Path integral and Statistical Physics

Consider the trace relation

\[ \text{Tr } K = \sum_n e^{-\frac{i}{\hbar} E_n t} \]

\[ t = t_b - t_a \]

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

\[ x_a = x_b \]

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

\[ K(\beta, q) = \lim_{\epsilon \to 0} \int dx_1 \ldots dx_{N-1} \left( \frac{m}{2 \pi \hbar i \epsilon} \right)^{\frac{N}{2}} \]

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

\[ x_a = x_b \]

\[ x_a \text{ and } x_b \text{ are different and not integrated in } K(\beta, q) \]
\[
\text{Tr } K = \int dx_a K(a, a)
\]

one extra integration

\[
x_a = x_b
\]

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

We want to make time variable \( t \) complex!

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

\[
t = -i \tau \quad \varepsilon \to -i \varepsilon'
\]

\[
Z(b, t_b; a, t_a) = K(b, t_b; a, i t_a)
\]

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

\[
\times \exp \left\{ -\frac{m}{2 \hbar \varepsilon'} \sum_{i=1}^{N} (x_i - x_{i-1})^2 - \frac{\varepsilon'}{t} \sum_{i=1}^{N} \sqrt{\frac{x_{i-1} + x_i}{2}} \right\}
\]

well defined gaussian type integral!
\[ Z = \text{Tr} \ Z(\theta, a) = \int dx_a \ Z(a, a) \]

This is just the Tr K continued to imaginary time.

\[ Z = \sum_n e^{-\frac{E_n \tau}{\hbar}} \]

\[ \mathcal{L} = \int A[x(\tau)] e^{-\frac{1}{\hbar} \int \left( \frac{1}{2} m \left( \frac{dx}{d\tau} \right)^2 + V(x(\tau)) \right) d\tau} \]

\[ X(\tau_0) \rightarrow X(\tau_0) \]

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

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:

\[
i \int_{t_0}^{t_1} \left( \frac{1}{2} m \left( \frac{dx}{dt} \right)^2 - V(x(t)) \right) dt
\]

\[
= - \int_{\tau_0}^{\tau_1} \left[ \frac{1}{2} m \left( \frac{d\tau}{dt} \right)^2 + V(x(\tau)) \right] d\tau
\]

\[
t = -i \tau
\]

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

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 classical statistical mechanical chain lends itself to modern simulation methods

Consider a closed ring:

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

\( x_i \) measures displacements of (an) harmonic chain from its null position.
\[ E \rightarrow \int \left( \frac{1}{2} m \left( \frac{dx}{dt} \right)^2 + V(x(t)) \right) dt \]

in the continuum limit

\[ \mathcal{Z} = \sum_{n} \frac{E_n}{kT} \]

Summation is actually an integration over all classical configurations

It is very much like a polymer chain
How do we integrate?

Consider the integral

\[
\langle x^2 \rangle = \frac{\int_{x_{\alpha}}^{x_6} x^2 e^{-S(x)} dx}{\int_{x_{\alpha}}^{x_6} e^{-S(x)} dx}
\]

\[S = \frac{1}{2} x^2\]

(would work for any \(S(x)\))

\[\frac{\text{e}^{-S}}{\text{e}^{-S(x)}}\]

can be viewed as a probability distribution

\[
\langle x^2 \rangle \approx \frac{1}{N \to \infty} \sum_{i=1}^{N} x_i^2
\]

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 \(\frac{\text{e}^{-S(x')}}{\text{e}^{-S(x)}}\) probability