Path integrals in statistical mechanics

Consider canonical ensemble for a single particle → generalization to N particles → lectures

Partition function $\qquad \beta = \frac{1}{k_B T}$, $\quad d = 1 \qquad [k_B] = \left[\frac{J}{K}\right]$

$$Z = \mathrm{Tr}\left[e^{-\beta \hat{H}}\right] = \int dx \, \langle x | e^{-\beta \hat{H}} | x \rangle =$$

$$\underset{0}{|}\!\!\text{---}\underset{\varepsilon}{\text{---}}\!\!\text{---}\underset{\beta\hbar}{|}\!\!\longrightarrow \qquad \varepsilon = \frac{\beta\hbar}{N} \qquad [\beta\hbar] = \left[\frac{J \cdot s}{J} = s\right]$$

$$Z = \int dx \, \langle x | \underbrace{e^{-\frac{\varepsilon \hat{H}}{\hbar}} \cdots\cdots e^{-\frac{\varepsilon \hat{H}}{\hbar}}}_{N} | x \rangle$$

using completeness relation in a momentum space

$$\hat{\mathbb{1}}_p = \int \frac{dp_i}{2\pi\hbar} |p_i\rangle\langle p_i| \qquad i = 1, \dots, N$$

and in a position space

$$\hat{\mathbb{1}}_x = \int dx_i \, |x_i\rangle\langle x_i| \qquad i = 1 \dots, N$$

$$Z = \int dx \langle x | \underset{\mathbb{1}_{p_N}}{\wedge} e^{-\frac{\varepsilon \hat{H}}{\hbar}} \underset{\mathbb{1}_{x_N}}{\wedge} \underset{\mathbb{1}_{p_{N-1}}}{\wedge} e^{-\frac{\varepsilon \hat{H}}{\hbar}} \underset{\mathbb{1}_{x_{N-1}}}{\wedge} \cdots\cdots \underset{\mathbb{1}_{p_2}}{\wedge} e^{-\frac{\varepsilon \hat{H}}{\hbar}} \underset{\mathbb{1}_{x_2}}{\wedge} \underset{\mathbb{1}_{p_1}}{\wedge} e^{-\frac{\varepsilon \hat{H}}{\hbar}} \underset{\mathbb{1}_{x_1}}{\wedge} | x \rangle$$

we get a typical matrix element

$$\langle x_{i+1} | p_i \rangle\langle p_i | e^{-\frac{\varepsilon}{\hbar}\hat{H}(\hat{p}, \hat{x})} | x_i \rangle =$$

$$= e^{i\frac{p_i x_{i+1}}{\hbar}} \langle p_i | e^{-\frac{\varepsilon}{\hbar}\hat{H}(p_i, x_i) + O(\varepsilon^2)} | x_i \rangle$$

(*) scalar product and normalization ← $p \rightleftarrows$

$\hat{L}$ Trotter and normal ordering

↳ $e^{-ip_i x_i/\hbar}$

$$\langle x|\hat{p}|p\rangle = p\langle x|p\rangle = -i\hbar\,\partial_x\langle x|p\rangle$$

$$\Rightarrow \quad \langle x|p\rangle = A e^{\frac{ipx}{\hbar}}$$

$$\int dx\,|x\rangle\langle x| = \hat{\mathbb{1}} \quad , \quad \int \frac{dp}{B}\,|p\rangle\langle p| = \hat{\mathbb{1}}$$

$$\hat{\mathbb{1}} = \int dx \int \frac{dp}{B}\int\frac{dp'}{B}\,|p\rangle\langle p|x\rangle\langle x|p'\rangle\langle p'| =$$

$$= \int dx \int \frac{dp}{B}\int\frac{dp'}{B}\,|p\rangle\,|A|^2\,e^{\frac{i(p'-p)x}{\hbar}}\langle p'| =$$

$$= \int \frac{dp}{B}\int\frac{dp'}{B}\,|p\rangle\,|A|^2\,2\pi\,\delta(p'-p)\langle p'| =$$

$$= \frac{2\pi\hbar|A|^2}{B}\int\frac{dp}{B}\,|p\rangle\langle p| = \frac{2\pi\hbar|A|^2}{B}\,\hat{\mathbb{1}}$$

$$\Rightarrow \quad \boxed{B = 2\pi\hbar\,|A|^2}$$

and we choose $\underline{A = 1}$, hence $\underline{B = 2\pi\hbar}$

Here,

$$\langle x_{i+1} | p_i \rangle \langle p_i | e^{-\frac{\varepsilon}{\hbar}\hat{H}(\hat{p},\hat{x})} | x_i \rangle =$$

$$= e^{-\frac{\varepsilon}{\hbar}\left[\frac{p_i^2}{2m} - i p_i \frac{x_{i+1}-x_i}{\varepsilon} + V(x_i) + \mathcal{O}(\varepsilon^2)\right]}$$

