

## 6.2. Path Integral and S-Matrix: Perturbation Theory

Consider

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) \quad (6.13)$$

with

$$\mathcal{A}_0(\mathbf{x}) = \int_{t'}^{t''} dt \frac{1}{2} m \dot{\mathbf{x}}^2 \quad \mathcal{A}(\mathbf{x}) = \int_{t'}^{t''} dt \left( \frac{1}{2} m \dot{\mathbf{x}}^2 - V(\mathbf{x}) \right) \quad (6.14)$$

Let

$$\begin{aligned} \langle \mathbf{x}'' | U(t'', t') | \mathbf{x}' \rangle &= \int_{\mathbf{x}(t')=\mathbf{x}'}^{\mathbf{x}(t'')=\mathbf{x}''} [d\mathbf{x}(t)] e^{i\mathcal{A}(\mathbf{x})/\hbar} \\ &= \int_{\mathbf{x}(t')=\mathbf{x}'}^{\mathbf{x}(t'')=\mathbf{x}''} [d\mathbf{x}(t)] e^{i\mathcal{A}_0(\mathbf{x})/\hbar} \sum_{l=0}^{\infty} \frac{(-i)^l}{l!} \left( \frac{1}{\hbar} \int_{t'}^{t''} dt V(\mathbf{x}) \right)^l \\ &= \sum_i \langle \mathbf{x}'' | U^{(l)}(t'', t') | \mathbf{x}' \rangle \end{aligned} \quad (6.15)$$

where

$$\langle \mathbf{x}'' | U^{(l)}(t'', t') | \mathbf{x}' \rangle = \int_{\mathbf{x}(t')=\mathbf{x}'}^{\mathbf{x}(t'')=\mathbf{x}''} [d\mathbf{x}(t)] e^{i\mathcal{A}_0(\mathbf{x})/\hbar} \frac{(-i)^l}{l!} \left( \frac{1}{\hbar} \int_{t'}^{t''} dt V(\mathbf{x}) \right)^l \quad (6.15a)$$

Let

$$V(\mathbf{x}) = \int \frac{d\mathbf{k}}{(2\pi)^d} e^{i\mathbf{k} \cdot \mathbf{x}} \tilde{V}(\mathbf{k}) \quad (6.16)$$

→

$$\begin{aligned} \left( \frac{1}{\hbar} \int_{t'}^{t''} dt V(\mathbf{x}) \right)^l &= \prod_{j=1}^l \left\{ \frac{1}{\hbar} \int_{t'}^{t''} dt \tau_j V[\mathbf{x}(\tau_j)] \right\} \\ &= \prod_{j=1}^l \left\{ \frac{1}{\hbar} \int_{t'}^{t''} dt \tau_j \int \frac{d\mathbf{k}_j}{(2\pi)^d} e^{i\mathbf{k}_j \cdot \mathbf{x}(\tau_j)} \tilde{V}(\mathbf{k}_j) \right\} \\ &= \int_{t'}^{t''} \prod_{j=1}^l d\tau_j \int \left( \prod_{j=1}^l \frac{d\mathbf{k}_j}{(2\pi)^d} \frac{\tilde{V}(\mathbf{k}_j)}{\hbar} \right) \exp \left( i \sum_{j=1}^l \mathbf{k}_j \cdot \mathbf{x}(\tau_j) \right) \end{aligned}$$

$$\therefore \langle \mathbf{x}'' | U^{(l)}(t'', t') | \mathbf{x}' \rangle = \frac{(-i)^l}{l!} \int_{t'}^{t''} \prod_{j=1}^l d\tau_j \int \left( \prod_{j=1}^l \frac{d\mathbf{k}_j}{(2\pi)^d} \frac{\tilde{V}(\mathbf{k}_j)}{\hbar} \right) \quad (6.17)$$

$$\times \int_{\mathbf{x}(t')=\mathbf{x}'}^{\mathbf{x}(t'')=\mathbf{x}''} [d\mathbf{x}(t)] \exp \left( i \left[ \frac{1}{\hbar} \int_{t'}^{t''} dt \frac{1}{2} m \dot{\mathbf{x}}(t)^2 + \sum_{j=1}^l \mathbf{k}_j \cdot \mathbf{x}(\tau_j) \right] \right)$$

