6.3. Path Integral & S-Matrix: Semi-Classical Expansions

6.3.1. Path Integral & S-matrix

For the *S*-matrix elements between 2 wave packets

$$\langle \psi_2 \mid S \mid \psi_1 \rangle = \lim_{\substack{t' \to -\infty \\ t'' \to +\infty}} \int d\boldsymbol{q}' \, d\boldsymbol{q}'' \langle \psi_2 \mid e^{i H_0 t''/\hbar} \mid \boldsymbol{q}'' \rangle \tag{6.19}$$

$$\times \langle \boldsymbol{q}'' \mid U(t'', t') \mid \boldsymbol{q}' \rangle \langle \boldsymbol{q}' \mid e^{-i H_0 t'/\hbar} \mid \psi_1 \rangle$$

Let

$$\psi_j(\boldsymbol{q}, t) = \langle \boldsymbol{q} \mid e^{-i H_0 t/\hbar} \mid \psi_j \rangle \qquad j = 1, 2$$

$$= \int d\boldsymbol{p} \, d\boldsymbol{p}' \langle \boldsymbol{q} \mid \boldsymbol{p} \rangle \langle \boldsymbol{p} \mid e^{-i H_0 t/\hbar} \mid \boldsymbol{p}' \rangle \langle \boldsymbol{p}' \mid \psi_j \rangle$$

$$= \int d\boldsymbol{p} \, d\boldsymbol{p}' \frac{e^{i \boldsymbol{p}\cdot\boldsymbol{q}/\hbar}}{(2\pi\hbar)^{d/2}} \exp\left(-i \frac{\boldsymbol{p}'^2}{2m\hbar} t\right) \langle \boldsymbol{p} \mid \boldsymbol{p}' \rangle \tilde{\psi}_j(\boldsymbol{p}')$$

$$= \int \frac{d\boldsymbol{p}}{(2\pi\hbar)^{d/2}} \tilde{\psi}_j(\boldsymbol{p}) \exp\left[\frac{i}{\hbar} \left(\boldsymbol{p}\cdot\boldsymbol{q} - \frac{\boldsymbol{p}^2}{2m} t \right) \right] \tag{6.20}$$

which differs from Zinn-Justin's version by a factor of $\left(\frac{2\pi}{\hbar}\right)^{d/2}$. This difference is due to the different normalization chosen for $\langle \boldsymbol{q} \mid \boldsymbol{p} \rangle$.

Our choice is

$$\int d\boldsymbol{q} \mid \boldsymbol{q} \rangle \langle \boldsymbol{q} \mid = 1 \qquad \int d\boldsymbol{p} \mid \boldsymbol{p} \rangle \langle \boldsymbol{p} \mid = 1$$

$$\langle \boldsymbol{q} \mid \boldsymbol{q}' \rangle = \delta(\boldsymbol{q} - \boldsymbol{q}') \qquad \langle \boldsymbol{p} \mid \boldsymbol{p}' \rangle = \delta(\boldsymbol{p} - \boldsymbol{p}')$$

$$\langle \boldsymbol{q} \mid \boldsymbol{p} \rangle = \frac{e^{i \boldsymbol{p}\cdot\boldsymbol{q}/\hbar}}{(2\pi\hbar)^{d/2}}$$

Consistency test:

$$\langle \boldsymbol{p} \mid \boldsymbol{p}' \rangle = \int d\boldsymbol{q} \langle \boldsymbol{p} \mid \boldsymbol{q} \rangle \langle \boldsymbol{q} \mid \boldsymbol{p}' \rangle$$

$$= \int d\boldsymbol{q} \frac{e^{-i \boldsymbol{p}\cdot\boldsymbol{q}/\hbar}}{(2\pi\hbar)^{d/2}} \frac{e^{i \boldsymbol{p}'\cdot\boldsymbol{q}/\hbar}}{(2\pi\hbar)^{d/2}} = \delta(\boldsymbol{p} - \boldsymbol{p}')$$

& similarly for $\langle \boldsymbol{q} \mid \boldsymbol{q}' \rangle$.

For $|t| \to \infty$, the phase of the exponential fluctuates wildly for small changes in $\boldsymbol{p}$. The integral is therefore dominated by the stationary points of the phase given by

$$\frac{\partial}{\partial \boldsymbol{p}} \left(\boldsymbol{p}\cdot\boldsymbol{q} - \frac{\boldsymbol{p}^2}{2m} t \right) = 0$$

$$\to \qquad \boldsymbol{p}_s = \frac{m}{t} \boldsymbol{q} \tag{6.21}$$

Hence, for $|t| \to \infty$,

$$\psi_j(\boldsymbol{q}, t) \approx \tilde{\psi}_j(\boldsymbol{p}_s) \int \frac{d\boldsymbol{p}}{(2\pi\hbar)^{d/2}} \exp\left[\frac{i}{\hbar} \left(\boldsymbol{p}\cdot\boldsymbol{q} - \frac{\boldsymbol{p}^2}{2m} t \right) \right]$$

$$= \tilde{\psi}_j(\boldsymbol{p}_s)\left(\frac{m}{i\,t}\right)^{d/2}\exp\left(i\,\frac{m\,\boldsymbol{q}^2}{2\,\hbar\,t}\right)$$

$$= \tilde{\psi}_j(\boldsymbol{p}_s)\left(\frac{m}{i\,t}\right)^{d/2}\exp\left(i\,\frac{\boldsymbol{p}_s^2}{2\,m\,\hbar}\,t\right)$$

$$= \tilde{\psi}_j(\boldsymbol{p}_s)\left(\frac{m}{|\,t\,|}\right)^{d/2}\exp\left(-i\,d\,\frac{\pi}{4}\,\mathrm{sgn}\,t + i\,\frac{\boldsymbol{p}_s^2}{2\,m\,\hbar}\,t\right) \qquad (6.22)$$

which differs from Zinn-Justin’s version by the coefficient of $\mathrm{sgn}\,t$.

