

Lecture 9-10

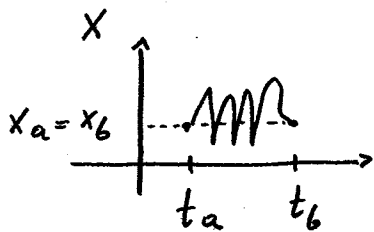
1.

Path Integral and Statistical Physics

Consider the trace relation

$$\text{Tr } K = \sum_n e^{-\frac{i}{\hbar} E_n t} \quad t = t_b - t_a$$

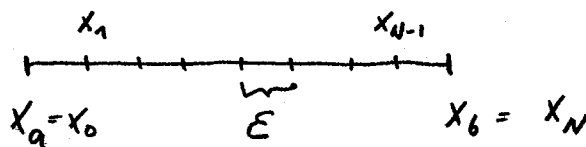
$$\hookrightarrow \int \mathcal{D}[x(t)] e^{\frac{i}{\hbar} S}$$



sum over all closed paths
(periodic paths with period t)

$$K(b, a) = \lim_{\epsilon \rightarrow 0} \int dx_1 \dots dx_{N-1} \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{\frac{N}{2}} x$$

$$\exp \left\{ \frac{im}{2\hbar\epsilon} \sum_{i=1}^N (x_i - x_{i-1})^2 - \frac{i}{\hbar} \epsilon \sum_{i=1}^N V \left(\frac{x_{i-1} + x_i}{2} \right) \right\}$$



x_a and x_b are different and not integrated in $K(b, a)$

$$\text{Tr } K = \int dx_a K(a, a)$$

one extra integration

$$x_a = x_b$$

$$\int = \int_{t_a}^{t_b} \left(\frac{1}{2} m \dot{x}^2 - V(x) \right) dt$$

We want to make time variable t complex!

It is easy to do that in zig-zag paths before continuum limit:

$$t = -i\tau$$

$$\varepsilon \rightarrow -i\varepsilon'$$

$$Z(b, \tau_b; a, \tau_a) = K(b, it_b; a, it_a)$$

$$= \lim_{\varepsilon' \rightarrow 0} \int dx_1 \dots dx_{N-1} \left(\frac{m}{2\pi\hbar\varepsilon'} \right)^{\frac{N}{2}} \times$$

$$\times \exp \left\{ -\frac{m}{2\hbar\varepsilon'} \sum_{i=1}^N (x_i - x_{i-1})^2 - \frac{\varepsilon'}{\hbar} \sum_{i=1}^N V\left(\frac{x_{i-1} + x_i}{2}\right) \right\}$$

well defined gaussian type integral!

$$Z = \text{Tr} Z(b, a) = \int dx_a Z(a, a)$$

This is just the $\text{Tr} K$ continued to imaginary time

$$Z = \sum_n e^{-\frac{E_n T}{\hbar}}$$

$$\hookrightarrow \int A[x(\tau)] e^{-\frac{1}{\hbar} \int_{\tau_a}^{\tau_b} \left(\frac{1}{2} m \left(\frac{dx}{d\tau} \right)^2 + V(x(\tau)) \right) d\tau}$$

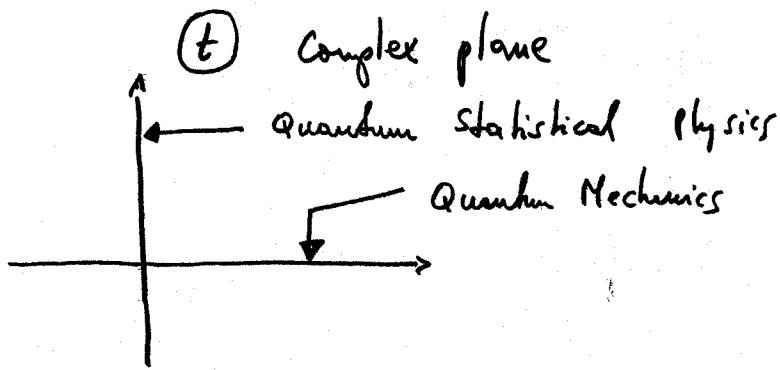
$$x(\tau_b) = x(\tau_a)$$

$$Z = \sum_n e^{-\frac{E_n}{kT}}$$

quantum partition function
of particle in heat bath
at temperature T

$$\frac{\tau}{\hbar} \rightarrow \frac{1}{kT}$$

Imaginary time path integral for periodic paths
is equivalent to quantum statistical physics of
particle