Since the integrand is symmetric in  $\tau_j$ , we can set

$$t'' = \tau_{l+1} \geq \tau_l \geq \tau_{l-1} \geq \dots \geq \tau_1 \geq \tau_0 = t' \quad (6.17a)$$

so that

$$\begin{aligned} \frac{1}{l!} \int_{t'}^{t''} \prod_{j=1}^l d\tau_j f(\tau) &= \int_{\tau_{l-1}}^{t''} d\tau_l \int_{\tau_{l-2}}^{\tau_l} d\tau_{l-1} \dots \int_{\tau_1}^{\tau_3} d\tau_2 \int_{t'}^{\tau_2} d\tau_1 f(\tau) \\ &= \prod_{j=1}^l \int_{\tau_{j-1}}^{\tau_{j+1}} d\tau_j f(\tau) \end{aligned}$$

The last factor in (6.17) is a path integral of the generating functional type [see §2.5.1].

Writing

$$\frac{1}{\hbar} \int_{t'}^{t''} dt \frac{1}{2} m \dot{\mathbf{x}}(t)^2 + \sum_{j=1}^l \mathbf{k}_j \cdot \mathbf{x}(\tau_j) = \frac{1}{\hbar} \int_{t'}^{t''} dt \left[ \frac{1}{2} m \dot{\mathbf{x}}(t)^2 + \sum_{j=1}^l \delta(t - \tau_j) \hbar \mathbf{k}_j \cdot \mathbf{x}(t) \right]$$

we have

$$L = \frac{1}{2} m \dot{\mathbf{x}}(t)^2 + \sum_{j=1}^l \delta(t - \tau_j) \hbar \mathbf{k}_j \cdot \mathbf{x}(t)$$

so that the Lagrange eq. is

$$m \ddot{\mathbf{x}} = \sum_{j=1}^l \delta(t - \tau_j) \hbar \mathbf{k}_j \tag{6.17b}$$

$$\rightarrow m \int_{t'}^t dt \ddot{\mathbf{x}} = m [\dot{\mathbf{x}}(t) - \dot{\mathbf{x}}(t')]$$

$$= \sum_{j=1}^l \int_{t'}^t dt \delta(t - \tau_j) \hbar \mathbf{k}_j$$

$$= \sum_{j=1}^n \hbar \mathbf{k}_j \quad \text{where} \quad \tau_{n+1} > t \geq \tau_n$$

$$\therefore \dot{\mathbf{x}}(t) = \dot{\mathbf{x}}(t') + \frac{1}{m} \sum_{j=1}^n \hbar \mathbf{k}_j$$

$$\rightarrow \dot{\mathbf{x}}(\tau_j) = \dot{\mathbf{x}}(t') + \frac{1}{m} \sum_{i=1}^j \hbar \mathbf{k}_i \quad \dot{\mathbf{x}}(\tau_{j-1}) = \dot{\mathbf{x}}(t') + \frac{1}{m} \sum_{i=1}^{j-1} \hbar \mathbf{k}_i$$

$$\therefore \dot{\mathbf{x}}(\tau_j) = \dot{\mathbf{x}}(\tau_{j-1}) + \frac{1}{m} \hbar \mathbf{k}_j \tag{6.17c}$$

Since

$$\dot{\mathbf{x}}(t) = \dot{\mathbf{x}}(\tau_j) \quad \text{for} \quad \tau_{j+1} \geq t \geq \tau_j$$

the particle is basically in free motion except for bumps at  $\tau_j$ 's.