Eq(6.19) becomes

$$\langle\,\psi_2\mid S\mid\psi_1\,\rangle = \lim_{\substack{t'\to-\infty\\ t''\to+\infty}}\int d\,\boldsymbol{q}''\,d\,\boldsymbol{q}'\;\overline{\tilde{\psi}}_2(\boldsymbol{p}_s'')\left(\frac{m}{-i\,t''}\right)^{d/2}\exp\left(-i\,\frac{\boldsymbol{p}_s''^{\,2}}{2\,m\,\hbar}\,t''\right)$$

$$\times\langle\,\boldsymbol{q}''\mid U(t'',t')\mid\boldsymbol{q}'\,\rangle\,\tilde{\psi}_1(\boldsymbol{p}_s')\left(\frac{m}{i\,t'}\right)^{d/2}\exp\left(i\,\frac{\boldsymbol{p}_s'^{\,2}}{2\,m\,\hbar}\,t'\right)$$

$$= \lim_{\substack{t'\to-\infty\\ t''\to+\infty}}\int d\,\boldsymbol{q}'\,d\,\boldsymbol{q}''\left(\frac{m^2}{t''\,t'}\right)^{d/2}\overline{\tilde{\psi}}_2(\boldsymbol{p}_s'')\,\tilde{\psi}_1(\boldsymbol{p}_s')$$

$$\times\exp\left(-\frac{i}{\hbar}\,\frac{\boldsymbol{p}_s''^{\,2}\,t''-\boldsymbol{p}_s'^{\,2}\,t'}{2\,m}\right)\langle\,\boldsymbol{q}''\mid U(t'',t')\mid\boldsymbol{q}'\,\rangle$$

$$= \lim_{\substack{t'\to-\infty\\ t''\to+\infty}}\int d\,\boldsymbol{q}'\,d\,\boldsymbol{q}''\left(\frac{m^2}{t''\,t'}\right)^{d/2}\overline{\tilde{\psi}}_2(\boldsymbol{p}_s'')\,\tilde{\psi}_1(\boldsymbol{p}_s')$$

$$\times\exp\left(-\frac{i}{\hbar}\,\frac{\boldsymbol{p}_s''^{\,2}\,t''-\boldsymbol{p}_s'^{\,2}\,t'}{2\,m}\right)\langle\,\boldsymbol{q}''\mid U(t'',t')\mid\boldsymbol{q}'\,\rangle$$

Setting

$$\boldsymbol{p}_s' = \frac{m}{t'}\,\boldsymbol{q}' \qquad\qquad \boldsymbol{p}_s'' = \frac{m}{t''}\,\boldsymbol{q}'' \qquad (6.23)$$

we have

$$\langle\,\psi_2\mid S\mid\psi_1\,\rangle = \lim_{\substack{t'\to-\infty\\ t''\to+\infty}}\left(\frac{t''\,t'}{m^2}\right)^{d/2}\int d\,\boldsymbol{p}_s'\,d\,\boldsymbol{p}_s''\;\overline{\tilde{\psi}}_2(\boldsymbol{p}_s'')\,\tilde{\psi}_1(\boldsymbol{p}_s') \qquad (6.24)$$

$$\times\exp\left(-\frac{i}{\hbar}\,\frac{\boldsymbol{p}_s''^{\,2}\,t''-\boldsymbol{p}_s'^{\,2}\,t'}{2\,m}\right)\left\langle\frac{t''}{m}\,\boldsymbol{p}_s''\,\middle|\,U(t'',t')\,\middle|\,\frac{t'}{m}\,\boldsymbol{p}_s'\right\rangle$$

which differs from Zinn-Justin’s version by a minus sign in the argument of the exponential function.

The evolution operator matrix element can be written in terms of a path integral [see eq(6.9) of §6.1] :

$$\left\langle\frac{t''}{m}\,\boldsymbol{p}_s''\,\middle|\,U(t'',t')\,\middle|\,\frac{t'}{m}\,\boldsymbol{p}_s'\right\rangle = \langle\,\boldsymbol{q}''\mid U(t'',t')\mid\boldsymbol{q}'\,\rangle$$

$$= \int_{\boldsymbol{q}(t')=t'\,\boldsymbol{p}_s'/m}^{\boldsymbol{q}(t'')=t''\,\boldsymbol{p}_s''/m}[\,d\,\boldsymbol{q}(t)\,]\,e^{i\,\mathcal{A}(\boldsymbol{q})/\hbar} \qquad (6.24a)$$

where $\mathcal{A}$ is given by eq(6.10) of §6.1.

Eqs(6.24 & 6.24a) give rise to the semi-classical approximation as will be illustrated in the following sections.

6.3.2. One-dimension: Semi-Classical Limit

Let

$$H = \frac{p^2}{2m} + V(x) \qquad \text{(a)}$$

We'll use the steepest descent method to calculate the S-matrix in the path integral representation for the case $\hbar \to 0$.

Forward Scattering

The classical eq. of motion is

$$m\ddot{x} = -\frac{dV}{dx} \qquad \text{(b)}$$

with the B.C.

$$x(\tau') = x' \qquad\qquad x(\tau'') = x''$$

Using

$$\ddot{x} = \frac{dx}{d\tau}\frac{d}{dx}\dot{x} = \frac{1}{2}\frac{d}{dx}\dot{x}^2$$

& integrating eq(b) once, we have

$$\frac{1}{2}m\dot{x}^2 + V = \text{const}$$

$$\overset{\text{set}}{=} E = \frac{\kappa^2}{2m} \qquad \text{(c)}$$

$$\to \qquad \dot{x} = \frac{1}{m}\sqrt{\kappa^2 - 2mV} \qquad \text{(d)}$$

Forward scattering, which requires $x = \pm\infty$ to be solutions to eqs(c), is possible classically only if $E \geq \max V$.

