1.12. Free-Particle Amplitudes

For a free particle,

$$\hat{H} = \frac{1}{2M}\hat{\boldsymbol{p}}^2$$

with eigenfunctions

$$\psi_{\boldsymbol{p}}(\boldsymbol{x}) = \langle \boldsymbol{x} \mid \boldsymbol{p} \rangle = e^{i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar} \qquad (1.189)$$

for eigenvalues

$$E(\boldsymbol{p}) = \frac{1}{2M}\boldsymbol{p}^2$$

Using the completeness relation

$$\int \frac{d^D p}{(2\pi\hbar)^D} \mid \boldsymbol{p}\rangle\langle \boldsymbol{p} \mid = \hat{1} \qquad (1.187)$$

where D is the dimension of space, we have

$$\begin{aligned}(\boldsymbol{x}\, t \mid \boldsymbol{x}'\, t') &= \left\langle \boldsymbol{x} \,\middle|\, e^{-i\hat{H}(t-t')/\hbar} \,\middle|\, \boldsymbol{x}' \right\rangle \\ &= \int \frac{d^D p}{(2\pi\hbar)^D} \left\langle \boldsymbol{x} \,\middle|\, e^{-i\hat{H}(t-t')/\hbar} \,\middle|\, \boldsymbol{p} \right\rangle \langle \boldsymbol{p} \mid \boldsymbol{x}' \rangle \\ &= \int \frac{d^D p}{(2\pi\hbar)^D} e^{-i\boldsymbol{p}^2(t-t')/2M\hbar} e^{i\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{x}')/\hbar} \qquad (1.329)\end{aligned}$$

Using

$$\begin{aligned}&\frac{1}{2M}\boldsymbol{p}^2(t-t') - \boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{x}') \\ &\qquad = \frac{1}{2M}\left(\boldsymbol{p} - M\frac{\boldsymbol{x}-\boldsymbol{x}'}{t-t'}\right)^2 (t-t') - \frac{M(\boldsymbol{x}-\boldsymbol{x}')^2}{2(t-t')} \qquad (1.330)\end{aligned}$$

(1.329) becomes

$$(\boldsymbol{x}\, t \mid \boldsymbol{x}'\, t') = F(t-t')\exp\left(\frac{i}{\hbar}\cdot\frac{1}{2}M\frac{(\boldsymbol{x}-\boldsymbol{x}')^2}{t-t'}\right) \qquad (1.331)$$

where

$$\begin{aligned}F(t-t') &= \int \frac{d^D p}{(2\pi\hbar)^D}\exp\left[-\frac{i}{2M\hbar}\left(\boldsymbol{p} - M\frac{\boldsymbol{x}-\boldsymbol{x}'}{t-t'}\right)^2 (t-t')\right] \\ &= \int \frac{d^D p'}{(2\pi\hbar)^D}\exp\left(-\frac{i}{\hbar}\cdot\frac{\boldsymbol{p}'^2}{2M}(t-t')\right) \qquad (1.332)\end{aligned}$$

Consider now the integral

$$\mathcal{I}(a) = \int_{-\infty}^{\infty} dp\, e^{iap^2} \qquad (1.331a)$$

Setting $i p^2 = -x^2$, we have

$$p = \sqrt{i}\, x$$

$$\mathcal{I} = \sqrt{i}\int_{-\infty}^{\infty} dx\, e^{-ax^2} = \sqrt{\frac{\pi i}{a}} \qquad (1.331b)$$

where use was made of the Gauss formula

$$\mathcal{J}(\alpha) = \int_{-\infty}^{\infty} d\,x\, e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}} \qquad \alpha > 0 \qquad (1.334)$$

(1.331b) can be written as

$$\int_{-\infty}^{\infty} d\,p\, e^{i\,a\,p^2} = \sqrt{\frac{\pi}{|\,a\,|}} \begin{cases} \sqrt{i} & \text{for } a > 0 \\ \frac{1}{\sqrt{i}} & \text{for } a < 0 \end{cases} \qquad (1.333)$$

which is known as the Fresnel integral formula.

Note that $\mathcal{I}(a)$ in (1.331a) can be considered as the analytic continuation of $\mathcal{J}(\alpha)$ in (1.334) with $\alpha \to -i\,a$, i.e., from the real axis to the $\mp$ imaginary axis for $a \gtrless 0$. Indeed, with the help of (1.333), we can relax the criterion $\alpha > 0$ in (1.334) to $\operatorname{Re}\alpha > 0$, as well as the Fresnel case of purely imaginary α.