Thus we can break up the path integral into  $l + 1$  segments:

$$\begin{aligned} \mathcal{P}_0 &= \int_{\mathbf{x}(t')=\mathbf{x}'}^{\mathbf{x}(t'')=\mathbf{x}''} [d\mathbf{x}(t)] \exp\left( i \left[ \frac{1}{\hbar} \int_{t'}^{t''} dt \frac{1}{2} m \dot{\mathbf{x}}(t)^2 \right] \right) \\ &= \int \prod_{j=1}^l \left( d\mathbf{x}_j \int_{\mathbf{x}(\tau_{j-1})=\mathbf{x}_{j-1}}^{\mathbf{x}(\tau_j)=\mathbf{x}_j} [d\mathbf{x}(t)] \right) \exp\left( i \left[ \frac{1}{\hbar} \sum_{j=1}^{l+1} \int_{\tau_{j-1}}^{\tau_j} dt \frac{1}{2} m \dot{\mathbf{x}}(t)^2 \right] \right) \end{aligned}$$

where

$$\mathbf{x}(\tau_j) = \mathbf{x}_j \quad \mathbf{x}_{l+1} = \mathbf{x}'' \quad \& \quad \mathbf{x}_0 = \mathbf{x}'$$

Setting

$$\mathbf{p}_j = m \dot{\mathbf{x}}_j \quad \mathbf{p}_{l+1} = m \dot{\mathbf{x}}_{l+1} \quad \& \quad \mathbf{p}_0 = m \dot{\mathbf{x}}_0$$

we have

$$\begin{aligned} \mathcal{P}_0 &= \int \left( \prod_{j=1}^l d\mathbf{x}_j \right) \prod_{j=1}^{l+1} \langle \mathbf{x}_j | U_0(\tau_j, \tau_{j-1}) | \mathbf{x}_{j-1} \rangle \\ &= \int \left( \prod_{j=1}^l d\mathbf{x}_j \right) \prod_{j=1}^{l+1} \langle \mathbf{x}_j | e^{-i \hat{\mathbf{p}}^2 (\tau_j - \tau_{j-1}) / 2m\hbar} | \mathbf{x}_{j-1} \rangle \end{aligned}$$

$$\begin{aligned}
&= \int \left( \prod_{j=1}^l d\mathbf{x}_j \right) \prod_{j=1}^{l+1} \int d\mathbf{p}' d\mathbf{p}_{j-1} \langle \mathbf{x}_j | \mathbf{p}' \rangle \langle \mathbf{p}' | e^{-i\hat{\mathbf{p}}^2(\tau_j - \tau_{j-1})/2m\hbar} | \mathbf{p}_{j-1} \rangle \langle \mathbf{p}_{j-1} | \mathbf{x}_{j-1} \rangle \\
&= \int \left( \prod_{j=1}^l d\mathbf{x}_j \right) \prod_{j=1}^{l+1} \int d\mathbf{p}' d\mathbf{p}_{j-1} \frac{e^{i\mathbf{p}' \cdot \mathbf{x}_j / \hbar}}{(2\pi\hbar)^{d/2}} e^{i\mathbf{p}_{j-1}^2(\tau_j - \tau_{j-1})/2m\hbar} \langle \mathbf{p}' | \mathbf{p}_{j-1} \rangle \frac{e^{-i\mathbf{p}_{j-1} \cdot \mathbf{x}_{j-1} / \hbar}}{(2\pi\hbar)^{d/2}} \\
&= \int \left( \prod_{j=1}^l d\mathbf{x}_j \right) \prod_{j=1}^{l+1} \int \frac{d\mathbf{p}_{j-1}}{(2\pi\hbar)^d} \exp \left\{ \frac{i}{\hbar} \left( -\frac{\mathbf{p}_{j-1}^2}{2m} (\tau_j - \tau_{j-1}) + \mathbf{p}_{j-1} \cdot (\mathbf{x}_j - \mathbf{x}_{j-1}) \right) \right\}
\end{aligned}$$