Let

$$X = x'' - x' \qquad\qquad T = \tau'' - \tau'$$

$$\& \qquad k = m\frac{X}{T} \qquad \text{(e)}$$

Forward scattering requires

$$\lim_{\substack{\tau'' \to \infty \\ \tau' \to -\infty}} \frac{X}{T} \equiv \frac{X_\infty}{T_\infty} = \frac{\kappa}{m}$$

be finite.

$$\kappa - k = m\left(\frac{X_\infty}{T_\infty} - \frac{X}{T}\right)$$

$$= \frac{m}{T\,T_\infty}\left(T X_\infty - T_\infty X\right)$$

$$= \frac{m}{T\,T_\infty}\left[(T_\infty - \Delta)\,X_\infty - T_\infty\frac{k}{m}(T_\infty - \Delta)\right] \qquad \Delta = T_\infty - T$$

$$= \frac{m}{T}\left(1 - \frac{\Delta}{T_\infty}\right)\left(X_\infty - T_\infty\frac{k}{m}\right)$$

$$\therefore \qquad \kappa = k + \frac{m}{T}\left(X_\infty - T_\infty \frac{k}{m}\right) + O\left(\frac{\Delta}{T}\right) \qquad \text{(f)}$$

Integrating eq(d) gives

$$T = m \int_{x'}^{x''} \frac{d\,x}{\sqrt{\kappa^2 - 2\,m\,V}} \qquad \text{(g)}$$

$$\rightarrow \qquad T_\infty = m \int_{-\infty}^{\infty} \frac{d\,x}{\sqrt{\kappa^2 - 2\,m\,V}}$$

$$X_\infty = \int_{-\infty}^{\infty} d\,x$$

Eq(f) thus becomes

$$\kappa = k + \frac{m}{T}\int_{-\infty}^{\infty} d\,x\left(1 - \frac{k}{\sqrt{\kappa^2 - 2\,m\,V}}\right) + O\left(\frac{\Delta}{T}\right) \qquad \text{(h)}$$

which differs from Zinn-Justin's version by a minus sign in the 2nd term.

$$\mathcal{A} = \int_{t'}^{t''} d\,\tau\,L = \int_{t'}^{t''} d\,\tau\left(\frac{1}{2} m\,\dot{x}^2 - V\right)$$

$$= \int_{t'}^{t''} d\,\tau\left(\frac{\kappa^2}{2\,m} - 2\,V\right) \qquad \text{[Eq(d) used.]}$$

$$= \frac{\kappa^2}{2\,m} T - 2\int_{t'}^{t''} d\,\tau\,V$$

Using

$$2\int_{t'}^{t''} d\,\tau\,V = 2\int_{x'}^{x''} d\,x\,\frac{d\,\tau}{d\,x} V$$

$$= \int_{x'}^{x''} d\,x\,\frac{2\,m\,V}{\sqrt{\kappa^2 - 2\,m\,V}} \qquad \text{[Eq(d) used.]}$$

$$= \int_{x'}^{x''} d\,x\left(-\sqrt{\kappa^2 - 2\,m\,V} + \frac{\kappa^2}{\sqrt{\kappa^2 - 2\,m\,V}}\right)$$

$$= -\int_{x'}^{x''} d\,x\sqrt{\kappa^2 - 2\,m\,V} + \kappa^2\frac{T}{m} \qquad \text{[Eq(g) used.]}$$

$$= -\int_{x'}^{x''} d\,x\left(\sqrt{\kappa^2 - 2\,m\,V} - \frac{1}{k}\kappa^2\right) \qquad \text{[Eq(e) used.]}$$

$$= -\int_{x'}^{x''} d\,x\left(\sqrt{\kappa^2 - 2\,m\,V} - \kappa\right) + O\left(T^{-1}\right) \qquad \text{[Eq(h) used.]}$$

we have

$$\mathcal{A} = \frac{\kappa^2}{2\,m} T + \int_{x'}^{x''} d\,x\left(\sqrt{\kappa^2 - 2\,m\,V} - \kappa\right) + O\left(T^{-1}\right) \qquad \text{(i)}$$

From eq(6.20), we see that if $\left|\,\psi_j\right\rangle$ is a plane wave $|\,\boldsymbol{k}\,\rangle$, then

$$\tilde{\psi}_j(\boldsymbol{p}) = \langle\,\boldsymbol{p}\mid\boldsymbol{k}\,\rangle = \delta(\boldsymbol{p} - \boldsymbol{k})$$

Eq(6.24) then simplifies to

$$\langle k'' \mid S \mid k' \rangle = \lim_{\substack{t' \to -\infty \\ t'' \to +\infty}} \left(\frac{t'' t'}{m^2} \right)^{1/2} \exp\left(-\frac{i}{\hbar} \frac{k''^2 t'' - k'^2 t'}{2m} \right) \left\langle \frac{t''}{m} k'' \,\middle|\, U(t'', t') \,\middle|\, \frac{t'}{m} k' \right\rangle$$

When we evaluate eq(6.24a) by means of the classical approximation [see §2.3] using eq(i), we have, to lowest order in T,

$$\langle x'' \mid U(t'', t') \mid x' \rangle = \mathcal{N}(t'' - t') \exp\left\{ \frac{i}{\hbar} \left[\frac{\kappa^2}{2m} T + \int_{x'}^{x''} dx \left(\sqrt{\kappa^2 - 2mV} - \kappa \right) \right] \right\}$$

$$\approx \mathcal{N}(t'' - t') \exp\left\{ \frac{i}{\hbar} \left[\frac{\kappa^2}{2m} T + \int_{-\infty}^{\infty} dx \left(\sqrt{\kappa^2 - 2mV} - \kappa \right) \right] \right\}$$

where $\mathcal{N}$ is independent of x'' & x'.

Using the free motion result of eq(2.10) of §2.2, we have

$$\mathcal{N}(t'' - t') = \left(\frac{m}{2\pi\hbar(t'' - t')} \right)^{1/2}$$

Setting

$$t'' = \frac{T}{2} = -t'$$

we have

$$\left(\frac{t'' t'}{m^2} \right)^{1/2} \mathcal{N}(t'' - t') = \left(\frac{T}{8\pi\hbar m} \right)^{1/2}$$

$$\rightarrow \qquad \langle k'' \mid S_+ \mid k' \rangle \propto \exp\left(-\frac{i}{2m\hbar} \left(k''^2 t'' - k'^2 t' - \kappa^2 T \right) \right) \qquad \text{(j)}$$

$$\times \exp\left\{ \frac{i}{\hbar} \int_{-\infty}^{\infty} dx \left(\sqrt{\kappa^2 - 2mV} - \kappa \right) \right\}$$

The 1st factor fluctuates wildly except for $k'' = k' = \kappa$ so that

$$k''^2 t'' - k'^2 t' - \kappa^2 T = 0$$

Thus, $\langle k'' \mid S_+ \mid k' \rangle$ vanishes except for

$$\langle \kappa \mid S_+ \mid \kappa \rangle \propto \exp\left\{ \frac{i}{\hbar} \int_{-\infty}^{\infty} dx \left(\sqrt{\kappa^2 - 2mV} - \kappa \right) \right\}$$

Neglecting the prefactor, we have

$$\ln S_+(\kappa) = \frac{i}{\hbar} \int_{-\infty}^{\infty} dx \left(\sqrt{\kappa^2 - 2mV} - \kappa \right)] \qquad \text{(k)}$$

Backward Scattering

For backward scattering, $E < \max V$.