Repeated differentiation on (1.334) with respect to α gives

$$-\frac{d\,\mathcal{J}(\alpha)}{d\,\alpha} = \int_{-\infty}^{\infty} d\,x\,x^2\, e^{-\alpha x^2} = \frac{1}{2}\sqrt{\frac{\pi}{\alpha^3}}$$

$$(-)^2 \frac{d^2\,\mathcal{J}(\alpha)}{d\,\alpha^2} = \int_{-\infty}^{\infty} d\,x\,x^4\, e^{-\alpha x^2} = \frac{1\cdot 3}{2\cdot 2}\sqrt{\frac{\pi}{\alpha^5}}$$

$$\to \qquad \int_{-\infty}^{\infty} d\,x\,x^{2n}\, e^{-\alpha x^2} = \frac{(2\,n-1)!!}{2^n}\sqrt{\frac{\pi}{\alpha^{2n+1}}} \qquad \operatorname{Re}\alpha > 0 \qquad (1.335)$$

Applying this to (1.332) gives

$$F(t-t') = \left(\frac{M}{2\,\pi\,i\,\hbar\,(t-t')}\right)^{D/2} \qquad (1.336)$$

so that (1.331) becomes

$$(\mathbf{x}\,t \mid \mathbf{x}'\,t') = \left(\frac{M}{2\,\pi\,i\,\hbar\,(t-t')}\right)^{D/2} \exp\left(\frac{i}{\hbar}\cdot\frac{1}{2}\,M\,\frac{(\mathbf{x}-\mathbf{x}')^2}{t-t'}\right) \qquad (1.337)$$

In the limit $t \to t'$, this becomes

$$\delta(\mathbf{x}-\mathbf{x}') = \lim_{t\to t'}\left(\frac{M}{2\,\pi\,i\,\hbar\,(t-t')}\right)^{D/2} \exp\left(\frac{i}{\hbar}\cdot\frac{1}{2}\,M\,\frac{(\mathbf{x}-\mathbf{x}')^2}{t-t'}\right) \qquad (1.338)$$

$$= \lim_{\tau\to 0}\left(\frac{1}{\pi\,\tau}\right)^{D/2} \exp\left(-\frac{(\mathbf{x}-\mathbf{x}')^2}{\tau}\right)$$

where

$$\tau = \frac{2\,i\,\hbar}{M}\,(t-t')$$

Taking the Fourier transform of (1.329) gives the fixed-energy amplitude

$$(\mathbf{x} \mid \mathbf{x}')_E = \int_0^{\infty} d\,(t-t') \int \frac{d^D p}{(2\,\pi\,\hbar)^D} \qquad (1.339)$$

$$\times\, e^{i\,(E+i\,\eta)\,(t-t')/\hbar}\, e^{-i\,\mathbf{p}^2\,(t-t')/2\,M\,\hbar}\, e^{i\,\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')/\hbar}$$

$$= \int \frac{d^D p}{(2\,\pi\,\hbar)^D}\,\frac{i\,\hbar}{E-\frac{\mathbf{p}^2}{2\,M}+i\,\eta}\, e^{i\,\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')/\hbar} \qquad (1.340)$$

Alternatively, one can take the Fourier transform of (1.337) and get

$$(\boldsymbol{x} \mid \boldsymbol{x}')_E = \int_0^\infty d(t-t') \left(\frac{M}{2\pi i \hbar (t-t')} \right)^{D/2} \quad (1.341)$$
$$\times \exp\left[\frac{i}{\hbar}\left((E+i\eta)(t-t') + \frac{1}{2} M \frac{(\boldsymbol{x}-\boldsymbol{x}')^2}{t-t'} \right) \right]$$