Eq(6.17) thus becomes

$$\begin{aligned}
\langle \mathbf{x}'' | U^{(l)}(t'', t') | \mathbf{x}' \rangle &= (-i)^l \int_{t'}^{t''} \prod_{j=1}^l d\tau_j \int \left( \prod_{j=1}^l d\mathbf{x}_j \frac{d\mathbf{k}_j}{(2\pi)^d} \frac{\tilde{V}(\mathbf{k}_j)}{\hbar} \right) \int \left( \prod_{j=1}^{l+1} \frac{d\mathbf{p}_{j-1}}{(2\pi\hbar)^d} \right) \\
&\quad \times \exp \left\{ \frac{i}{\hbar} \left( \sum_{j=1}^{l+1} \left[ -\frac{\mathbf{p}_{j-1}^2}{2m} (\tau_j - \tau_{j-1}) + \mathbf{p}_{j-1} \cdot (\mathbf{x}_j - \mathbf{x}_{j-1}) \right] + \sum_{j=1}^l \hbar \mathbf{k}_j \cdot \mathbf{x}_j \right) \right\}
\end{aligned}$$

with the constraints on  $\tau_j$  given by eq(6.17a).

Collecting all terms involving a given  $\mathbf{x}_j$  in the exponential of eq(6.17g), we get

$$\int d\mathbf{x}_j \exp \left[ i \left( \frac{\mathbf{p}_{j-1} - \mathbf{p}_j}{\hbar} + \mathbf{k}_j \right) \cdot \mathbf{x}_j \right] = (2\pi)^d \delta \left( \frac{\mathbf{p}_{j-1} - \mathbf{p}_j}{\hbar} + \mathbf{k}_j \right) \quad j = 1, \dots, l$$

Performing the  $\mathbf{k}_j$  integrals then gives

$$\begin{aligned}
\langle \mathbf{x}'' | U^{(l)}(t'', t') | \mathbf{x}' \rangle &= (-i)^l \int_{t'}^{t''} \prod_{j=1}^l d\tau_j \int \left( \prod_{j=1}^{l+1} \frac{d\mathbf{p}_{j-1}}{(2\pi\hbar)^d} \right) \left( \prod_{j=1}^l \frac{\tilde{V}(\mathbf{p}_j - \mathbf{p}_{j-1})}{\hbar} \right) \\
&\quad \times \exp \left\{ \frac{i}{\hbar} \left( -\sum_{j=1}^{l+1} \frac{\mathbf{p}_{j-1}^2}{2m} (\tau_j - \tau_{j-1}) + \mathbf{p}_l \cdot \mathbf{x}'' - \mathbf{p}_0 \cdot \mathbf{x}' \right) \right\}
\end{aligned}$$

Consider now the matrix elements with respect to the momentum eigenstates

$$\begin{aligned}
\langle \mathbf{p}'' | U^{(l)}(t'', t') | \mathbf{p}' \rangle &= \int d\mathbf{x}'' d\mathbf{x}' \langle \mathbf{p}'' | \mathbf{x}'' \rangle \langle \mathbf{x}'' | U^{(l)}(t'', t') | \mathbf{x}' \rangle \langle \mathbf{x}' | \mathbf{p}' \rangle \\
&= \int d\mathbf{x}'' d\mathbf{x}' \frac{e^{-i\mathbf{p}'' \cdot \mathbf{x}'' / \hbar}}{(2\pi\hbar)^{d/2}} \langle \mathbf{x}'' | U^{(l)}(t'', t') | \mathbf{x}' \rangle \frac{e^{i\mathbf{p}' \cdot \mathbf{x}' / \hbar}}{(2\pi\hbar)^{d/2}}
\end{aligned}$$

The  $\mathbf{x}''$  &  $\mathbf{x}'$  integrals give

$$\begin{aligned}
\int d\mathbf{x}'' e^{i(\mathbf{p}'' - \mathbf{p}') \cdot \mathbf{x}'' / \hbar} &= (2\pi\hbar)^d \delta(\mathbf{p}'' - \mathbf{p}') \\
\int d\mathbf{x}' e^{i(\mathbf{p}' - \mathbf{p}_0) \cdot \mathbf{x}' / \hbar} &= (2\pi\hbar)^d \delta(\mathbf{p}' - \mathbf{p}_0)
\end{aligned}$$

