Relation Between Quantum and Classical Stat. Mech

We have already noted a similarity between quantum and classical stat mech.

$$Z = \sum_{\{\phi\}} e^{-\beta E(\phi)} \quad \leftarrow \text{classical}$$

$\{\phi\}$ ← classical degrees of freedom with energy E

$$Z = \sum_n e^{-\beta E_n} \quad \longleftarrow \text{quantum}$$

sum over eigenenergies of quantum $\hat{H}$

We now explore a much more profound relationship which allows us to map any quantum stat mech problem onto a classical one (in one higher dimension).

The method is based on <u>path integrals</u>.

Consider a single quantum oscillator. (We can regard this as a $d=0$ dimensional system)

$$\hat{H} = \hat{p}^2/2m + 1/2\, m\omega^2 \hat{x}^2$$

The expression for Z is

$$Z = \sum_n e^{-\beta E_n} = \mathrm{Tr}\, e^{-\beta \hat{H}}$$

working in basis of eigenstates $\hat{H}|n\rangle = E_n|n\rangle$ makes this obvious.

But can evaluate Tr in any basis. Let's use eigenstates of position operator $\hat{x}|x\rangle = x|x\rangle$

$$Z = \int dx \, \langle x| e^{-\beta \hat{H}} |x\rangle$$

We are not allowed to write $e^{-\beta\hat{H}} = e^{-\beta \hat{p}^2/2m} e^{-\beta m\omega^2 \hat{x}^2/2}$

because $[\hat{x},\hat{p}] \neq 0$. However, this expression is approximately true if β is small — the errors are order β^2.

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Recall why this is

$$e^{\lambda(\hat{A}+\hat{B})} = 1 + \lambda(\hat{A}+\hat{B}) + \frac{1}{2}\lambda^2(\hat{A}+\hat{B})^2 + \ldots$$

$$\hat{A}^2 + \hat{A}\hat{B} + \hat{B}\hat{A} + \hat{B}^2$$

$$e^{\lambda\hat{A}} e^{\lambda\hat{B}} = \left(1 + \lambda\hat{A} + \tfrac{1}{2}\lambda^2\hat{A}^2 + \ldots\right)\left(1 + \lambda\hat{B} + \frac{\lambda^2}{2}\hat{B}^2 + \ldots\right)$$

$$= 1 + \lambda(\hat{A}+\hat{B}) + \frac{1}{2}\lambda^2(\hat{A}^2 + 2\hat{A}\hat{B} + \hat{B}^2) + \ldots$$

So the error is

$$e^{\lambda(\hat{A}+\hat{B})} - e^{\lambda\hat{A}} e^{\lambda\hat{B}} = \frac{1}{2}\lambda^2(\hat{B}\hat{A} - \hat{A}\hat{B}) + \ldots$$

$$= \frac{1}{2}\lambda^2[B,\hat{A}] + \ldots$$

order λ^2.

Actually it is even better than this because one can easily show

$$e^{\lambda(\hat{A}+\hat{B})} - e^{\lambda\hat{A}/2} e^{\lambda\hat{B}} e^{\lambda\hat{A}/2} = \text{order}(\lambda^3)$$

and (because the trace is cyclic) we will in a moment see the error is this smaller value.

The idea of the path integral method is to subdivide β into smaller values τ so we can approximate $e^{-\beta\hat{H}}$ accurately. More precisely, if $\hat{H} = \hat{A} + \hat{B}$ we write $\beta = L\tau$ (L large, τ small)

$$Z = \mathrm{Tr}\, e^{-\beta\hat{H}} = \mathrm{Tr}\, e^{-L\tau(\hat{A}+\hat{B})}$$

$$= \mathrm{Tr}\Big[\underbrace{e^{-\tau(\hat{A}+\hat{B})}\, e^{-\tau(\hat{A}+\hat{B})} \cdots e^{-\tau(\hat{A}+\hat{B})}}_{L \text{ factors}}\Big]$$

$$\underset{\uparrow}{\approx} \mathrm{Tr}\left[e^{-\tau\hat{A}} e^{-\tau\hat{B}} e^{-\tau\hat{A}} e^{-\tau\hat{B}} \cdots e^{-\tau\hat{A}} e^{-\tau\hat{B}}\right]$$

This is a "well controlled" approximation meaning it can be systematically improved by increasing L (decreasing τ). This is in contrast to MFT which is "uncontrolled". Once you ~~a~~ commit to MFT there is no way to improve it.