This can be evaluated using [see Gradshteyn & Ryzhik, “Table of Integrals, Series, & Products”, Formulas 3.471.10-11, 8.432.6 and 8.421.7, with some change of variables]

$$\int_0^\infty d\,t\, t^{\nu-1}\, e^{-i\gamma t + i\beta/t} = 2\left(\frac{\beta}{\gamma}\right)^{\nu/2} e^{-i\nu\pi/2} K_{-\nu}\left(2\sqrt{\beta\gamma}\right) \quad (1.343)$$

$$\int_0^\infty d\,t\, t^{\nu-1}\, e^{i\gamma t + i\beta/t} = i\pi\left(\frac{\beta}{\gamma}\right)^{\nu/2} e^{-i\nu\pi/2} H^{(1)}_{-\nu}\left(2\sqrt{\beta\gamma}\right) \quad (1.350)$$

where $0 < \mathrm{Re}\,\nu < 1$ and all other coefficients are real and positive. K_ν is the modified Bessel function and $H^{(1)}_\nu$ the Hankel function of the 1st kind.

An easier way to obtain (1.343) & (1.350) is via the following *Mathematica* code :

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Assuming[γ > 0 && β > 0, ∫_0^∞ t^(ν-1) e^(-i γ t + i β / t) dt]

Assuming[γ > 0 && β > 0, ∫_0^∞ t^(ν-1) e^(i γ t + i β / t) dt]
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Setting

$$\tau = t - t' \qquad R = |\,\boldsymbol{x} - \boldsymbol{x}'\,|$$
$$A = \frac{E}{\hbar} \qquad \beta = \frac{M R^2}{2\hbar}$$

(1.341) becomes

$$(\boldsymbol{x} \mid \boldsymbol{x}')_E = \left(\frac{M}{2\pi i \hbar} \right)^{D/2} \int_0^\infty d\tau\, \tau^{-D/2}\, e^{iA\tau + i\beta/\tau} \quad (1.341a)$$

Comparing with (1.343) & (1.350), we have

$$\nu = 1 - \frac{D}{2} = \begin{cases} 1/2 & \text{for } D = 1 \\ 0 & \text{for } D = 2 \\ -1/2 & \text{for } D = 3 \end{cases}$$

Since the integrals (1.343) & (1.350) are defined only for $0 < \mathrm{Re}\,\nu < 1$, the case $D = 3$ requires invoking the technique of analytic continuation..

$E < 0$

For $E < 0$, we set $\gamma = -A$ and use (1.343) to get

$$(\boldsymbol{x} \mid \boldsymbol{x}')_E = \left(\frac{M}{2\pi i \hbar} \right)^{D/2} 2\left(-\frac{\beta}{A}\right)^{(1-D/2)/2} e^{-i(1-D/2)\pi/2} K_{1-D/2}\left(2\sqrt{-\beta A}\right)$$
$$= -2i\left(\frac{1}{\pi\hbar}\right)^{D/2} \left(\sqrt{\frac{M}{2}}\right)^{1+D/2} \left(\frac{R}{\sqrt{-E}}\right)^{1-D/2} K_{1-D/2}\left(\sqrt{-\frac{2MR^2E}{\hbar^2}}\right)$$

where

$$1 - \frac{D}{2} \geq 0 \qquad \text{for} \qquad D \leq 2.$$

and we’ve used [G&R, Formula 8.486.16]

$$K_\nu(z) = K_{-\nu}(z)$$

Setting

$$\kappa = \sqrt{-\frac{2\,M\,E}{\hbar^2}} \tag{1.342}$$

gives

$$(\boldsymbol{x} \mid \boldsymbol{x}')_E = -i\,\frac{M}{\pi\,\hbar}\left(\frac{2\,\pi\,R}{\kappa}\right)^{1-D/2} K_{1-D/2}(\kappa\,R) \tag{1.344}$$

Comment: Kleinert's version of (1.344) is designed for the case $D = 3$.

Of special interest to us are

$$K_{1/2}(z) = K_{-1/2}(z) = \sqrt{\frac{\pi}{2\,z}}\;e^{-z} \tag{1.345}$$

If we assume (1.344) is valid for all D, then

$$(\boldsymbol{x} \mid \boldsymbol{x}')_E = \begin{cases} -i\,\dfrac{M}{\hbar\,\kappa}\,e^{-\kappa\,R} & \text{for } D = 1 \\ -i\,\dfrac{M}{\hbar\,\pi}\,K_0(\kappa\,R) & \text{for } D = 2 \\ -i\,\dfrac{M}{2\,\pi\,\hbar}\,\dfrac{e^{-\kappa\,R}}{R} & \text{for } D = 3 \end{cases} \tag{1.346}$$

