

PI-1

Relation Between Quantum and Classical Stat. Mech

We have already noted a similarity between

quantum and classical stat mech.

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

↑  
classical degrees of freedom with energy E

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

↑  
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 path integrals.

PI-2

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

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



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

But can evaluate  $\text{Tr}$  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  $\beta$  is small — the errors

are order  $\beta^2$ .

PI-3

Recall why this is

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

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

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

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

So the error is

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

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

↑  
order  $\lambda^2$

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.

PI-4

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  $\beta = L\tau$   $\left\{ \begin{array}{l} \leftarrow \text{large} \\ \leftarrow \text{small} \end{array} \right.$

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

$$= \text{Tr} \left[ \underbrace{e^{-\tau(\hat{A} + \hat{B})} e^{-\tau(\hat{A} + \hat{B})} \dots e^{-\tau(\hat{A} + \hat{B})}}_{L \text{ factors}} \right]$$

$$\approx \text{Tr} \left[ e^{-\tau\hat{A}} e^{-\tau\hat{B}} e^{-\tau\hat{A}} e^{-\tau\hat{B}} \dots e^{-\tau\hat{A}} e^{-\tau\hat{B}} \right]$$

$\uparrow$

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

$$\text{Tr} \left[ \underbrace{e^{-\tau\hat{A}/2} e^{-\tau\hat{A}/2} e^{-\tau\hat{B}} e^{-\tau\hat{A}/2} e^{-\tau\hat{A}/2} e^{-\tau\hat{B}} \dots e^{-\tau\hat{A}/2} e^{-\tau\hat{A}/2} e^{-\tau\hat{B}}}_{L \text{ terms}} \right]$$

and because Tr is cyclic

can move first term to end

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

PI-5

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

$$\approx \int dx_1 \langle x_1 | e^{-\tau/2 m \omega^2 \hat{x}^2} e^{-\tau \hat{p}^2 / 2m} e^{-\tau/2 m \omega^2 \hat{x}^2} e^{-\tau \hat{p}^2 / 2m} \dots | x_1 \rangle$$

$\underbrace{\qquad\qquad\qquad}_{e^{-\tau/2 m \omega^2 x_1^2} \langle x_1 |}$ 
↖ ↗
 $\int dx_2 |x_2\rangle \langle x_2|$

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  $|x_1\rangle$ )

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

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

All the  $\hat{x}$  operators are gone. We can get rid of

$\hat{p}$  also because we can evaluate each  $\langle x_2 | e^{-\tau \hat{p}^2 / 2m} | x_{2+1} \rangle$

PI-6

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

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

$$\underbrace{|p\rangle e^{-\tau p^2 / 2m}}_{\substack{\uparrow \\ \text{a number!}}} \quad \underbrace{e^{-i p x_{e+1} / \hbar}}_{\substack{\uparrow \\ \text{I'm going to forget} \\ \text{about normalization,} \\ \text{since constants} \\ \text{are irrelevant to} \\ \text{derivatives of } \ln Z}}$$

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

$\uparrow$   
all observables

Complete the square

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

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

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

$p_0$  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:

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

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

PI-7

Putting this all together

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

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

where

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

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

instead of  $e^{-\beta\hat{H}}$ . when you do that you get ( $t = L\epsilon$ )

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

where  $S =$  classical action

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

"T"

- "V"

discretized version of

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

Units check!

$\tau = \beta/\omega$  has units  $1/\omega$

So  $\tau \frac{1}{2} m \omega^2 x^2$  dimensionless  
 as it must be up in exponent

Meanwhile  $\tau \frac{x}{\hbar}$  has units  $\frac{1}{p}$

$$\text{So } \tau m \left( \frac{x_{l+1} - x_l}{\epsilon} \right)^2 \frac{1}{k^2} \sim \frac{m}{\tau p^2}$$