Note that we can also rewrite this as

$$\mathrm{Tr}\left[e^{-\tau\hat{A}/2} e^{-\tau\hat{A}/2} e^{-\tau\hat{B}} e^{-\tau\hat{A}/2} e^{-\tau\hat{A}/2} e^{-\tau\hat{B}} \cdots e^{-\tau\hat{A}/2} e^{-\tau\hat{A}/2} e^{-\tau\hat{B}}\right]$$

and because Tr is cyclic can move first term to end

and actually have product of L terms $e^{-\tau\hat{A}/2} e^{-\tau\hat{B}} e^{-\tau\hat{A}/2}$

Lets apply this to the harmonic oscillator and see why this is so useful

$$Z = \int dx_1 \, \langle x_1 | e^{-\beta \hat{H}} | x_1 \rangle$$

We'll see why I am labeling the states $|x_1\rangle$ in a moment

$$\approx \int dx_1 \underbrace{\langle x_1 | e^{-\tau \frac{1}{2} m\omega^2 \hat{x}^2}}_{e^{-\tau \frac{1}{2} m\omega^2 x_1^2} \langle x_1 |} e^{-\tau \hat{p}^2/2m} e^{-\tau \frac{1}{2} m\omega^2 \hat{x}^2} e^{-\tau \hat{p}^2/2m} \ldots | x_1 \rangle$$

$\int dx_2 \, |x_2\rangle\langle x_2|$

Notice the operator $\hat{x}$ gets replaced by a number x_1

Can we do more elimination of yucky operators?! Sure! Just introduce complete sets of states all over the place (now you see why we used $|x_1\rangle$)

$$Z \approx \int dx_1 \, e^{-\tau \frac{1}{2} m\omega^2 (x_1^2 + x_2^2 + \ldots x_L^2)} \langle x_1 | e^{-\tau \hat{p}^2/2m} | x_2 \rangle$$

$$\langle x_2 | e^{-\tau \hat{p}^2/2m} | x_3 \rangle \ldots \langle x_L | e^{-\tau \hat{p}^2/2m} | x_1 \rangle$$

All the $\hat{x}$ operators are gone. We can get rid of $\hat{p}$ also because we can evaluate each $\langle x_\ell | e^{-\tau \hat{p}^2/2m} | x_{\ell+1} \rangle$

$$\langle x_\ell | e^{-\tau \hat{p}^2/2m} | x_{\ell+1} \rangle$$

$$= \int dp \; \underbrace{\langle x_\ell | e^{-\tau \hat{p}^2/2m}}_{|p\rangle e^{-\tau p^2/2m}} | p \rangle \langle p | x_{\ell+1} \rangle$$

$e^{-i p x_{\ell+1}/\hbar}$

a number!

I'm going to forget about normalization, since constants are irrelevant to derivatives of $\ln Z$ ← all observables

$$= \int dp \; e^{-i(x_{\ell+1} - x_\ell) p/\hbar} \; e^{-\tau \hat{p}^2/2m}$$

Complete the square

$$-\tau p^2/2m - i(x_{\ell+1} - x_\ell) p/\hbar$$

$$= -\frac{\tau}{2m}\left[\left(p + \frac{i(x_{\ell+1} - x_\ell) m}{\tau \hbar} \right)^2 \right] + \frac{\tau}{2m} \left(\frac{i(x_{\ell+1} - x_\ell) m}{\tau \hbar} \right)^2$$

Now $\int dp \; e^{-a(p - p_0)^2} = \sqrt{\frac{\pi}{a}}$

p_0 is irrelevant (even if imaginary...) and again we will ignore the constant factor $\sqrt{\pi/a}$ which are irrelevant to derivatives of $\ln Z$. Upshot:

$$\langle x_\ell | e^{-\tau \hat{p}^2/2m} | x_{\ell+1} \rangle \sim e^{-\frac{1}{2} m \left(\frac{x_{\ell+1} - x_\ell}{\tau} \right)^2 \tau \, 1/\hbar^2}$$

Looks a lot like $\frac{1}{2} m v^2$ eh?!