Let x_0 & t_0 be the turning point & time, respectively, i.e.,

$$\frac{\kappa^2}{2m} = V(x_0) \qquad\qquad t_0 = m \int_{x'}^{x_0} \frac{dx}{\sqrt{\kappa^2 - 2mV}}$$

In a back-scattering, the motion connsists of 2 segments:

1. The incidence segment:

   x goes from $x(t') = x' \approx -\infty$ to $x(t_0) = x_0$ with $\dot{x} > 0$.

2. The reflection segment:

   x goes from $x(t_0) = x_0$ to $x(t'') = x'' \approx -\infty$ with $\dot{x} < 0$.

Hence, for x', $x'' < x_0$, we have

$$T = \left(\int_{x'}^{x_0} - \int_{x_0}^{x''} \right) \frac{dx}{|\dot{x}|}$$

$$= m\left(\int_{x'}^{x_0} + \int_{x''}^{x_0}\right)\frac{dx}{\sqrt{\kappa^2 - 2mV}}$$
$$= T' + T''$$

where

$T'' = t'' - t_0 > 0 \qquad T' = t_0 - t' > 0$

denote the time-lapse in each segment.

$$\therefore \qquad T_\infty = 2m\int_{-\infty}^{x_0}\frac{dx}{\sqrt{\kappa^2 - 2mV}}$$

Similarly, let the distance travelled in each segment be

$X'' = x_0 - x'' > 0 \qquad X' = x_0 - x' > 0$

The corresponding momenta are

$$k'' = -m\frac{X''}{T''} < 0 \qquad k' = m\frac{X'}{T'} > 0$$

$$\to \qquad T = m\left(-\frac{X''}{k''} + \frac{X'}{k'}\right)$$

For $k' = -k'' = \kappa$, we have

$$T = \frac{m}{\kappa}(X'' + X') = \frac{m}{\kappa}(2x_0 - x'' - x')$$
$$\kappa = \frac{m}{T}(2x_0 - x'' - x')$$

where $X'' + X'$ is the total distance travelled.

Following closely the derivation of eq(i), we have

$$\mathcal{A} = \left(\int_{t'}^{t_0} + \int_{t_0}^{t''}\right)d\tau\left(\frac{\kappa^2}{2m} - 2V\right)$$
$$= T\frac{\kappa^2}{2m} + \left(\int_{x'}^{x_0} - \int_{x_0}^{x''}\right)dx\,\frac{2V}{|\dot{x}|}$$
$$= \frac{m}{2T}(2x_0 - x'' - x')^2 + \left(\int_{x'}^{x_0} + \int_{x''}^{x_0}\right)dx\left(\sqrt{\kappa^2 - 2mV} - \kappa\right) + O(T^{-1})$$
$$= \frac{m}{2T}(2x_0 - x'' - x')^2 + 2\int_{-\infty}^{x_0}dx\left(\sqrt{\kappa^2 - 2mV} - \kappa\right) + O(T^{-1})$$
$$= \frac{\kappa}{2}(2x_0 - x'' - x') + 2\int_{-\infty}^{x_0}dx\left(\sqrt{\kappa^2 - 2mV} - \kappa\right) + O(T^{-1})$$

Using

$$x'' = -\frac{\kappa}{m}t'' \qquad x' = \frac{\kappa}{m}t' \qquad \text{as } t'' \to \infty \ \& \ t' \to -\infty$$

we have [c.f. eq(j)]

$$\langle k'' \,|\, S_- \,|\, k' \rangle \propto \exp\left(-\frac{i}{2m\hbar}\left(k''^2 t'' - k'^2 t' - \kappa^2 t'' + \kappa^2 t'\right) + \frac{i}{\hbar}\kappa x_0\right)$$
$$\times \exp\left\{\frac{2i}{\hbar}\int_{-\infty}^{x_0}dx\left(\sqrt{\kappa^2 - 2mV} - \kappa\right)\right\}$$

Thus, $\langle k'' \,|\, S_- \,|\, k' \rangle$ vanishes except for

$$\langle \kappa \,|\, S_- \,|\, \kappa \rangle \propto \exp\left\{\frac{2i}{\hbar}\int_{-\infty}^{x_0}dx\left(\sqrt{\kappa^2 - 2mV} - \kappa\right) + \frac{i}{\hbar}\kappa x_0\right\}$$

$$\to \qquad \ln S_{-}(\kappa) = \frac{2i}{\hbar}\int_{-\infty}^{x_0} dx\left(\sqrt{\kappa^2 - 2mV} - \kappa\right) + \frac{i}{\hbar}\kappa x_0$$

which differs from Zinn-Justin's version by a prefactor of 2 in the last term.

6.3.3. Eikonal Approximation and Path Integral

The eikonal approximation deals with the high energy, low momentum transfer regime.

For the free hamiltonian

$$H_0 = \frac{\boldsymbol{p}^2}{2m}$$

the classical path is

$$\boldsymbol{q}(t) = \boldsymbol{q}' + (\boldsymbol{q}'' - \boldsymbol{q}')\frac{t - t'}{t'' - t'} \qquad (6.25)$$

$$\to \qquad \dot{\boldsymbol{q}}(t) = \frac{\boldsymbol{q}'' - \boldsymbol{q}'}{t'' - t'}$$

In the classical approximation [see §2.3], we have

$$\langle \boldsymbol{q}'' \mid U(t'', t') \mid \boldsymbol{q}' \rangle = \int_{\boldsymbol{q}(t')=q'}^{\boldsymbol{q}(t'')=q''} [d\,\boldsymbol{q}(t)] \exp\left(\frac{i}{\hbar}\mathcal{A}(\boldsymbol{q})\right)$$

$$= \mathcal{N}(t'', t') \exp\left(\frac{i}{\hbar}\mathcal{A}(\boldsymbol{q}_c)\right)$$

where $\mathcal{N}(t'', t')$ is usually treated as a normalization "constant" to be dropped or estimated by other means.