Let us investigate what happened in action integral:

$$iS = i \int_{t_a}^{t_b} \left(\frac{1}{2} m \left(\frac{dx}{dt} \right)^2 - V(x(t)) \right) dt$$

$$= - \int_{\tau_a}^{\tau_b} \left[\frac{1}{2} m \left(\frac{dx}{d\tau} \right)^2 + V(x(\tau)) \right] d\tau$$

$$t = -i\tau$$

$$\left(\frac{dx}{dt} \right)^2 = - \left(\frac{dx}{d\tau} \right)^2$$

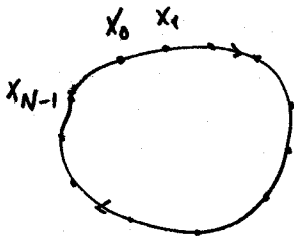
The imaginary time period for the closed paths can be chosen to relate to the heatbath temperature:

$$\tau = \frac{\hbar}{kT}$$

Imaginary time path integral has three great advantages:

- (1) It is a well-behaved real integral
No complicated phase cancellations
- (2) Direct information on Quantum Statistical Behavior of particle at finite temperature
- (3) New analogy with a classical statistical mechanical chain lends itself to modern simulation methods

Consider a closed ring:



x_i measures displacements of (an) harmonic chain from its null position

$$E = \sum_{i=1}^N \frac{1}{2\varepsilon'} m (x_i - x_{i-1})^2 + \varepsilon' \sum_{i=1}^N V\left(\frac{x_{i-1} + x_i}{2}\right)$$

$$E \rightarrow \int \left(\frac{1}{2} m \left(\frac{dx}{dt} \right)^2 + V(x(t)) \right) dt$$

in the continuum limit

$$Z = \sum_n - \frac{E_n}{kT}$$

↑

summation is actually an integration
over all classical configurations

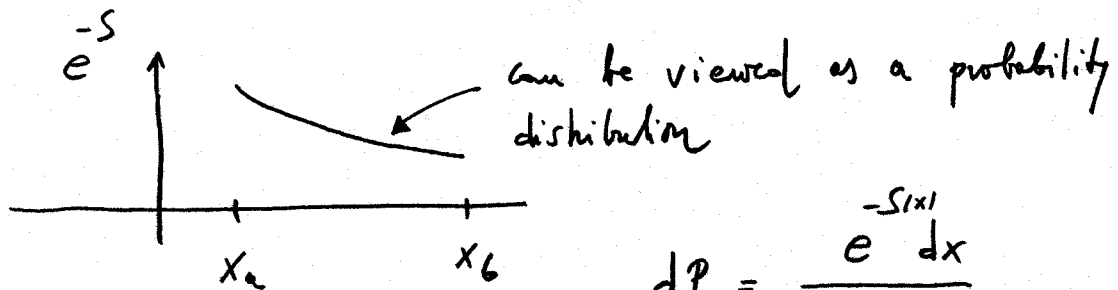
It is very much like a polymer chain

How do we integrate?

Consider the integral

$$\langle x^2 \rangle = \frac{\int_{x_a}^{x_b} x^2 e^{-S(x)} dx}{\int_{x_a}^{x_b} e^{-S} dx}$$

$S = \frac{1}{2} x^2$
(would work for any $S(x)$)



$$dP = \frac{e^{-S(x)} dx}{\int_{x_a}^{x_b} e^{-S(x)} dx}$$

$$\langle x^2 \rangle = \lim_{N \rightarrow \infty} \frac{1}{N} \sum x_i^2$$

↑
points distributed accordingly

Metropolis procedure:

choose x' from $x \pm \Delta x$ interval randomly

if $S(x') < S(x)$ accept

if $S(x') > S(x)$ accept with $\frac{e^{-S(x')}}{e^{-S(x)}}$ probability