Putting this all together

$$Z = \int dx_1\, dx_2 \ldots dx_L\; e^{-S(x_1, x_2 \ldots x_L)}$$

Understand $x_{L+1} \equiv x_1$
which reflects
Trace $= \int dx_1 \langle x_1 | \ldots | x_1 \rangle$
last x = first x

where

$$S = \tau \left[\frac{1}{2} m\omega^2 \sum_{l=1}^{L} x_l^2 + \frac{1}{2} m \sum_{l=1}^{L} \left(\frac{x_{l+1} - x_l}{\tau} \right)^2 \frac{1}{\hbar^2} \right]$$

Comment: Feynman originally did this for $e^{-i\hat{H}t/\hbar}$
instead of $e^{-\beta \hat{H}}$. When you do that you get $(t = L\epsilon)$

$$\langle x | e^{-i\hat{H}t/\hbar} | x' \rangle = \int dx_1 \ldots dx_L\; e^{iS/\hbar}$$

where S = classical action

$$= \epsilon \left\{ \sum \frac{1}{2} m \left(\frac{x_{l+1} - x_l}{\epsilon} \right)^2 - \sum \frac{1}{2} m\omega^2 x_l^2 \right\}$$

"T" − "V"

~~discretized version of~~

$$\int (T - V)\, dt$$

Units check!
$\tau = \beta/L$ has units $1/E$
So $\tau \frac{1}{2} m\omega^2 x^2$ dimensionless
as it must be up in exponent
Meanwhile $x/\hbar$ has units $\frac{1}{p}$
so $\tau m \left(\frac{x_{l+1} - x_l}{\tau} \right)^2 \frac{1}{\hbar^2} \sim \frac{m}{\tau} \frac{1}{p^2}$
$\sim \frac{1}{\tau (p^2/2m)} \sim$ dimensionless

Going back to stat mech problem,

Think about the structure of this expression

$$Z = \int dx_1 dx_2 \ldots dx_L \, e^{-S}$$

$$S = \tau \left\{ \frac{1}{2} m\omega^2 \sum x_\ell^2 + \frac{1}{2} m \sum \left(\frac{x_{\ell+1} - x_\ell}{\tau} \right)^2 \frac{1}{\hbar^2} \right\}$$

This is precisely the partition function of a classical system of L masses, each of which is connected to equilibrium position with spring $\frac{1}{2} m\omega^2$ and connected to its neighbors with spring $\frac{1}{2} m \frac{1}{\tau^2} \frac{1}{\hbar^2}$

$$Z_{\text{single quantum oscillator}} \longleftrightarrow Z_{\text{chain of } L \text{ classical oscillators}}$$

"0 dimensional" — "1 dimensional"

Amazingly, this can always be done

Quantum Z in d dimensions $\longleftrightarrow$ classical Z in $(d+1)$ dimensions.

A natural question to ask is whether we can recover the quantum expression for Z

$$Z = \sum_n e^{-\beta E_n} = \sum_{n=0}^{\infty} e^{-\beta(n+1/2)\hbar\omega}$$

$$= e^{-\beta 1/2 \hbar\omega}\left(1-e^{-\beta\hbar\omega}\right)^{-1}$$

To do so involves doing a multidimensional Gaussian integral

$$Z = \int dx_1\, dx_2 \ldots dx_L \; e^{-\vec{x}^T \mathbb{M} \vec{x}}$$

where $\vec{x}^T = (x_1\ x_2 \ldots x_L)$ and $\mathbb{M}$ is the matrix

$$\mathbb{M} = \begin{bmatrix} A & B & 0 & 0 & \\ B & A & B & 0 & \\ 0 & B & A & 0 & \\ & & & \ddots & \\ & & & & A \end{bmatrix}$$

$$A \equiv \tfrac{1}{2} m\omega^2 \tau + m \, 1/\hbar^2 \tau$$

$$B \equiv 1/2\, m\, 1/\hbar^2 \tau$$

Think about factors of 2 carefully

$(x_{e+1} - x_e)^2$

$\sim x_{e+1}^2 - 2x_{e+1}x_e + x_e^2$

Each $(x_{e+1}-x_e)^2$ contributes 2 x^2 terms to A

placed into two B terms

A very useful identity is — dimension of matrix/vector

$$\int d\vec{x}\, e^{-\vec{x}^T \mathbb{M} \vec{x}} = \pi^{N/2}\, 1/\sqrt{\det \mathbb{M}}$$

