2.1. Path Integrals: The General Idea

Introduction

This section corresponds roughly to the “Abstract & Keywords” section in Zinn-Justin’s text.

The quantum partition function $\mathcal{Z}(\beta)$ is defined as the trace of the quantum statistical operator $e^{-\beta H}$.

$$\mathcal{Z}(\beta) \equiv \text{tr}\, e^{-\beta H} \qquad (2.1)$$

Comparing with the quantum evolution operator $e^{-\frac{i}{\hbar} H t}$, we see that $e^{-\beta H}$ can be treated as an evolution in imaginary time with $\beta = \frac{i}{\hbar} t$.

Working with $e^{-\beta H}$ instead of $e^{-\frac{i}{\hbar} H t}$ is known as the Euclidean formulation of quantum field theory. The preferred mathematical tools are then path & functional integrals.

If H is bounded below, the minimum of the energy spectrum is called the ground state energy E_0. By definition

$$E_0 = \langle 0 \mid H \mid 0 \rangle$$

where $\mid 0 \rangle$ is (or one of) the ground state(s).

For a discrete spectrum, we have

$$\text{tr}\, e^{-\beta H} = g_0\, e^{-\beta E_0} + g_1\, e^{-\beta E_1} + \ldots$$

where g_i is the degeneracy of the i^{th} excited state.

Hence,

$$\begin{aligned}
\lim_{\beta \to \infty} \left(-\frac{1}{\beta} \ln \text{tr}\, e^{-\beta H} \right) &= \lim_{\beta \to \infty} \left\{ -\frac{1}{\beta} \ln \left[e^{-\beta E_0} \left(g_0 + g_1\, e^{-\beta (E_1 - E_0)} + \ldots \right) \right] \right\} \\
&= \lim_{\beta \to \infty} \left\{ -\frac{1}{\beta} \ln \left(e^{-\beta E_0}\, g_0 \right) \right\} \\
&= E_0
\end{aligned}$$

Replacing the sum with integral when dealing with a continuous spectrum, the above result still holds so that we have in general

$$E_0 = \lim_{\beta \to \infty} \left(-\frac{1}{\beta} \ln \text{tr}\, e^{-\beta H} \right) \qquad (2.2)$$

If the ground state is non-degenerate ($g_0 = 1$) & isolated (discrete spectrum), we have

$$\lim_{\beta \to \infty} \text{tr}\, e^{-\beta H} = e^{-\beta E_0} = \left\langle 0 \,\middle|\, e^{-\beta H} \,\middle|\, 0 \right\rangle$$

$$\to \qquad \lim_{\beta \to \infty} e^{-\beta H} = e^{-\beta E_0} \mid 0 \rangle \langle 0 \mid \qquad (2.3)$$

The General Idea

Let $\mathcal{U}(t, t')$, with $t \geq t'$, be a bounded operator in the Hilbert space that describes the evolution from time t' to t, i.e.,

$$\begin{aligned}
\mid t \rangle &= \mathcal{U}(t, t') \mid t' \rangle \qquad (a) \\
&= \mathcal{U}(t, t'') \mid t'' \rangle \\
&= \mathcal{U}(t, t'')\, \mathcal{U}(t'', t') \mid t' \rangle \qquad \forall\ t'' \geq t'
\end{aligned}$$

Thus, $\mathcal{U}$ satisfies the Markov (no memory) property

$$\mathcal{U}(t, t'')\, \mathcal{U}(t'', t') = \mathcal{U}(t, t') \qquad \text{with} \qquad t \geq t'' \geq t' \qquad (b)$$

with

$$\mathcal{U}(t, t) = 1 \tag{c}$$

From eq(a), we have

$$i\hbar\frac{\partial}{\partial t}\left| t\right\rangle = i\hbar\frac{\partial}{\partial t}\mathcal{U}(t, t')\left| t'\right\rangle$$
$$= H\,|\,t\rangle$$
$$= H\,\mathcal{U}(t, t')\,|\,t'\rangle$$

$$\rightarrow \qquad i\hbar\frac{\partial}{\partial t}\mathcal{U}(t, t') = H\,\mathcal{U}(t, t') \tag{d}$$

If H is t-independent,

$$\mathcal{U}(t, t') = \exp\left(-\frac{i}{\hbar}H\,(t - t')\right) \tag{e}$$

For the imaginary time version, we set $\tau = i\,t$ with

$$(\tau = i\,t) > (\tau' = i\,t') \qquad \text{if} \qquad t > t'$$

to get

$$|\,\tau\rangle = U(\tau, \tau')\,|\,\tau'\rangle \tag{2.4a}$$
$$= U(\tau, \tau'')\,|\,\tau''\rangle$$
$$= U(\tau, \tau'')\,U(\tau'', \tau')\,|\,\tau'\rangle \qquad \forall\ \tau'' \geq \tau'$$

$$U(\tau, \tau'')\,U(\tau'', \tau') = U(\tau, \tau') \qquad \text{with} \qquad \tau \geq \tau'' \geq \tau' \tag{2.4}$$