Performing the  $\mathbf{p}_l$  &  $\mathbf{p}_0$  integrals then gives

$$\begin{aligned}
\langle \mathbf{p}'' | U^{(l)}(t'', t') | \mathbf{p}' \rangle &= (2\pi\hbar)^d (-i)^l \int_{t'}^{t''} \prod_{j=1}^l d\tau_j \int \left( \prod_{j=2}^l \frac{d\mathbf{p}_{j-1}}{(2\pi\hbar)^d} \right) \left( \prod_{j=1}^l \frac{\tilde{V}(\mathbf{p}_j - \mathbf{p}_{j-1})}{\hbar} \right) \\
&\quad \times \exp \left( -\frac{i}{\hbar} \sum_{j=1}^{l+1} \frac{\mathbf{p}_{j-1}^2}{2m} (\tau_j - \tau_{j-1}) \right)
\end{aligned}$$

$$= (2\pi\hbar)^d (-i)^l \int_{t'}^{t''} \prod_{j=1}^l d\tau_j \int \left( \prod_{j=1}^{l-1} \frac{d\mathbf{p}_j}{(2\pi\hbar)^d} \right) \left( \prod_{j=1}^l \frac{\tilde{V}(\mathbf{p}_j - \mathbf{p}_{j-1})}{\hbar} \right) \times \exp\left(-\frac{i}{\hbar} \sum_{j=0}^l \frac{\mathbf{p}_j^2}{2m} (\tau_{j+1} - \tau_j)\right)$$

with the B.C.'s

$$\mathbf{p}_l = \mathbf{p}'' \quad \& \quad \mathbf{p}' = \mathbf{p}_0 \tag{6.18a}$$

The S-matrix is

$$\langle \mathbf{p}'' \mid S^{(l)} \mid \mathbf{p}' \rangle = \lim_{\substack{t'' \rightarrow \infty \\ t' \rightarrow -\infty}} e^{iE''t''/\hbar} \langle \mathbf{p}'' \mid U^{(l)}(t'', t') \mid \mathbf{p}' \rangle e^{-iE't'/\hbar} \tag{6.18b}$$

with

$$E'' = \frac{\mathbf{p}_l^2}{2m} \quad \& \quad E' = \frac{\mathbf{p}_0^2}{2m}$$

so that the  $\tau_{l+1}$  &  $\tau_0$  terms in the exponential are cancelled out. This effect can be emulated by setting

$$\tau_{l+1} = \tau_0 = 0 \tag{6.18c}$$

whereupon

$$\langle \mathbf{p}'' \mid S^{(l)} \mid \mathbf{p}' \rangle = (2\pi\hbar)^d (-i)^l \int_{-\infty}^{\infty} \prod_{j=1}^l d\tau_j \int \left( \prod_{j=1}^{l-1} \frac{d\mathbf{p}_j}{(2\pi\hbar)^d} \right) \left( \prod_{j=1}^l \frac{\tilde{V}(\mathbf{p}_j - \mathbf{p}_{j-1})}{\hbar} \right) \times \exp\left(-\frac{i}{\hbar} \sum_{j=0}^l \frac{\mathbf{p}_j^2}{2m} (\tau_{j+1} - \tau_j)\right) \tag{6.18}$$

Collecting all terms involving a given  $\tau_j$  in the exponential, we get

$$\begin{aligned} \mathcal{I}_j &= \int_{\tau_{j-1}}^{\tau_{j+1}} d\tau_j \exp\left(-\frac{i}{\hbar} \frac{(\mathbf{p}_{j-1}^2 - \mathbf{p}_j^2)}{2m} \tau_j\right) \\ &= \int_{\tau_{j-1}}^{\tau_{j+1}} d\tau_j \exp\left(\frac{i}{\hbar} [E(\mathbf{p}_j) - E(\mathbf{p}_{j-1})] \tau_j\right) \quad \text{where } E(\mathbf{p}) = \frac{\mathbf{p}^2}{2m} \end{aligned}$$

Since  $\tau_{j+1}$  &  $\tau_{j-1}$  can assume any values satisfying the only restriction  $\tau_{j+1} \geq \tau_{j-1}$ , we can write

$$\mathcal{I}_j = \int_0^{\infty} d\tau_j \exp\left(\frac{i}{\hbar} [E'' - E(\mathbf{p}_{j-1})] \tau_j\right) \quad \forall j = 2, \dots, l$$

where we've incorporated the fact that  $\tau_j = \infty$  is possible only if  $\tau_k = \infty \quad \forall k > j$ .