This is the multidimensional analog of

$$\int dx\, e^{-ax^2} = \sqrt{\frac{\pi}{a}} \leftarrow a^{1/2}$$

a = det of 1×1 "matrix" a

Note also $\det \mathbb{M} = \prod_l \lambda_l$

$\uparrow$ eigenvalues.

So we can evaluate the classical Z because

we know eigenvalues of $\mathbb{M}$ $\doteq$ $A + 2B\cos k$

$\uparrow \frac{2\pi}{L}\{1, 2, \ldots L\}$

$$Z_{\text{classical}} = \pi^{L/2} \left[\prod_l \left(A + 2B\cos\frac{2\pi l}{L}\right) \right]^{-1/2}$$

$$A = \frac{1}{2} m\omega^2 \tau + m/\hbar^2\tau$$

$$B = \cancel{}\ 1/2\, m/\hbar^2\tau$$

Recall $\tau = \beta/L$

We'll explore this further in the homework.

Sketching things a bit:

$$\ln Z = C' - \tfrac{1}{2} \sum_{\ell} \ln\left(A + 2B\cos \frac{2\pi\ell}{L}\right)$$

If we are willing to write a little program to evaluate the sum we can compare with

$$\ln \, e^{-\frac{1}{2}\beta\hbar\omega}\left(1-e^{-\beta\hbar\omega}\right)^{-1}$$

We would need to keep track of constants C' more carefully to do this.

It's better to compare $\langle E\rangle$ because we avoid tracking all the constants. Anyway Energy is more interesting.

$\sum x^n = 1/1-x$

$\sum n x^n = x/(1-x)^2$

The exact result is, of course, $\langle E\rangle = \hbar\omega \, \frac{1}{e^{\beta\hbar\omega}-1} + \frac{1}{2}\hbar\omega$

Derivation:

$$\langle E\rangle = Z^{-1}\sum E_n e^{-\beta E_n} = Z^{-1}\sum_n (n+\tfrac{1}{2})\hbar\omega \, e^{-\beta(n+\frac{1}{2})\hbar\omega}$$

$$= \tfrac{1}{2}\hbar\omega + Z^{-1}e^{-\beta\frac{1}{2}\hbar\omega}\sum_n n e^{-\beta n\hbar\omega}$$

$$= \tfrac{1}{2}\hbar\omega + e^{\beta\hbar\omega/2}\left(1-e^{-\beta\hbar\omega}\right) e^{-\beta\hbar\omega}/\left(1-e^{-\beta\hbar\omega}\right)^2 e^{-\beta\frac{1}{2}\hbar\omega} \, \hbar\omega \checkmark\checkmark$$

We'll want also to evaluate things like

$$\int dx_1 dx_2 \ldots dx_L \, e^{-\vec{x}^T M \vec{x}} \, x_i x_j \Big/ \int dx_1 dx_2 \ldots e^{-\vec{x}^T M \vec{x}}$$

which, amazingly, turns out to be $\frac{1}{2}(M^{-1})_{ij}$!

As a preview to Quantum Field Theory:

$$\int dx_1 dx_2 \ldots dx_L \, e^{-\vec{x}^T M \vec{x}} \, x_i x_j x_k x_l \Big/ \int dx_1 dx_2 \ldots e^{-\vec{x}^T M \vec{x}}$$

$$= \tfrac{1}{2}(M^{-1})_{ij} \, \tfrac{1}{2}(M^{-1})_{kl} + \tfrac{1}{2}(M^{-1})_{ik} \left(\tfrac{1}{2} M^{-1}\right)_{jl}$$

$$+ \tfrac{1}{2}(M^{-1})_{il} \, \tfrac{1}{2}(M^{-1})_{jk}$$

In QFT you'll call this "doing all the contractions"