Using

$$K_\nu(z) = K_{-\nu}(z) \underset{z\to 0}{\approx} \frac{1}{2}\,\Gamma(\nu)\left(\frac{z}{2}\right)^{-\nu} \qquad \text{for} \qquad \mathrm{Re}\,\nu > 0 \tag{1.347}$$

on (1.344) gives, for $D \le 2$,

$$(\boldsymbol{x} \mid \boldsymbol{x}')_E \approx -i\,\frac{M}{\pi\,\hbar}\left(\frac{2\,\pi\,R}{\kappa}\right)^{1-D/2} \frac{1}{2}\,\Gamma\!\left(1-\frac{D}{2}\right)\left(\frac{\kappa\,R}{2}\right)^{-\left(1-\frac{D}{2}\right)} \qquad \text{for } R \to 0$$
$$= -i\,\frac{2\,M}{\hbar}\,\frac{1}{(4\,\pi)^{D/2}\,\kappa^{2-D}}\,\Gamma\!\left(1-\frac{D}{2}\right) \tag{1.348}$$

Thus, we've shown that $(\boldsymbol{x} \mid \boldsymbol{x}')_E$ is finite at $R = 0$ for $D \le 2$. This result is made applicable to $D > 2$ by the means of analytic continuation.

$E > 0$

For $E > 0$, we set $\gamma = A$ and use (1.350) to get

$$(\boldsymbol{x} \mid \boldsymbol{x}')_E = \left(\frac{M}{2\,\pi\,i\,\hbar}\right)^{D/2} i\,\pi\left(\frac{\beta}{A}\right)^{(1-D/2)/2} e^{-i\,(1-D/2)\,\pi/2}\,H^{(1)}_{-1+D/2}\!\left(2\sqrt{\beta\,A}\right)$$
$$= \pi\left(\frac{1}{\pi\,\hbar}\right)^{D/2}\left(\sqrt{\frac{M}{2}}\right)^{1+D/2}\left(\frac{R}{\sqrt{E}}\right)^{1-D/2} H^{(1)}_{-1+D/2}\!\left(\sqrt{\frac{2\,M\,R^2\,E}{\hbar^2}}\right)$$

Setting

$$k = \sqrt{\frac{2\,M\,E}{\hbar^2}} \tag{1.349}$$

gives

$$(\boldsymbol{x} \mid \boldsymbol{x}')_E = \frac{M}{2\hbar}\left(\frac{2\pi R}{k}\right)^{1-D/2} H^{(1)}_{-1+D/2}(kR) \qquad (1.351)$$

The relation [see G&R, Formula 8.407.1 with $z \to -iz$].

$$K_\nu(-iz) = \frac{\pi}{2}\, i\, e^{i\nu\pi/2} H^{(1)}_\nu(z) \qquad (1.352)$$

connects (1.344) for $E < 0$ with (1.351) for $E > 0$ via $\kappa \leftrightarrow -ik$.

For large distances, we have [see G&R, Formulas 8.451.6 & 8.451.3]

$$K_\nu(z) \approx \sqrt{\frac{\pi}{2z}}\, e^{-z} \qquad H^{(1)}_\nu(z) \approx \sqrt{\frac{2}{\pi z}}\, e^{i(z-\nu\pi/2-\pi/4)} \qquad (1.353)$$

(1.344) thus becomes, for $E < 0$,

$$\begin{aligned}(\boldsymbol{x} \mid \boldsymbol{x}')_E &\approx -i\frac{M}{\pi\hbar}\left(\frac{2\pi R}{\kappa}\right)^{1-D/2}\sqrt{\frac{\pi}{2\kappa R}}\, e^{-\kappa R} \\ &= -i\frac{M}{\hbar\kappa}\left(\frac{\kappa}{2\pi R}\right)^{(D-1)/2} e^{-\kappa R} \qquad (1.354)\end{aligned}$$

Setting $\kappa \leftrightarrow -ik$ gives the result for $E > 0$,

$$(\boldsymbol{x} \mid \boldsymbol{x}')_E \approx \frac{M}{\hbar k}\left(\frac{k}{2\pi i R}\right)^{(D-1)/2} e^{ikR} \qquad (1.355)$$

Comparing (1.345) with (1.353), we see that these asymptotic expressions actually hold for all R if $D = 1$ or 3.