Note, on the very right $\langle x_1 | x \rangle = \delta(x_1 - x)$

& on the very left $\langle x | = \langle x_{N+1} | = \langle x_1 |$

Thus,

$$\boxed{Z = \lim_{N\to\infty} \int \prod_{i=1}^{N} \frac{dx_i\, dp_i}{2\pi\hbar} e^{-\frac{1}{\hbar}\sum_{i=1}^{N} \varepsilon\left[\frac{p_i^2}{2m} - i p_i \frac{x_{i+1}-x_i}{\varepsilon} + V(x_i)\right]}\Bigg|_{\substack{x_{N+1}=x_1\\ \varepsilon = \frac{\beta\hbar}{N}}}}$$

Symbolically

$$\boxed{Z = \int_{x(\beta\hbar)=x(0)} \frac{\mathcal{D}[x]\,\mathcal{D}[p]}{2\pi\hbar} e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \left[\frac{p(\tau)^2}{2m} - i p(\tau)\dot{x}(\tau) + V(x(\tau))\right]}}$$

We can integrate out p_i if $V(x)$ is fnctn of x only

$$\int_{-\infty}^{\infty} \frac{dp_i}{2\pi\hbar} e^{-\frac{\varepsilon}{\hbar}\left[\frac{p_i^2}{2m} - i p_i \frac{x_{i+1}-x_i}{\varepsilon}\right]} = \underbrace{\sqrt{\frac{m}{2\pi\hbar\varepsilon}}\, e^{-\frac{m(x_{i+1}-x_i)^2}{2\hbar\varepsilon}}}_{\text{Gaussian}}$$

$$\boxed{Z = \lim_{N\to\infty} \int \prod_{i=1}^{N} \frac{dx_i}{\sqrt{\frac{2\pi\hbar\varepsilon}{m}}} e^{-\frac{1}{\hbar}\sum_{i=1}^{N} \varepsilon\left[\frac{m}{2}\left(\frac{x_{i+1}-x_i}{\varepsilon}\right)^2 + V(x_i)\right]}\Bigg|_{\substack{x_{N+1}=x_1\\ \varepsilon = \frac{\beta\hbar}{N}}}}$$

the measure constant

$$C = \left(\sqrt{\frac{m}{2\pi\hbar\varepsilon}}\right)^N = e^{\frac{N}{2}\ln\left(\frac{mN}{2\pi\hbar^2\beta}\right)}$$ appears to diverge at large N.

However, it does to depend on $V(x)$, so it does not contain any dynamics → dont worry yet!

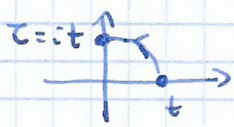
Symbolically

$$\boxed{Z = C \int\limits_{x(\beta\hbar)=x(0)} \mathcal{D}[x(\tau)]\, e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \left[\frac{m}{2}\left(\frac{dx(\tau)}{d\tau}\right)^2 + V(x(\tau))\right]}}$$

Interpretation:

in QM $\quad e^{\frac{i}{\hbar}\int dt\, L_M}$, $\quad$ Classical Lagrangian $\quad L_M = \frac{m}{2}\left(\frac{dx}{dt}\right)^2 - V(x)$

°) "Wick rotation" $\quad \tau = it$



°°) introduce

$$L_E = -L_M(\tau = it) = \frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x)$$

°°°) restrict $\quad \tau \in [0, \beta\hbar]$

°°°°) periodicity : $\quad x(\beta\hbar) = x(0)$

$$e^{\frac{i}{\hbar}\int dt\, L_M} \xrightarrow[(\cdot)\to(-)]{} \underbrace{e^{-\frac{1}{\hbar}S_E} = e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\, L_E}}_{\substack{\text{Euclidian action,} \\ \text{imaginary-time formalism}}}$$

$$\{i\,dt = d\tau\}$$