To make the exponential vanish at  $\tau_j = \infty$ , we set, with  $\epsilon \rightarrow 0^+$ ,

$$\begin{aligned} \mathcal{I}_j &= \int_0^{\infty} d\tau_j \exp\left(\frac{i}{\hbar} [E'' - E(\mathbf{p}_{j-1}) + i\epsilon] \tau_j\right) \\ &= \frac{i\hbar}{E'' - E(\mathbf{p}_{j-1}) + i\epsilon} \quad \forall j = 2, \dots, l \end{aligned}$$

Since  $\tau_0 = -\infty$ , the case  $j = 1$  gives

$$\mathcal{I}_1 = \int_{-\infty}^{\infty} d\tau_j \exp\left(\frac{i}{\hbar} (E'' - E') \tau_j\right) = 2\pi\hbar \delta(E'' - E')$$

Thus, eq(6.18) beocmes

$$\begin{aligned} \langle \mathbf{p}'' \mid S^{(l)} \mid \mathbf{p}' \rangle &= (2\pi\hbar)^d 2\pi\hbar \delta(E'' - E') (-i)^l \\ &\times \int \left( \prod_{j=1}^{l-1} \frac{d\mathbf{p}_j}{(2\pi\hbar)^d} \right) \left( \prod_{j=1}^l \frac{\tilde{V}(\mathbf{p}_j - \mathbf{p}_{j-1})}{\hbar} \right) \left( \prod_{j=2}^l \frac{i\hbar}{E'' - E(\mathbf{p}_{j-1}) + i\epsilon} \right) \end{aligned}$$

$$\begin{aligned}
&= -i (2\pi\hbar)^d 2\pi \delta(E'' - E') \\
&\quad \times \int \left( \prod_{j=1}^{l-1} \frac{d\mathbf{p}_j}{(2\pi\hbar)^d} \right) \left( \prod_{j=1}^l \tilde{V}(\mathbf{p}_j - \mathbf{p}_{j-1}) \right) \left( \prod_{j=1}^{l-1} \frac{1}{E'' - E(\mathbf{p}_j) + i\epsilon} \right) \\
&= -i (2\pi\hbar)^d 2\pi \delta(E'' - E') \quad (6.18d) \\
&\quad \times \int \tilde{V}(\mathbf{p}'' - \mathbf{p}_{l-1}) \prod_{j=1}^{l-1} \frac{d\mathbf{p}_j}{(2\pi\hbar)^d} \frac{\tilde{V}(\mathbf{p}_j - \mathbf{p}_{j-1})}{E'' - E(\mathbf{p}_j) + i\epsilon}
\end{aligned}$$

Note: The  $(2\pi\hbar)^d$  factor would be absent if we used normalized plane waves in eq(6.18b).

Eq(6.18b) can also be obtained by solving the Lippman-Schwinger (integral) eq. by iteration.

The equivalent operator eq. is usually written in terms of the  $T$ -matrix [ see e.g., §4.1 of E.N.Economou, "Green's Functions in Quantum Physics" ] :

$$T(E) = V - V G_0(E) T(E) \quad G_0(E) = \frac{1}{H_0 - E}$$

with

$$T(\mathbf{p}'', \mathbf{p}') = \langle \mathbf{p}'' | T(E + i\epsilon) | \mathbf{p}' \rangle \quad E = \frac{\mathbf{p}'^2}{2m} = \frac{\mathbf{p}''^2}{2m}$$