For example, using

$$\mathcal{A}_0(\boldsymbol{q}_c) = \int_{t'}^{t''} dt\,\frac{1}{2} m \dot{\boldsymbol{q}}_c^2$$

$$= \int_{t'}^{t''} dt\,\frac{1}{2} m \left(\frac{\boldsymbol{q}'' - \boldsymbol{q}'}{t'' - t'}\right)^2$$

$$= \frac{1}{2} m \frac{(\boldsymbol{q}'' - \boldsymbol{q}')^2}{t'' - t'} \qquad (6.25a)$$

we have

$$\langle \boldsymbol{q}'' \mid U_0(t'', t') \mid \boldsymbol{q}' \rangle = \mathcal{N}_0(t'', t') \exp\left(i\frac{m(\boldsymbol{q}'' - \boldsymbol{q}')^2}{2\hbar(t'' - t')}\right)$$

which agrees with the exact result eq(6.5b).

Consider now

$$H = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{q})$$

and

$$\langle \boldsymbol{p}'' \mid U(t'', t') \mid \boldsymbol{p}' \rangle = \left\langle \boldsymbol{p}'' \mid e^{-iH(t''-t')/\hbar} \mid \boldsymbol{p}' \right\rangle$$

$$= \int \frac{d\,\boldsymbol{q}''\,d\,\boldsymbol{q}'}{(2\pi\hbar)^d} e^{-i(\boldsymbol{p}''\cdot\boldsymbol{q}'' - \boldsymbol{p}'\cdot\boldsymbol{q}')/\hbar} \langle \boldsymbol{q}'' \mid U(t'', t') \mid \boldsymbol{q}' \rangle$$

Let

$$\boldsymbol{p}'' = \boldsymbol{p} + \frac{1}{2}\boldsymbol{k} \qquad \boldsymbol{p}' = \boldsymbol{p} - \frac{1}{2}\boldsymbol{k} \qquad (6.25b)$$

$$\boldsymbol{s} = \boldsymbol{q}'' - \boldsymbol{q}' \qquad \boldsymbol{x} = \frac{1}{2}(\boldsymbol{q}'' + \boldsymbol{q}')$$

$$\to \qquad \boldsymbol{p}''\cdot\boldsymbol{q}'' - \boldsymbol{p}'\cdot\boldsymbol{q}' = \left(\boldsymbol{p}+\frac{1}{2}\boldsymbol{k}\right)\cdot\boldsymbol{q}'' - \left(\boldsymbol{p}-\frac{1}{2}\boldsymbol{k}\right)\cdot\boldsymbol{q}'$$
$$= \boldsymbol{p}\cdot\boldsymbol{s} + \boldsymbol{k}\cdot\boldsymbol{x}$$

$$\therefore \qquad \langle \boldsymbol{p}'' \mid U(t'', t') \mid \boldsymbol{p}' \rangle = \left\langle \boldsymbol{p}+\frac{1}{2}\boldsymbol{k} \;\middle|\; U(t'', t') \;\middle|\; \boldsymbol{p}-\frac{1}{2}\boldsymbol{k} \right\rangle$$
$$= \int \frac{d\boldsymbol{s}\, d\boldsymbol{x}}{(2\pi\hbar)^d} e^{-i(\boldsymbol{p}\cdot\boldsymbol{s}+\boldsymbol{k}\cdot\boldsymbol{x})/\hbar} \left\langle \boldsymbol{x}+\frac{\boldsymbol{s}}{2} \;\middle|\; U(t'', t') \;\middle|\; \boldsymbol{x}-\frac{\boldsymbol{s}}{2} \right\rangle$$
$$= \mathcal{N}(t'', t') \int \frac{d\boldsymbol{s}\, d\boldsymbol{x}}{(2\pi\hbar)^d} e^{-i(\boldsymbol{p}\cdot\boldsymbol{s}+\boldsymbol{k}\cdot\boldsymbol{x})/\hbar} \exp\left(\frac{i}{\hbar}\mathcal{A}(\boldsymbol{q}_c)\right) \qquad (6.26)$$

For

$$\boldsymbol{p}^2 \to \infty \text{ so that } \frac{\boldsymbol{p}^2}{2m} >> |V| \qquad (6.26a)$$

the classical path should be close to the free path.

Since

$$\mathcal{A}(\boldsymbol{q}) = \int_{t'}^{t''} dt \left[\frac{1}{2} m \dot{\boldsymbol{q}}^2 - V(\boldsymbol{q})\right]$$

we can use eqs(6.25, 6.25a & 6.25b) to get

$$\mathcal{A}(\boldsymbol{q}_c) \approx \frac{1}{2} m \frac{(\boldsymbol{q}''-\boldsymbol{q}')^2}{t''-t'} - \int_{t'}^{t''} dt\, V\left(\boldsymbol{q}' + (\boldsymbol{q}''-\boldsymbol{q}')\frac{t-t'}{t''-t'}\right)$$
$$= \frac{1}{2} m \frac{\boldsymbol{s}^2}{t''-t'} - \int_{t'}^{t''} dt\, V\left(\boldsymbol{x} - \frac{\boldsymbol{s}}{2} + \boldsymbol{s}\frac{t-t'}{t''-t'}\right) \qquad (6.27)$$
$$= \mathcal{A}(\boldsymbol{s}, \boldsymbol{x})$$

Moreover, $\mathcal{N}(t'', t')$ in eq(6.26) should be close to the free motion value of eq(6.5b).

