Path integral and Statistical Physics

Consider the trace relation

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

with $t = t_f - t_0$

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

Sum over all closed paths (periodic paths with period $t$)

$$K(6,9) = \lim_{\varepsilon \to 0} \int dx_1 \ldots dx_{N-1} \left( \frac{m}{2\pi i \hbar \varepsilon} \right)^N x$$

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

$$x_{N+1} = x_1$$

$x_0$ and $x_6$ are different and not integrated in $K(6,9)$
\[ \text{Tr} \ K = \int dx_a \ K(a, a) \]

one extra integration

\[ x_b = x_6 \]

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

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

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

\[ Z \left( b, t_6 ; a, t_a \right) = K \left( b, i t_6 ; a, i t_a \right) \]

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

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

well defined gaussian type integral!
\[ Z = \text{Tr} \exp \left( i \int_{x(a)} Z(a,a) \right) \]

This is just the Tr KE continued to imaginary time

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

\[ \int A[x(t)] e^{-\frac{1}{2} \int_0^T \left( \frac{1}{2} m \left( \frac{dx}{dt} \right)^2 + V(x(t)) \right) dt} \]

\[ \tau_b \rightarrow \tau_a \]

\[ X(\tau_b) = X(\tau_a) \]

\[ Z = \sum_n e^{-\frac{E_n}{kT}} \] quantum partition function of particle in heat bath at temperature \( T \)

\[ \frac{T}{kT} \rightarrow \frac{1}{kT} \]

Imaginary time path integral for periodic paths is equivalent to quantum statistical physics of particle
Let us investigate what happened in action integral:

\[ i \mathcal{S} = i \int_{t_a}^{t_b} \left( \frac{1}{2} m \left( \frac{dX}{dt} \right)^2 - V(X(t)) \right) dt \]

\[ = -\int_{T_a}^{T_b} \left[ \frac{1}{2} m \left( \frac{dX}{dT} \right)^2 + V(X(T)) \right] dT \]

\[ t = -i \tau \]

\[ \left( \frac{dX}{dt} \right)^2 = - \left( \frac{dX}{dT} \right)^2 \]

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:

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

\( x_i \) 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

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

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 $S(x)$)

$$e^{-S}$$

can be viewed as a probability distribution

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

$$\langle x^2 \rangle \approx \frac{1}{N} \sum_{N \to \infty} x_i^2$$

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