2.6. Free-Particle and Oscillator Wave Functions

The evolution amplitude of a free particle was expressed in (1.331) as a Fourier integral

$$(x_b\, t_b \mid x_a\, t_a) = \int \frac{d\,p}{2\,\pi\,\hbar}\, e^{i\,p\,(x_b - x_a)/\hbar} \exp\left(-\frac{i}{\hbar}\frac{p^2}{2\,M}(t_b - t_a) \right) \tag{2.291}$$

On the other hand, §1.7 showed that for a time-independent Hamiltonian H, the evolution amplitude has a spectral representation

$$(x_b\, t_b \mid x_a\, t_a) = \sum_{n=0}^{\infty} \psi_n(x_b)\, \psi_n^*(x_a) \exp\left(-\frac{i}{\hbar} E_n (t_b - t_a) \right) \tag{2.292}$$

where

$$H\,\psi_n(x) = E_n\,\psi_n(x)$$

For the free particle, the spectrum is continuous so the sum in (2.292) must be replaced by an integral. Comparing (2.291) with (2.292), we have

$$E_n \to E_p = \frac{p^2}{2\,M}$$

$$\sum_n = C \int d\,p \qquad\qquad \psi_n(x) \to \psi_p(x) = C'\, e^{i\,p\,x/\hbar} \tag{2.293a}$$

where C, C' are constants satisfying

$$\frac{C\,\mid C' \mid^2}{2\,\pi\,\hbar} = 1$$

Kleinert's choice was

$$C = 1 \qquad\qquad C' = \frac{1}{\sqrt{2\,\pi\,\hbar}} \qquad\qquad \to \qquad\qquad \psi_p(x) = \frac{1}{\sqrt{2\,\pi\,\hbar}}\, e^{i\,p\,x/\hbar} \tag{2.293}$$

so that

$$\langle p \mid p' \rangle = \int d\,x\, \psi_p^*(x)\, \psi_{p'}(x) \;= \frac{1}{2\,\pi\,\hbar} \int d\,x\, e^{i\,(p' - p)\,x/\hbar} \;= \delta(p - p')$$

For the harmonic oscillator, (2.173) gives

$$(x_b\, t_b \mid x_a\, t_a) = \sqrt{\frac{M\,\omega}{2\,\pi\,i\,\hbar \sin\omega\,(t_b - t_a)}} \tag{2.294}$$

$$\times \exp\left\{ \frac{i}{\hbar} \frac{M\,\omega}{2\,\sin\omega(t_b - t_a)} \left[\left(x_b^2 + x_a^2\right) \cos\omega(t_b - t_a) \; - 2\,x_b\,x_a \right] \right\}$$

The extraction of the wave functions is achieved using a summation formula [see Morse & Feshbach, "Methods of Theoretical Physics", Vol I, p.781] :

$$\frac{1}{\sqrt{1 - a^2}} \exp\left\{ -\frac{1}{2\left(1 - a^2\right)} \left[\left(x^2 + x'^2\right) \left(1 + a^2\right) - 4\,a\,x\,x' \right] \right\} \tag{2.295}$$

$$= \exp\left[-\frac{1}{2}\left(x^2 + x'^2\right) \right] \sum_{n=0}^{\infty} \frac{a^n}{2^n\, n!} H_n(x)\, H_n(x')$$

where $H_n(x)$ are the Hermite polynomials [see Appendix 2C] with

$$H_n(x) = (-)^n\, e^{x^2} \frac{d^n}{d\,x^n} e^{-x^2} \tag{2.296}$$

so that

$$H_0(x) = 1 \qquad H_1(x) = 2\,x \qquad H_2(x) = 4\,x^2 - 2$$

Setting

$$x = C\,x_b \qquad x' = C\,x_a$$

we have

$$-\frac{1+a^2}{1-a^2}\,C^2 = \frac{i}{\hbar}\,M\,\omega\cot\omega(t_b - t_a) \qquad \frac{2\,a}{1-a^2}\,C^2 = -\frac{i}{\hbar}\,\frac{M\,\omega}{\sin\omega(t_b - t_a)} \qquad (2.297a)$$

$$\rightarrow \qquad \frac{2\,a}{1+a^2} = \frac{1}{\cos\omega(t_b - t_a)}$$

i.e., $a^2 - 2\,a\cos\omega(t_b - t_a) + 1 = 0$

$$\therefore \qquad a = \cos\omega(t_b - t_a) \pm \sqrt{\cos^2\omega(t_b - t_a) - 1} = e^{\pm i\,\omega\,(t_b - t_a)}$$