By eq(6.26a), we assume the V term is negligible compared to the $\boldsymbol{p}\cdot\boldsymbol{s}$ term. Thus, for large times, the $\boldsymbol{s}$ integral can be replaced by its value at the saddle point give by

$$\frac{\partial}{\partial \boldsymbol{s}}\left(-\boldsymbol{p}\cdot\boldsymbol{s} + \frac{1}{2} m \frac{\boldsymbol{s}^2}{t''-t'}\right) = 0$$

$$\to \qquad -\boldsymbol{p} + m\frac{\boldsymbol{s}}{t''-t'} = 0$$

$$\boldsymbol{s} = \frac{\boldsymbol{p}}{m}(t''-t') \qquad (6.28)$$

so that

$$-\boldsymbol{p}\cdot\boldsymbol{s} + \frac{1}{2} m \frac{\boldsymbol{s}^2}{t''-t'} = -\frac{\boldsymbol{p}^2}{2m}(t''-t')$$

$$-\frac{\boldsymbol{s}}{2} + \boldsymbol{s}\frac{t-t'}{t''-t'} = \frac{\boldsymbol{p}}{m}(t''-t')\left[-\frac{1}{2} + \frac{t-t'}{t''-t'}\right]$$
$$= \frac{\boldsymbol{p}}{m}\left[t - \frac{1}{2}(t''+t')\right]$$

$$\therefore \qquad \langle \boldsymbol{p}'' \mid U(t'', t') \mid \boldsymbol{p}' \rangle = \mathcal{N} \int \frac{d\boldsymbol{x}}{(2\pi\hbar)^d} e^{-i\,\boldsymbol{k}\cdot\boldsymbol{x}/\hbar}$$
$$\times \exp\left(\frac{i}{\hbar}\left\{-\frac{\boldsymbol{p}^2}{2m}(t''-t') - \int_{t'}^{t''} dt\, V\left(\boldsymbol{x} + \frac{\boldsymbol{p}}{m}\left[t - \frac{1}{2}(t''+t')\right]\right)\right\}\right)$$

$$= \mathcal{N} \int \frac{d\,\boldsymbol{x}}{(2\,\pi\,\hbar)^d} \exp\left(\frac{i}{\hbar} \left\{ -\boldsymbol{k}\cdot\boldsymbol{x} - \frac{\boldsymbol{p}^2}{2\,m} T - \int_{-T/2}^{T/2} d\,t\, V\left(\boldsymbol{x} + \frac{\boldsymbol{p}}{m} t \right) \right\} \right) \tag{6.28a}$$

where $T = t'' - t'$.

Let $\boldsymbol{b}$ be the component of $\boldsymbol{x}$ orthogonal to $\boldsymbol{p}$, i.e.,

$$\boldsymbol{b} = \boldsymbol{x} - \frac{\boldsymbol{x}\cdot\boldsymbol{p}}{\boldsymbol{p}^2} \boldsymbol{p} \tag{6.29}$$

$$\rightarrow \qquad \boldsymbol{x} + \frac{\boldsymbol{p}}{m} t = \boldsymbol{b} + \frac{\boldsymbol{p}}{m} \left(m \frac{\boldsymbol{x}\cdot\boldsymbol{p}}{\boldsymbol{p}^2} + t \right)$$

$$= \boldsymbol{b} + \frac{\boldsymbol{p}}{m} \tau$$

where

$$\tau = m \frac{\boldsymbol{x}\cdot\boldsymbol{p}}{\boldsymbol{p}^2} + t$$

Also,

$$d\,\boldsymbol{x} = J\, d\,\boldsymbol{b}\, d\,\boldsymbol{x}_{\boldsymbol{p}}$$

where $\boldsymbol{x}_{\boldsymbol{p}}$ is the component of $\boldsymbol{x}$ along $\boldsymbol{p}$ & J is the Jacobian.

Writing

$$\boldsymbol{k}\cdot\boldsymbol{x} = \boldsymbol{k}\cdot\boldsymbol{b} + \boldsymbol{k}\cdot\boldsymbol{x}_{\boldsymbol{p}}$$

we integral over $\boldsymbol{x}_{\boldsymbol{p}}$ to get a delta function $\delta(\hat{\boldsymbol{p}}\cdot\boldsymbol{k})$.

Thus, for $T \to \infty$, we have

$$\left\langle \boldsymbol{p} + \frac{1}{2}\boldsymbol{k} \,\middle|\, U(t'', t') \,\middle|\, \boldsymbol{p} - \frac{1}{2}\boldsymbol{k} \right\rangle = \mathcal{N}(\boldsymbol{p})\, \delta(\hat{\boldsymbol{p}}\cdot\boldsymbol{k}) \tag{6.30}$$

$$\times \int \frac{d^{d-1}\,b}{(2\,\pi\,\hbar)^{d-1}} \exp\left(-\frac{i}{\hbar} \left[\boldsymbol{k}\cdot\boldsymbol{b} + \int_{-\infty}^{\infty} d\,\tau\, V\left(\boldsymbol{b} + \frac{\boldsymbol{p}}{m}\tau \right) \right] \right)$$

where

$$\mathcal{N}(\boldsymbol{p}) = \mathcal{N}\, J \exp\left(-i \frac{\boldsymbol{p}^2}{2\,m\,\hbar} T \right) \tag{6.31}$$

Inserting eq(6.30) into eq(6.6), the exponential in $\mathcal{N}(\boldsymbol{p})$ got cancelled so that

$$\left\langle \boldsymbol{p} + \frac{1}{2}\boldsymbol{k} \,\middle|\, S \,\middle|\, \boldsymbol{p} - \frac{1}{2}\boldsymbol{k} \right\rangle \propto \delta(\hat{\boldsymbol{p}}\cdot\boldsymbol{k})$$

$$\times \int \frac{d^{d-1}\,b}{(2\,\pi\,\hbar)^{d-1}} \exp\left(-\frac{i}{\hbar} \left[\boldsymbol{k}\cdot\boldsymbol{b} + \int_{-\infty}^{\infty} d\,\tau\, V\left(\boldsymbol{b} + \frac{\boldsymbol{p}}{m}\tau \right) \right] \right)$$

