Quantum Mechanics as a Path Integral (I)

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References

- Laine and Vuorinen, "Basics of Thermal Field Theory", Chapter 1: https://arxiv.org/pdf/1701.01554.pdf

Partition Function

Recall from Lecture 2:

- Partition Function

$$\mathrm{Z}(T) = \mathrm{Tr}\left[e^{-\beta \hat{\mathrm{H}}}\right] . \tag{3.1}$$

- Tr is trace over Hilbert space, $\beta = T^{-1}$ is inverse temperature, $\hat{\mathrm{H}}$ is Hamiltonian
- For instance, when using energy-basis $|n\rangle$ with $n = 0, 1, 2, \ldots$

$$\mathrm{Z}(T) = \sum_{n=0}^{\infty} \langle n | e^{-\beta \hat{\mathrm{H}}} | n \rangle \tag{3.2}$$

Partition Function

- We can also use a different basis for Tr, e.g. position basis:

$$Z(T) = \int dx \langle x | e^{-\beta \hat{\mathrm{H}}} | x \rangle \,. \tag{3.3}$$

- Now let's split Boltzmann factor into a product of $N \gg 1$ pieces:

$$e^{-\beta \hat{\mathrm{H}}} = e^{-\epsilon \hat{\mathrm{H}}} e^{-\epsilon \hat{\mathrm{H}}} e^{-\epsilon \hat{\mathrm{H}}} \ldots e^{-\epsilon \hat{\mathrm{H}}} \,, \tag{3.4}$$

where $\epsilon \equiv \frac{\beta}{N}$. Since $\hat{\mathrm{H}}$ commutes with itself, there are no commutators to consider.

Partition Function

- Next we want to insert "unity" in-between these different products
- "Unity" can be expressed in different ways, for instance in x-basis as

$$\mathbf{1} = \int_{-\infty}^{\infty} dx |x\rangle\langle x| \,, \tag{3.5}$$

or in momentum ("p") basis as

$$\mathbf{1} = \int_{-\infty}^{\infty} \frac{dp}{2\pi} |p\rangle\langle p| \,. \tag{3.6}$$

- [Homework: derive the normalization factor $\frac{1}{2\pi}$ for the p-basis when using $\langle x|p\rangle = e^{ipx}$].

Partition Function

- We want to insert many "unities", so we need to distinguish them
- Let's give them labels, e.g. $x_1, x_2, x_3 \ldots, x_N$ for inserting x-basis number $1, 2, 3, \ldots, N$ (and the same for the p-basis).
- Let's start at the very right-hand-side of $\mathrm{Z}(T)$:

$$Z(T) = \int dx dx_1 dx_2 \frac{dp_1}{2\pi} \langle x | e^{-\epsilon \hat{\mathrm{H}}} \ldots e^{-\epsilon \hat{\mathrm{H}}} | x_2 \rangle \langle x_2 | p_1 \rangle \langle p_1 | e^{-\epsilon \hat{\mathrm{H}}} | x_1 \rangle \langle x_1 | x \rangle \tag{3.7}$$

- Let's repeat this procedure by putting $|x_i\rangle\langle x_i|$ to the right of every $e^{-\epsilon \hat{\mathrm{H}}}$ and $|p_i\rangle\langle p_i|$ to the left of every $e^{-\epsilon \hat{\mathrm{H}}}$, we end up with $2N+1$ integrals for Z(T): $\int \frac{dx dx_1 dx_2 \ldots dx_N dp_1 dp_2 \ldots dp_N}{(2\pi)^N}$.

Partition Function

- The integrand is a product of matrix elements of the type

$$\langle x_{i+1}|p_i\rangle\langle p_i|e^{-\epsilon\hat{\mathrm{H}}}|x_i\rangle = e^{ip_i x_{i+1}}\langle p_i|e^{-\epsilon\hat{\mathrm{H}}}|x_i\rangle \tag{3.8}$$

- Assuming the Hamiltonian to be of the form

$$\hat{\mathrm{H}} = \frac{\hat{p}^2}{2m} + \hat{\mathrm{V}}\left(\hat{x}\right)\,, \tag{3.9}$$

we can write

$$\langle p_i|e^{-\epsilon\hat{\mathrm{H}}}|x_i\rangle = \langle p_i|e^{-\epsilon\left[\frac{p_i^2}{2m}+V(x_i)\right]+\mathcal{O}(\epsilon^2)}|x_i\rangle \tag{3.10}$$

because $\epsilon = \frac{\beta}{N} \ll 1$ for $N \gg 1$.

Partition Function

- Ignoring contributions of order $\mathcal{O}(\epsilon^2)$ therefore

$$
\begin{aligned}
\langle x_{i+1}|p_i\rangle\langle p_i|e^{-\epsilon\hat{\mathrm{H}}}|x_i\rangle &= e^{ip_i x_{i+1}}\langle p_i|e^{-\epsilon\left[\frac{p_i^2}{2m}+V(x_i)\right]}|x_i\rangle\,,\\
&= e^{ip_i x_{i+1}}e^{-\epsilon\left[\frac{p_i^2}{2m}+V(x_i)\right]}\langle p_i|x_i\rangle\,,\\
&= e^{ip_i x_{i+1}}e^{-\epsilon\left[\frac{p_i^2}{2m}+V(x_i)\right]}e^{-ip_i x_i}\,,\\
&= e^{-\epsilon\left[\frac{p_i^2}{2m}+V(x_i)-ip_i\frac{x_{i+1}-x_i}{\epsilon}\right]}\,. \qquad (3.11)
\end{aligned}
$$

Partition Function

- We are now ready to assemble all the pieces in (3.7):

$$Z(T) = \lim_{N\to\infty} \int dx \left[\prod_{i=1}^{N} \frac{dx_i dp_i}{(2\pi)}\right] e^{-\epsilon \sum_{j=1}^{N}\left[\frac{p_j^2}{2m}+V(x_j)-ip_j\frac{x_{j+1}-x_j}{\epsilon}\right]} \langle x_1|x\rangle \,, \tag{3.12}$$

  where on the very left we identified $x = x_{N+1}$.

- Noting that $\langle x_1|x\rangle = \delta(x_1 - x)$, the integral over dx can be performed, which gives

$$Z(T) = \lim_{N\to\infty} \int \left[\prod_{i=1}^{N} \frac{dx_i dp_i}{(2\pi)}\right] e^{-\epsilon \sum_{j=1}^{N}\left[\frac{p_j^2}{2m}+V(x_j)-ip_j\frac{x_{j+1}-x_j}{\epsilon}\right]} \,, \tag{3.13}$$

  together with $x_{N+1} = x_1$.