$$\rightarrow \qquad \frac{1+a^2}{1-a^2} = \frac{1+e^{\pm 2\,i\,\omega\,(t_b-t_a)}}{1-e^{\pm 2\,i\,\omega\,(t_b-t_a)}} = \frac{e^{\mp\,i\,\omega\,(t_b-t_a)} + e^{\pm\,i\,\omega\,(t_b-t_a)}}{e^{\mp\,i\,\omega\,(t_b-t_a)} - e^{\pm\,i\,\omega\,(t_b-t_a)}} = \frac{\cos\omega(t_b - t_a)}{\mp\,i\sin\omega(t_b - t_a)}$$

$$\frac{a}{1-a^2} = \frac{e^{\pm i\,\omega\,(t_b-t_a)}}{1-e^{\pm 2\,i\,\omega\,(t_b-t_a)}} = \frac{1}{e^{\mp\,i\,\omega\,(t_b-t_a)} - e^{\pm\,i\,\omega\,(t_b-t_a)}} = \frac{1}{\mp\,2\,i\sin\omega(t_b - t_a)}$$

$$C^2 = -\frac{1-a^2}{2\,a}\,\frac{i}{\hbar}\,\frac{M\,\omega}{\sin\omega(t_b - t_a)} = \mp\,\frac{M\,\omega}{\hbar}$$

Setting C to be real, we must choose the lower sign so that

$$x = \sqrt{\frac{M\,\omega}{\hbar}}\;x_b \qquad x' = \sqrt{\frac{M\,\omega}{\hbar}}\;x_a \qquad a = e^{-i\,\omega\,(t_b-t_a)} \qquad (2.297)$$

$$1 - a^2 = 2\,a\,i\sin\omega(t_b - t_a) = 2\,i\,e^{-i\,\omega\,(t_b-t_a)}\sin\omega(t_b - t_a)$$

(2.294) then becomes

$$(x_b\,t_b \mid x_a\,t_a) = \sqrt{\frac{M\,\omega}{\pi\,\hbar}}\;e^{-i\,\omega\,(t_b-t_a)/2}\exp\left[-\frac{1}{2}\,\frac{M\,\omega}{\hbar}\,(x_b^2 + x_a^2)\right]$$

$$\times\sum_{n=0}^{\infty}\frac{e^{-i\,n\,\omega\,(t_b-t_a)}}{2^n\,n!}\,H_n\!\left(\sqrt{\frac{M\,\omega}{\hbar}}\;x_b\right)H_n\!\left(\sqrt{\frac{M\,\omega}{\hbar}}\;x_a\right)$$

Setting

$$\lambda_\omega = \sqrt{\frac{\hbar}{M\,\omega}} \qquad (2.301)$$

we have

$$(x_b\,t_b \mid x_a\,t_a) = \frac{1}{\sqrt{\pi}\;\lambda_\omega}\exp\left[-\frac{1}{2\,\lambda_\omega^2}\,(x_b^2 + x_a^2)\right]$$

$$\times\sum_{n=0}^{\infty}\frac{e^{-i\,(n+1/2)\,\omega\,(t_b-t_a)}}{2^n\,n!}\,H_n\!\left(\frac{x_b}{\lambda_\omega}\right)H_n\!\left(\frac{x_a}{\lambda_\omega}\right)$$

$$= \sum_{n=0}^{\infty}\psi_n(x_b)\,\psi_n(x_a)\,e^{-i\,(n+1/2)\,\omega\,(t_b-t_a)} \qquad (2.298)$$

where

$$\psi_n(x) = \frac{1}{\sqrt{\sqrt{\pi}\ \lambda_\omega\, 2^n\, n!}} \exp\left(-\frac{1}{2\,\lambda_\omega^2}\, x^2\right) H_n\left(\frac{x}{\lambda_\omega}\right)$$
$$= N_n\, \frac{1}{\sqrt{\lambda_\omega}} \exp\left(-\frac{1}{2\,\lambda_\omega^2}\, x^2\right) H_n\left(\frac{x}{\lambda_\omega}\right) \qquad (2.300)$$

with

$$N_n = \frac{1}{\sqrt{\sqrt{\pi}\ 2^n\, n!}} \qquad (2.302)$$

Using the orthogonality of the Hermite polynomials [see Gradshteyn & Ryzhik, Formula 7.374.1]

$$\frac{1}{\sqrt{\pi}\ 2^n\, n!} \int_{-\infty}^{\infty} d\,x\, e^{-x^2}\, H_n(x)\, H_m(x) = \delta_{n\,m} \qquad (2.304)$$

we see that ψ_n are orthonormal:

$$\int_{-\infty}^{\infty} d\,x\, \psi_n^*(x)\, \psi_m(x) = \delta_{n\,m} \qquad (2.204)$$