Relation Between Quantum and Classical Stat. Mech

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

\[ Z = \sum e^{-\beta E(\Phi)} \quad \leftarrow \text{classical} \]
\[ \sum_{\Phi} \quad \text{classical degrees of freedom with energy } E \]

\[ Z = \sum e^{-\beta E_n} \quad \leftarrow \text{quantum} \]
\[ \sum_{n} \quad \text{sum over eigenenergies of quantum } \Phi \]

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

\[ \hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2 \]

The expression for Z is

\[ Z = \sum_n e^{-\beta E_n} = Tr e^{-\beta \hat{H}} \]

working in basis of eigenstates \( \hat{H} | n \rangle = E_n | n \rangle \)

makes this obvious.

But can evaluate Tr in any basis. So let 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 \( e^{-\beta \hat{H}} = e^{-\beta \frac{\hat{p}^2}{2m}} e^{-\beta m \omega^2 \hat{x}^2 / 2} \)

because \( [\hat{x}, \hat{p}] \neq 0 \). However, this expression is approximately true if \( \beta \) is small — the errors are order \( \beta^2 \).
Recall why this is
\[ e^{\lambda (\hat{A} + \hat{B})} = 1 + \lambda (\hat{A} + \hat{B}) + \frac{1}{2} \lambda^2 (\hat{A} + \hat{B})^2 + \ldots \]
\[ \hat{A}^2 + \hat{A} \hat{B} + \hat{B} \hat{A} + \hat{B}^2 \]
\[ e^{\lambda \hat{A}} e^{\lambda \hat{B}} = (1 + \lambda \hat{A} + \frac{1}{2} \lambda^2 \hat{A}^2 + \ldots) (1 + \lambda \hat{B} + \frac{1}{2} \lambda^2 \hat{B}^2 + \ldots) \]
\[ = 1 + \lambda (\hat{A} + \hat{B}) + \frac{1}{2} \lambda^2 (\hat{A}^2 + 2 \hat{A} \hat{B} + \hat{B}^2) + \ldots \]

So the error is
\[ ed(\hat{A} + \hat{B}) = e^{\frac{\lambda}{2} \hat{A}} e^{\frac{\lambda}{2} \hat{B}} - e^{\lambda \hat{A}} e^{\lambda \hat{B}} = \frac{1}{2} \lambda^2 (\hat{B} \hat{A} - \hat{A} \hat{B}) + \ldots \]
\[ = \frac{1}{2} \lambda^2 [\hat{B}, \hat{A}] + \ldots \]
\[ \uparrow \]
\[ \text{order } \lambda^2 \]

Actually it is even better than this because one can easily show
\[ ed(\hat{A} + \hat{B}) = e^{\frac{\lambda}{2} \hat{A}} e^{\frac{\lambda}{2} \hat{B}} e^{\frac{\lambda}{2} \hat{A}} = \text{order } (\lambda^3) \]

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 \( \beta \) into smaller values \( \tau \) so we can approximate \( e^{-\beta \hat{H}} \) accurately. More precisely, if \( \hat{H} = \hat{A} + \hat{B} \) we write \( \beta = L \tau \) so small:

\[
Z = \text{Tr} e^{-\beta \hat{H}} = \text{Tr} e^{-L \tau (\hat{A} + \hat{B})} = \text{Tr} \left[ e^{-\tau (\hat{A} + \hat{B})} e^{-\tau (\hat{A} + \hat{B})} \ldots e^{-\tau (\hat{A} + \hat{B})} \right]
\]

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

Note that we can also rewrite this as:

\[
\text{Tr} \left[ e^{-\tau \hat{A}/2} e^{-\tau \hat{B}/2} e^{-\tau \hat{B}/2} \ldots e^{-\tau \hat{A}/2} e^{-\tau \hat{B}/2} \right]
\]

and because \( \text{Tr} \) is cyclic and actually have product of \( L \) terms \( e^{-\tau \hat{A}/2} e^{-\tau \hat{B}} \).
Let's apply this to the harmonic oscillator and see why this is so useful.

\[ Z = \int dx_1 \langle x_1 | e^{-\hat{p}^2/2m} | x_1 \rangle \]

We'll see why I am labeling the states \( |x_i\rangle \) in a moment.

\[ \approx \int dx_1 \langle x_1 | e^{-\frac{1}{2} \hbar \omega x_1^2} e^{-\hat{p}_1^2/2m} e^{-\frac{1}{2} \hbar \omega x_1^2} e^{-\hat{p}_2^2/2m} \cdots | x_1 \rangle \]

Notice the operator \( \hat{x} \) gets replaced by a number \( x_1 \).

