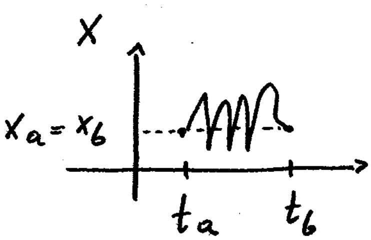
Lecture 5

Path Integral and Statistical Physics

Consider the trace relation

$$\mathrm{Tr}\, K = \sum_n e^{-\frac{i}{\hbar} E_n t} \qquad t = t_b - t_a$$

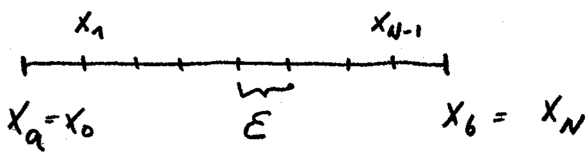
$$\hookrightarrow \int \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar} S}$$



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

$$K(b,a) = \lim_{\varepsilon \to 0} \int dx_1 \cdots dx_{N-1} \left(\frac{m}{2\pi i \hbar \varepsilon}\right)^{\frac{N}{2}} \times$$

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



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

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

one extra integration

$x_a = x_b$

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

We want to make time variable t complex!
It is easy to do that in zig-zag paths before continuum limit:

$$t = -i\tau \qquad\qquad \varepsilon \to -i\varepsilon'$$

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

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

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

well defined gaussian type integral!

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

this is just the Tr K continued to imaginary time

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

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

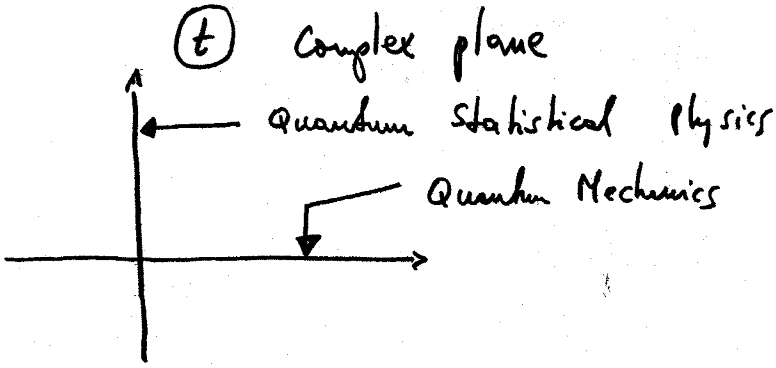
$$x(\tau_b) = x(\tau_a)$$

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

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 heat bath temperature :

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

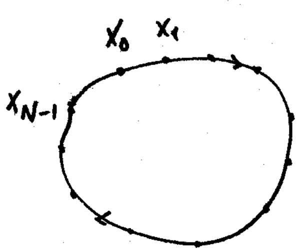
Imaginary time path integral has three great advantages:

(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 <u>classical</u> 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

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

$$E \to \int \left(\frac{1}{2} m \left(\frac{dx}{d\tau}\right)^2 + V(x(\tau)) \right) d\tau$$

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

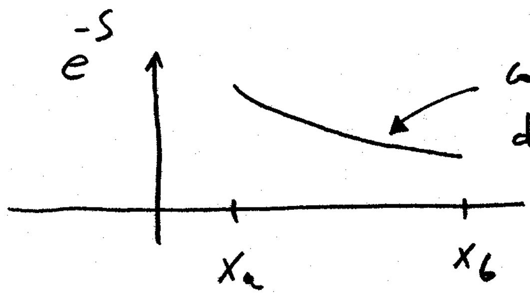
How do we integrate?

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 $S(x)$)



can be viewed as a probability distribution

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

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

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 $\dfrac{e^{-S(x')}}{e^{-S(x)}}$ probability