With

$$\delta(\boldsymbol{p}'' - \boldsymbol{p}') = \delta(\boldsymbol{k}) = \delta(\hat{\boldsymbol{p}}\cdot\boldsymbol{k}) \int \frac{d^{d-1}\,b}{(2\,\pi\,\hbar)^{d-1}} e^{-i\,\boldsymbol{k}\cdot\boldsymbol{b}/\hbar}$$

putting into eq(6.7), we have

$$i \left\langle \boldsymbol{p} + \frac{1}{2}\boldsymbol{k} \,\middle|\, \mathcal{T} \,\middle|\, \boldsymbol{p} - \frac{1}{2}\boldsymbol{k} \right\rangle = \delta(\boldsymbol{k}) - \left\langle \boldsymbol{p} + \frac{1}{2}\boldsymbol{k} \,\middle|\, S \,\middle|\, \boldsymbol{p} - \frac{1}{2}\boldsymbol{k} \right\rangle$$

$$\propto -\delta(\hat{\boldsymbol{p}}\cdot\boldsymbol{k}) \int \frac{d^{d-1}\,b}{(2\,\pi\,\hbar)^{d-1}} e^{-i\,\boldsymbol{k}\cdot\boldsymbol{b}/\hbar} \left\{ \exp\left[-\frac{i}{\hbar} \int_{-\infty}^{\infty} d\,\tau\, V\left(\boldsymbol{b} + \frac{\boldsymbol{p}}{m}\tau \right) \right] - 1 \right\}$$

Note: we've tacitly assumed $\mathcal{N}\, J = 1$.

With

$$\delta(E'' - E') = \delta\left(\frac{\boldsymbol{p}\cdot\boldsymbol{k}}{m}\right) = \frac{m}{|\,\boldsymbol{p}\,|}\,\delta(\hat{\boldsymbol{p}}\cdot\boldsymbol{k})$$

Eq(6.8) then gives

$$T\left(\boldsymbol{p} + \frac{1}{2}\boldsymbol{k},\, \boldsymbol{p} - \frac{1}{2}\boldsymbol{k}\right) = i\,\frac{|\,\boldsymbol{p}\,|}{m}\int \frac{d^{d-1}b}{(2\pi\hbar)^d}\,e^{-i\,\boldsymbol{k}\cdot\boldsymbol{b}/\hbar} \qquad (6.32)$$

$$\times\left\{\exp\left[-\frac{i}{\hbar}\int_{-\infty}^{\infty} d\tau\, V\left(\boldsymbol{b} + \frac{\boldsymbol{p}}{m}\tau\right)\right] - 1\right\}$$

It's easy to check that for $d = 1$, eq(6.32) is still valid if we set $\boldsymbol{b} = 0$.

Application to the Coulomb Potential

For a Coulomb-like potential

$$V(\boldsymbol{q}) = \frac{\alpha}{|\,\boldsymbol{q}\,|} \qquad (6.33)$$

the integral in eq(6.32) diverges.

Integrating over finite time interval, we have

$$\int_{-T/2}^{T/2} dt\, V\left(\boldsymbol{b} + \frac{\boldsymbol{p}}{m}t\right) = \int_{-T/2}^{T/2} dt\,\frac{\alpha}{\left|\,\boldsymbol{b} + \frac{\boldsymbol{p}}{m}t\,\right|}$$

Since $\boldsymbol{b}\cdot\boldsymbol{p} = 0$, we have

$$\left|\,\boldsymbol{b} + \frac{\boldsymbol{p}}{m}t\,\right| = \sqrt{b^2 + \left(\frac{p\,t}{m}\right)^2}$$

$$\rightarrow \quad \int_{-T/2}^{T/2} dt\, V\left(\boldsymbol{b} + \frac{\boldsymbol{p}}{m}t\right) = \frac{m\,\alpha}{p}\int_{-T/2}^{T/2} dt\,\frac{1}{\sqrt{t^2 + \left(\frac{m\,b}{p}\right)^2}}$$

$$= \frac{m\,\alpha}{p}\ln\left(t + \sqrt{t^2 + \left(\frac{m\,b}{p}\right)^2}\right)_{-T/2}^{T/2}$$

Using

$$t + \sqrt{t^2 + \left(\frac{m\,b}{p}\right)^2} \approx t + |\,t\,|\left\{1 + \frac{1}{2}\left(\frac{m\,b}{p\,t}\right)^2\right\}$$

we have

$$\left(t + \sqrt{t^2 + \left(\frac{m\,b}{p}\right)^2}\right)_{T/2} \approx T$$

$$\left(t + \sqrt{t^2 + \left(\frac{m\,b}{p}\right)^2}\right)_{-T/2} \approx T\left(\frac{m\,b}{p\,T}\right)^2$$

so that

$$\int_{-T/2}^{T/2} dt\, V\left(\boldsymbol{b} + \frac{\boldsymbol{p}}{m}t\right) = \frac{2\,m\,\alpha}{p}\ln\left(\frac{p\,T}{m\,b}\right) \qquad (6.34)$$

This infinite phase makes T ill-defined so that only cross-section is well-defined.

Eq(6.34) applies only if $d \geq 2$. For $d = 1$, we have $\boldsymbol{b} = 0$ so that

$$\int_{-T/2}^{T/2} dt\, V\left(\frac{p}{m} t\right) = \frac{m\alpha}{p} \int_{-T/2}^{T/2} dt \frac{1}{|t|}$$

$$= \frac{m\alpha}{p} \left(\int_0^{T/2} dt \frac{1}{t} - \int_{-T/2}^{0} dt \frac{1}{t} \right)$$

$$= \frac{m\alpha}{p} \left[\ln \frac{T}{2} + \ln\left(-\frac{T}{2} \right) \right]$$

$$= \frac{m\alpha}{p} (\ln T + i\pi) \tag{6.34a}$$

$$\rightarrow \quad T\left(p + \frac{1}{2}k,\, p - \frac{1}{2}k\right) = i \frac{p}{2\pi\hbar m} \left\{ \exp\left[-\frac{i}{\hbar} \frac{m\alpha}{p} (\ln T + i\pi) \right] - 1 \right\} \tag{6.34b}$$

For $d \geq 2$, eq(6.32) becomes

$$T\left(\boldsymbol{p} + \frac{1}{2}\boldsymbol{k},\, \boldsymbol{p} - \frac{1}{2}\boldsymbol{k}\right) = i \frac{p}{m} \int \frac{d^{d-1} b}{(2\pi\hbar)^d} e^{-i\boldsymbol{k}\cdot\boldsymbol{b}/\hbar} \left\{ \exp\left[-i \frac{2m\alpha}{p\hbar} \ln\left(\frac{pT}{mb} \right) \right] - 1 \right\}$$

where, by construction, both $\boldsymbol{k}$ & $\boldsymbol{b}$ are perpendicular to $\boldsymbol{p}$.