Can we do more elimination of yucky operators?!

Sure! Just introduce complete set of states all over the place (now you see why we used \( |x_i\rangle \))

\[ Z \approx \int dx_1 e^{-\frac{1}{2} \hbar \omega (x_1^2 + x_2^2 + \cdots x_n^2)} \langle x_1 | e^{-\hat{p}_2^2/2m} | x_2 \rangle \]

\[ \langle x_2 | e^{-\hat{p}_2^2/2m} | x_3 \rangle \cdots \langle x_n | e^{-\hat{p}_n^2/2m} | x_1 \rangle \]

All the \( \hat{x} \) operators are gone. We can get rid of \( \hat{p} \) also because we can evaluate each \( \langle x_2 | e^{-\hat{p}_2^2/2m} | x_1 \rangle \).
\[ \langle x_e | e^{-\frac{i}{2m} \hat{p}^2} | x_{e+1} \rangle \]

\[ = \int dp \langle x_e | e^{-\frac{i}{2m} \hat{p}^2} | p \rangle \langle p | x_{e+1} \rangle \]

\[ = \int dp e^{-\frac{i}{2m} \hat{p}^2} e^{-i \frac{p(x_{e+1} - x_e)}{\hbar}} \]

\[ = \int dp e^{i \frac{(x_{e+1} - x_e)p}{\hbar}} e^{-\frac{p^2}{2m} - \frac{i}{\hbar} \frac{(x_{e+1} - x_e)^2}{2m}} \]

All observables

Complete the square

\[ -\frac{p^2}{2m} - i \frac{(x_{e+1} - x_e)p}{\hbar} \]

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

Now \[ \int dp e^{-\frac{(p - p_0)^2}{\hbar}} = \sqrt{\frac{\pi}{\hbar}} \]

\[ p_0 \text{ is irrelevant (even if imaginary...)} \text{ and again we will ignore the constant factor } \sqrt{\frac{\pi}{\hbar}} \text{ which are irrelevant to derivatives of } \ln Z. \]

\[ \text{Upshot:} \]

\[ \langle x_e | e^{-\frac{i}{2m} \hat{p}^2} | x_{e+1} \rangle \sim e^{-\frac{1}{2} m \left( \frac{x_{e+1} - x_e}{\hbar} \right)^2 - 2 \frac{1}{2} \hbar^2} \]

\[ \sqrt{\frac{\pi}{\hbar}} \]

Looks a lot like \[ \frac{1}{2} m v^2 \text{ e}^{\frac{\hbar^2}{2m}}. \]
Putting this all together

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

where

\[ S' = T \left( \frac{1}{2} m w^2 \sum_{j=1}^{L} x_j^2 + \frac{1}{2} m \sum_{\ell=1}^{L} \left( \frac{x_{\ell+1} - x_\ell}{\ell} \right)^2 \right) \]

Comment: Feynman originally did this for \( e^{-i\hat{H}t/\hbar} \)

instead of \( e^{-\hat{H}t/\hbar} \). When you do that you get (t = Lε)

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

where \( S' = \text{classical action} \)

\[ = e^{\left( \sum \frac{1}{2} m \left( \frac{x_{\ell+1} - x_\ell}{\ell} \right)^2 - \sum \frac{1}{2} m w^2 x_\ell^2 \right)} \]

\[ \equiv T - V \]

Units check!

\[ T = \theta/\hbar \text{ has units } \frac{1}{\hbar} \]

So \( T \frac{1}{2} m w^2 x^2 \text{ dimensionless} \)

as it must be in exp term

\[ \text{Mean while } \frac{x}{\hbar} \text{ has units } \frac{1}{\hbar} \]

So \( T \frac{1}{2} m \left( \frac{x_{\ell+1} - x_\ell}{\ell} \right)^2 \frac{1}{\hbar^2} \sim m \frac{1}{T \hbar^2} \)

\( \sim \frac{1}{T} (p^2/2m) \text{ ~dimensionless} \)
Going back to stat mech problem.

Think about the structure of this expression

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

$$S = T \left\{ \frac{1}{2} m \omega^2 \sum x_i^2 + \frac{1}{2} m \sum \frac{(x_{i+1} - x_i)^2}{\epsilon^2} \right\}$$

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

$$Z \quad \leftrightarrow \quad Z$$

single quantum oscillator \quad chain of $n$ classical oscillators

"$n$ dimensional" \quad "1-dimensional"

Amazingly, this can always be done.