with

$$U(\tau, \tau) = 1 \tag{2.5a}$$

From eq(24.a), we have

$$-\hbar\frac{\partial}{\partial \tau}\left| \tau\right\rangle = -\hbar\frac{\partial}{\partial \tau}U(\tau, \tau')\left| \tau'\right\rangle$$
$$= H\,|\,\tau\rangle$$
$$= H\,U(\tau, \tau')\,|\,\tau'\rangle$$

$$\rightarrow \qquad -\hbar\frac{\partial}{\partial \tau}U(\tau, \tau') = H\,U(\tau, \tau') \tag{2.5}$$

$$\therefore \qquad -\hbar\frac{\partial}{\partial \tau}U(\tau, \tau')\Big|_{\tau=\tau'} = H$$

If H is τ-independent,

$$U(\tau, \tau') = \exp\left(-\frac{1}{\hbar}H\,(\tau - \tau')\right)$$

Dividing $\tau'' - \tau'$ into n steps of length ε, we have

$$\tau'' = \tau' + n\,\varepsilon$$
$$U(\tau'', \tau') = U[\,\tau' + n\,\varepsilon,\ \tau' + (n-1)\,\varepsilon\,] \ldots U(\tau' + \varepsilon, \tau')$$
$$\equiv \prod_{m=1}^{n} U[\,\tau' + m\,\varepsilon,\ \tau' + (m-1)\,\varepsilon\,] \tag{2.6}$$

Position Operator and Matrix Elements

The eigenstates $\{\,|\,\boldsymbol{q}\rangle\}$ of the position operator $\hat{\boldsymbol{q}}$ forms a distinguished basis in which $\hat{q}$ is diagonal.

Using the completeness condition

$$\int d\,\boldsymbol{q}\ |\,\boldsymbol{q}\rangle\langle\boldsymbol{q}\,| = 1$$

and setting

$$\tau_k = \tau' + k\,\varepsilon \qquad \boldsymbol{q}_0 = \boldsymbol{q}' \qquad \boldsymbol{q}_n = \boldsymbol{q}''$$

we get from eq(2.6) the matrix elements

$$\langle \boldsymbol{q}'' \mid U(\tau'', \tau') \mid \boldsymbol{q}' \rangle = \int d\,\boldsymbol{q}_{n-1} \ldots \int d\,\boldsymbol{q}_1 \langle \boldsymbol{q}'' \mid U(\tau'', \tau_{n-1}) \mid \boldsymbol{q}_{n-1} \rangle \ldots \langle \boldsymbol{q}_1 \mid U(\tau_1, \tau') \mid \boldsymbol{q}' \rangle$$

$$= \int \prod_{j=1}^{n-1} d\,\boldsymbol{q}_j \prod_{k=1}^{n} \langle \boldsymbol{q}_k \mid U(\tau_k, \tau_{k-1}) \mid \boldsymbol{q}_{k-1} \rangle \qquad (2.7)$$

Setting $n \to \infty$, the calculation of $\langle \boldsymbol{q}'' \mid U(\tau'', \tau') \mid \boldsymbol{q}' \rangle$ is reduced to that of $\langle \boldsymbol{q} \mid U(\tau + \varepsilon, \tau) \mid \boldsymbol{q}' \rangle$ with $\varepsilon \to 0$.

Locality of Short Time Evolution

If H is local in the basis $\{ \mid \boldsymbol{q} \rangle \}$, i.e.,

$$\langle \boldsymbol{q} \mid H(\tau) \mid \boldsymbol{q}' \rangle = \delta(\boldsymbol{q} - \boldsymbol{q}') \langle \boldsymbol{q} \mid H(\tau) \mid \boldsymbol{q} \rangle$$

only $\langle \boldsymbol{q} \mid U(\tau + \varepsilon, \tau) \mid \boldsymbol{q}' \rangle$'s with small $\mid \boldsymbol{q} - \boldsymbol{q}' \mid$ contribute significantly in eq(2.7).

This means we can construct a path integral representation of $\langle \boldsymbol{q}'' \mid U(\tau'', \tau') \mid \boldsymbol{q}' \rangle$.

Local H's include those of the form $H = K(\hat{\boldsymbol{p}}) + V(\hat{\boldsymbol{q}}, \tau)$ where $K(\hat{\boldsymbol{p}})$ is a polynomial in $\hat{\boldsymbol{p}}$.

The Operator *H*

We have derive the properties of U explicitly from the hamiltonian.

Another approach, which Zinn-Justin took, is to take eq(2.5) as the defining equation for U associated with an aritrary operator H. Furthermore, τ, now written as t, is taken as the real part of a complex time variable. Setting $\tau = i\,t$ to get the time evolution becomes an analytic continuation from the real axis t to the imaginary axis $i\,t$.

Notation Change

From here-on, we shall follow Zinn-Justin and use t, instead of τ, to denote imaginary time.