Let

$$\theta = -i \frac{\alpha m}{p\hbar} \tag{6.36}$$

$$\rightarrow \quad T\left(\boldsymbol{p} + \frac{1}{2}\boldsymbol{k},\, \boldsymbol{p} - \frac{1}{2}\boldsymbol{k}\right) = i \frac{p}{m} \int \frac{d^{d-1} b}{(2\pi\hbar)^d} e^{-i\boldsymbol{k}\cdot\boldsymbol{b}/\hbar} \left\{ b^{-2\theta} \exp\left[-i \frac{2m\alpha}{p\hbar} \ln\left(\frac{pT}{m} \right) \right] - 1 \right\}$$

Let Ω_d be the solid angle or surface area of a sphere of unir radius in d-D Euclidean space. Then [see "n-Sphere.pdf" in Chap.3 & §A1.5 of I.D.Lawrie, "A Unified Grand Tour of Theoretical Physics"],

$$\Omega_d = \frac{2\pi^{d/2}}{\Gamma(d/2)}$$

$$d^d r = r^{d-1}\, dr\, d\Omega_d$$

$$d\Omega_d = \sin^{d-2}\theta_1 \sin^{d-3}\theta_2 \ldots \sin\theta_{d-2}\, d\theta_1\, d\theta_2 \ldots d\theta_{d-2}\, d\phi$$

where

$$\theta_j \in [0, \pi] \qquad \& \qquad \phi \in [0, 2\pi]$$

$$\int_{-\infty}^{\infty} d^d x\, e^{-r^2} = \left(\int_{-\infty}^{\infty} dx\, e^{-x^2} \right)^d = \pi^{d/2}$$

$$= \Omega_d \int_0^{\infty} dr\, r^{d-1} e^{-r^2} = \frac{1}{2} \Omega_d \Gamma\left(\frac{d}{2}\right)$$

$$\rightarrow \quad \Omega_d = \frac{2\pi^{d/2}}{\Gamma(d/2)}$$

Setting

$$\boldsymbol{k}\cdot\boldsymbol{b} = k\, b \cos\phi$$

we have

$$\int d^{d-1} b\, e^{-i\boldsymbol{k}\cdot\boldsymbol{b}/\hbar} = \frac{\Omega_{d-1}}{2\pi} \int_0^{\infty} db\, b^{d-2} \int_0^{2\pi} d\phi\, e^{-ikb\cos\phi/\hbar}$$

$$= \frac{\pi^{(d-1)/2}}{\Gamma\left(\frac{d-1}{2}\right)} \int_0^{\infty} db\, b^{d-2} J_0\left(\frac{kb}{\hbar}\right)$$

where J_0 is the Bessel function of order 0 & we've used

$$J_0(\rho) = \frac{1}{2\pi} \int_0^{2\pi} d\,\phi\, e^{-i\rho\cos\phi}$$

Using

$$\int_0^\infty d\,x\, x^\mu J_\nu(a\,x) = 2^\mu a^{-\mu-1} \frac{\Gamma\left(\frac{1}{2}(1+\nu+\mu)\right)}{\Gamma\left(\frac{1}{2}(1+\nu-\mu)\right)} \qquad \text{[see G-R, eq(6.561.14)]}$$

we have

$$\int d^{d-1} b\, e^{-i\,\boldsymbol{k}\cdot\boldsymbol{b}/\hbar} = \frac{\pi^{(d-1)/2}}{\Gamma\left(\frac{d-1}{2}\right)} 2^{d-2} \left(\frac{k}{\hbar}\right)^{-d+1} \frac{\Gamma\left(\frac{1}{2}(d-1)\right)}{\Gamma\left(\frac{1}{2}(3-d)\right)}$$

$$\int d^{d-1} b\, e^{-i\,\boldsymbol{k}\cdot\boldsymbol{b}/\hbar}\, b^{-2\theta} = \frac{\pi^{(d-1)/2}}{\Gamma\left(\frac{d-1}{2}\right)} 2^{d-2-2\theta} \left(\frac{k}{\hbar}\right)^{-d+1+2\theta} \frac{\Gamma\left(\frac{1}{2}(d-1-2\theta)\right)}{\Gamma\left(\frac{1}{2}(3-d+2\theta)\right)}$$

Keeping only the infinite-phse term. we have

$$T\left(\boldsymbol{p} + \frac{1}{2}\boldsymbol{k},\, \boldsymbol{p} - \frac{1}{2}\boldsymbol{k}\right) = i\,\frac{p}{m} \frac{\pi^{(d-1)/2}}{(2\pi\hbar)^d} \exp\left[-i\,\frac{2\,m\,\alpha}{p\,\hbar} \ln\left(\frac{p\,T}{m}\right)\right]$$

$$\times \frac{\Gamma\left(\frac{1}{2}(d-1)-\theta\right)}{\Gamma\left(\frac{d-1}{2}\right)\Gamma\left(1-\frac{1}{2}(d-1)+\theta\right)} \left(\frac{k^2}{4\hbar}\right)^{\theta+(1-d)/2}$$

(6.35a)

which coincides with Zinn-Justin’s version if $d = 3$.

For $d \geq 2$, the poles of T are the poles of $\Gamma\left(\frac{1}{2}(d-1)-\theta\right)$, which occur at

$$\frac{1}{2}(d-1) - \theta = -n \qquad \text{where } n = 0, 1, 2, \ldots$$

$$\rightarrow \qquad \theta_n = \frac{1}{2}(d-1) + n$$

These poles represent bound states of the (attractive) Coulomb potential when $\alpha < 0$.
Their energies are given by

$$E_n = \frac{\boldsymbol{p}^2}{2\,m} = \frac{1}{2\,m}\left(-i\,\frac{\alpha\,m}{\theta_n\,\hbar}\right)^2 \qquad \text{[Eq(6.36) used]}$$

$$= -\frac{2\,m\,\alpha^2}{(d-1+2\,n)^2}$$

(6.37)