Quantum $Z \quad \leftrightarrow \quad$ classical $Z$

in $d$ dimensions \quad in $(d+1)$ dimensions.
A natural question to ask is whether we can recover the quantum expression for $Z$

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

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

To do so involves doing a multidimensional Gaussian integral

$$Z = \int_{\mathbb{R}^L} e^{-\frac{1}{2} M \vec{x} \vec{x}^T}$$

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

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

$$A = \frac{1}{2} m \omega^2 - \frac{\hbar}{\sqrt{2}} m \frac{1}{\hbar^2} \omega$$

$$B = \frac{1}{2} m \frac{1}{\hbar^2} \omega$$

Think about factors of 2 carefully

$$\left(\frac{X_{e+1} - X_e}{\hbar}\right)^2$$

$$\frac{X_{e+1}^2 - X_{e+1} X_e + X_e^2}{\hbar^2}$$

Each $(X_{e+1} - X_e)^2$ contributes $2 \frac{X_{e+1}^2 - X_{e+1} X_e + X_e^2}{\hbar^2}$ terms to $A$
A very useful identity is for the dimension of matrix/vector

$$\int d\mathbf{x} e^{-\frac{1}{2} \mathbf{x}^T M \mathbf{x}} = \pi^{n/2} \frac{1}{\sqrt{\det M}}$$

This is the multidimensional analog of

$$\int dx e^{-ax^2} = \sqrt{\frac{\pi}{a}} \left( \frac{a}{2} \right)^{1/2}$$

$$a = \det \text{of } 1 \times 1 \text{ "matrix" } a$$

Note also that $M = \prod \lambda_i$ is eigenvalues.

So we can evaluate the classical $Z$ because we know eigenvalues of $M = A + 2B\cos k L$

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

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

$$B = \frac{1}{2} m \omega^2 \tau$$

Recall $\tau = \beta/L$
We will explore this further in the homework.

Sketching things a bit:

\[ \ln Z = C - \frac{1}{2} \sum \ln \left( 1 + 2 \beta \cos \frac{2\pi n}{L} \right) \]

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

\[ \ln e^{-\frac{1}{2} \beta \mu} \left( 1 - e^{-\beta \mu} \right)^{-1} \]

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

It's better to compare \(<E>\) because we avoid tracking all the constants. Anyway, energy is more interesting.

\[ \sum x^n = \frac{1}{1-x} \]
\[ \sum nx^n = \frac{x}{(1-x)^2} \]

The exact result is, of course:

\[ <E> = \hbar \omega \sum \frac{1}{e^{\beta \hbar \omega} - 1} + \frac{1}{2} \hbar \omega \]

Derivation:

\[ <E> = 2^{-1} \sum E_n e^{-\beta E_n} = 2^{-1} \sum (n + \frac{1}{2}) \hbar \omega e^{-\beta (n + \frac{1}{2}) \hbar \omega} \]

\[ = \frac{1}{2} \hbar \omega + 2^{-1} e^{-\beta \hbar \omega} \sum n e^{-\beta n \hbar \omega} \]

\[ = \frac{1}{2} \hbar \omega + e^{\beta \hbar \omega / 2} \left( 1 - e^{-\beta \hbar \omega} \right) e^{-\beta \hbar \omega} / \left( 1 - e^{-\beta \hbar \omega} \right)^2 e^{-\beta \hbar \omega} \]
we'll want also to evaluate things like

\[
\int dx_1 dx_2 \ldots dx_N \exp \left( -\frac{1}{2} \mathbf{x}^T \mathbf{M} \mathbf{x} \right) \frac{x_i \cdot x_j}{\int dx_1 dx_2 \ldots e^{-\frac{1}{2} \mathbf{x}^T \mathbf{M} \mathbf{x}}}
\]

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

As a preview to Quantum Field Theory:

\[
\int dx_1 dx_2 \ldots dx_N \exp \left( -\frac{1}{2} \mathbf{x}^T \mathbf{M} \mathbf{x} \right) \frac{x_i \cdot x_j 
\cdot x_k \cdot x_l}{\int dx_1 dx_2 \ldots e^{-\frac{1}{2} \mathbf{x}^T \mathbf{M} \mathbf{x}}}
\]

\[
= \frac{1}{2} (\mathbf{M}^{-1})_{ij} \cdot \frac{1}{2} (\mathbf{M}^{-1})_{kl} + \frac{1}{2} (\mathbf{M}^{-1})_{ik} \cdot \frac{1}{2} (\mathbf{M}^{-1})_{lj} + \frac{1}{2} (\mathbf{M}^{-1})_{il} \cdot \frac{1}{2} (\mathbf{M}^{-1})_{jk}
\]

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