$$\sim \frac{1}{\tau (p^2/m)} \sim \text{dimensionless}$$

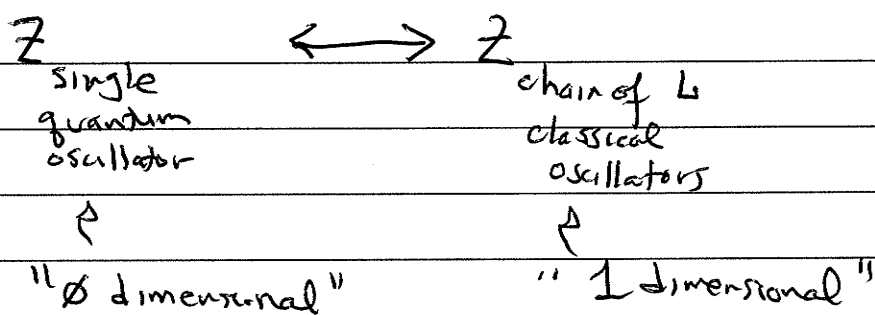
PI-8

Going back to stat mech problem,  
Think about the structure of this expression

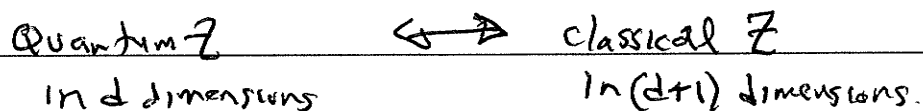
$$Z = \int dx_1 dx_2 \dots dx_L e^{-\mathcal{J}}$$

$$\mathcal{J} = L \left\{ \frac{1}{2} m \omega^2 \sum x_0^2 + \frac{1}{2} m \sum \left( \frac{x_{e+1} - x_e}{b} \right)^2 \frac{1}{k} \right\}$$

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  $\frac{1}{2} m \frac{1}{L} \frac{1}{k}$



Amazingly, this can always be done





PI-9

A natural question to ask is whether we can recover

the quantum expression for  $Z$

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

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

To do so involves doing a multidimensional Gaussian integral

$$Z = \int dx_1 dx_2 \dots dx_L e^{-\vec{x}^T M \vec{x}}$$

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

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

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

$$B \equiv \frac{1}{2} m \frac{1}{\hbar^2} \tau$$

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 in two B terms

PI-10

A very useful identity is  $\int d\vec{x} e^{-\vec{x}^T M \vec{x}} = \pi^{L/2} / \sqrt{\det M}$  ↙ dimension of matrix/vector

$$\int d\vec{x} e^{-\vec{x}^T M \vec{x}} = \pi^{L/2} / \sqrt{\det M}$$

This is the multidimensional analog of

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

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

Note also  $\det M = \prod_e \lambda_e$   
↙ eigenvalues.

So we can evaluate the classical  $Z$  because

we know eigenvalues of  $M \equiv A + 2B \cos k$   
↙  $\frac{2\pi}{L} \{1, 2, \dots, L\}$

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

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

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

Recall  $\tau = \beta/L$

PI-11

We'll explore this further in the homework.

Sketching things a bit:

$$\ln Z = C - \frac{1}{2} \sum_l \ln \left( 4 + 2B \cos \frac{2\pi l}{L} \right)$$

If we are willing to write a little program to

evaluate the sum we can compare with

$$\ln e^{-\frac{1}{2}\beta k w} (1 - e^{-\beta k w})^{-1}$$

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.

$$\sum x^n = \frac{1}{1-x}$$

$$\sum n x^n = \frac{x}{(1-x)^2}$$

Derivation:

$$\langle E \rangle = Z^{-1} \sum E_n e^{-\beta E_n} = Z^{-1} \sum_n (n + \frac{1}{2}) k w e^{-\beta (n + \frac{1}{2}) k w}$$

$$= \frac{1}{2} k w + Z^{-1} e^{-\beta \frac{1}{2} k w} \sum_n n e^{-\beta n k w}$$

$$= \frac{1}{2} k w + e^{\beta k w / 2} (1 - e^{-\beta k w})^{-1} e^{-\beta k w} / \left( (1 - e^{-\beta k w})^2 e^{-\beta \frac{1}{2} k w} k w \right)$$

PI-12

We'll want also to evaluate things like

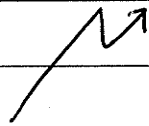
$$\int dx_1 dx_2 \dots dx_L e^{-\vec{x}^T M \vec{x}} x_i x_j / \int dx_1 dx_2 \dots dx_L e^{-\vec{x}^T M \vec{x}}$$

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

As a preview to Quantum Field Theory =

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

$$= \frac{1}{2} (M^{-1})_{ij} \frac{1}{2} (M^{-1})_{kl} + \frac{1}{2} (M^{-1})_{ik} \frac{1}{2} (M^{-1})_{jl} \\ + \frac{1}{2} (M^{-1})_{il} \frac{1}{2} (M^{-1})_{jk}$$



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