Lecture 9-10

Path integral and Statistical Physics

Consider the trace relation

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

\[ t = t_b - t_a \]

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

\[ x_a = x_b \]

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

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

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

\[ x_a = x_b \]

\[ X_a \text{ and } X_b \text{ are different and not integrated in } K(b, a) \]
\[
\text{Tr } K = \int \! \! \! \int dx_a \, K(a, a)
\]

one extra integration

\[x_a = x_b\]

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

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

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

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

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

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

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

well defined gaussian type integral!
\[ Z = \text{Tr} \ Z(b, a) = \int \! dx_0 \ Z(a, a) \]

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

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

\[ \sim \int \! \mathcal{A}[x(\tau)] \ e^{-\frac{1}{\hbar} \int_0^{\tau_b} \left( \frac{i}{2} m \left( \frac{dx}{d\tau} \right)^2 + V(x(\tau)) \right) \, d\tau} \]

\[ X(\tau_b) = X(\tau_0) \]

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

quantum partition function of particle in heat bath at temperature \( T \)

\[ \frac{\tau}{\hbar} \to \frac{1}{kT} \]

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

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

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

\[ t = -i \tau \]

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

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

\[ \tau = \frac{t}{kT} \]
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:

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

\[ x_0 \quad x_1 \quad x_N \quad x_{N-1} \]

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

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

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

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

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

\[
e^{-S}
\]

\[
\begin{array}{c}
\text{can be viewed as a probability distribution}
\end{array}
\]

\[
\begin{array}{c}
\text{points distributed accordingly}
\end{array}
\]

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

Metropolis procedure:

choose \(x'\) from \(x \pm \Delta x\) interval randomly

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

if \(S(x') > S(x)\) accept with \(\exp(-S(x')) / \exp(-S(x))\) probability