

$$Z_T(\beta = \frac{1}{T}) = \mathrm{Tr}(e^{-\beta \hat{H}}) = e^{-\beta F(\beta)}$$
$$F = -T \log Z(\beta)$$

In quantum mechanics, we have

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar} = \sum_{n,s} e^{-i\hat{H}t/\hbar} |E_n, s\rangle\langle E_n, s| = \sum_{n,s} e^{-i\hat{H}t/\hbar} \mathcal{P}_n$$

and we define similar to statistical mechanics,

$$\begin{aligned} Z_{\mathrm{QM}}(t) = \mathrm{Tr}\, \hat{U}(t) &= \sum_n g_n e^{-iE_n t/\hbar} \\ &= \int dx\ \langle x|\hat{U}(t)|x\rangle \\ &= \int dx\ K(x,t;x,0) \end{aligned}$$

Recall that

$$K(x_2,t_2;x_1,t_1) = \sum_{n,s} e^{-iE_n(t_2-t_1)/\hbar} \psi_{ns}(x_2)\psi^*_{ns}(x_1)$$

Let us work with the simple harmonic oscillator. The partition function now becomes

$$\begin{aligned} Z^{\mathrm{SHO}}_{\mathrm{QM}}(\Delta t) &= \int_{-\infty}^{\infty} dx\ \sqrt{\frac{m\omega}{2\pi i\hbar \sin\omega\Delta t}} \exp\left(\frac{i}{\hbar}\left(\frac{m\omega}{\sin\omega\Delta t}\right) 2x^2 \left(\cos\omega\Delta t - 1\right)\right) \\ &= \sqrt{\frac{m\omega}{2\pi i\hbar \sin\omega\Delta t}} \left(i\pi \frac{2\hbar \sin\omega\Delta t}{2m\omega(\cos\omega\Delta t - 1)}\right) \\ &= \frac{1}{2a \sin\frac{\omega\Delta t}{2}} = e^{-i\omega\Delta t/2}\left(\frac{1}{1-e^{-i\omega\Delta t}}\right) \\ &= e^{-i\omega\Delta t/2} \sum_{n=0}^{\infty} e^{-in\omega\Delta t} = \sum_n g_n e^{-iE_n^{\mathrm{HO}}\Delta t/\hbar} \end{aligned}$$

This can be extended to the D-dimensional harmonic oscillator very simply as the integrals over each dimension decouple and we are left with the simple relation:

$$Z^{\mathrm{D(HO)}}_{\mathrm{QM}} = \left(Z^{\mathrm{HO}}_{\mathrm{QM}}\right)^D$$

Note that we can relate the thermal partition function to the quantum mechanical one as follows:

$$Z_T(\beta = +i\Delta t/\hbar) = Z_{\text{QM}}(\Delta t = -i\hbar\beta)$$

The thermal dynamics is thus a complex analytic continuation of quantum mechanical evolution. This corresponds to a **Wick rotation**. If we Wick rotate $Z_{\text{QM}}^{\text{SHO}}$, for example, we will recover the statistcal mechanics partition function.

1.2 Time lattice approximation

If we have an anharmonic oscillator $V(x(t))$ the action is given by

$$\begin{aligned}
S[x(t)] &= \frac{m}{2}\int_{t_1}^{t_2} d\tau\, \left(\dot{x}^2 - \frac{2}{m}V(X(t))\right) \\
S[x = x_{\text{cl}} + y] &= S_{\text{cl}} + \frac{m}{2}\int_{t_1}^{t_2} d\tau\, \left(\dot{y}^2 - \frac{2}{m}\frac{1}{2}V''\left(x_{\text{cl}}(t)\right)y^2\right) + \cdots = \omega_{\text{cl}}^2 \\
\delta S^{(2)} &= -\frac{m}{2}\int_{t_1}^{t_2} d\tau\, y(\tau)\left(\frac{d^2}{d\tau^2} + \omega_{\text{cl}}^2(\tau)\right)y(\tau)
\end{aligned}$$

But how the hell do we evaluate this integral? We make the time lattice approximation where we discretize time with lattice spacing a. The frequencies are trivially $\omega(\tau_n) = \omega_n$, and of course $y_0 = y_{N+1} = 0$ with

$$y(t) = \begin{pmatrix} y_N \\ \vdots \\ y_1 \end{pmatrix}$$

$$y(\tau)\hat{D}y(\tau) = y_i M_{nj} y_j$$

where $\hat{D}$ is the differential operator present in the integral above and M can be found to be a tri-diagonal matrix (by simple discretization). It turns out, then that we can compute the path integral prefactor

$$\begin{aligned}
\mathcal{A}_{\text{AHO}} &= \left(\frac{m}{2\pi i\hbar a}\right)^{N+\frac{1}{2}} \int dy_1 \dots dy_N\; e^{\frac{im}{2\hbar a} y_i M_{ij} y_j} \\
&= \left(\frac{m}{2\pi i\hbar a}\right)^{1/2}\left(\frac{1}{\det M}\right)^{1/2}.
\end{aligned}$$

Depending on the dimension of the problem, we can express the determinant as a recursion relation involving determinants for the lower dimensional problems (Kleiner 2.189),

$$(d_{N+1} - 2d_N + d_{N-1}) + a^2\omega_{N+1}d_N = 0$$

After some black magic, one reaches $d_N = C_+(1+ia\omega)^N + C_-(1-ia\omega)^N$, which, in the limit of the lattice spacing getting finer and finer, yields

$$d_\infty = C_+ e^{i\omega\Delta t} + C_- e^{-i\omega\Delta t}$$

To recover the free propogator, we must have $ad_N \to \Delta t$ as $\omega \to 0$ in the denominator. This implies that $C_+ = -C_- = 1/2i\omega$, and we have essentially solved the problem by reducing the computation of the path integral prefactor to the computation of an infinite-dimensional determinant.

1.3 Van Vleck approximation