CHAPTER I

PROPAGATOR METHODS

I.1 BASIC QUANTUM MECHANICS

The fundamental problem of quantum mechanics is to determine the time development of quantum states. That is, given a state vector $|\psi(0)\rangle$ at time $t = 0$, what is the state at a later time $t - |\psi(t)\rangle$? The answer is provided by the Schrödinger equation

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \tag{1.1}$$

where $\hat{H}$ is the Hamiltonian operator. Usually one sees this equation expressed in terms of the coordinate space projection of the state vector — *i.e.* the wavefunction $\psi(x,t)$ where†

$$\psi(x,t) \equiv \langle x|\psi(t)\rangle \quad . \tag{1.2}$$

The time-evolution of the wavefunction is then given by

$$i\frac{\partial}{\partial t}\langle x|\psi(t)\rangle = \left\langle x \left| \hat{H} \right| \psi(t) \right\rangle \quad . \tag{1.3}$$

In order to evaluate the matrix element on the right we can insert a complete set of co-ordinate states

$$\mathbf{1} = \int_{-\infty}^{\infty} dx' \, |x'\rangle\langle x'| \tag{1.4}$$

yielding

$$i\frac{\partial}{\partial t}\langle x|\psi(t)\rangle = \int_{-\infty}^{\infty} dx' \left\langle x \left| \hat{H} \right| x' \right\rangle \langle x'|\psi(t)\rangle \quad . \tag{1.5}$$

Finally we need to interpret the operator matrix element $\left\langle x|\hat{H}|x' \right\rangle$. In general, the Hamiltonian $\hat{H}$ can be written in terms of kinetic and potential energy components as

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \quad . \tag{1.6}$$

Here $\hat{x}|x >= x|x >$ with $< x|x' >= \delta(x - x')$ so

$$\langle x \left| V(\hat{x}) \right| x' \rangle = V(x) \langle x|x' \rangle = V(x)\delta(x - x') \quad . \tag{1.7}$$

In order to represent the kinetic energy piece we can insert a complete set of momentum states such that $\hat{p}|p >= p|p >$ with $< p|p' >= 2\pi\delta(p - p')$. Then

$$\mathbf{1} = \int_{-\infty}^{\infty} \frac{dp}{2\pi}|p\rangle\langle p| \tag{1.8}$$

† For simplicity of notation, we shall work here in one dimension. However, generalization to three dimensions is obvious.

yielding

$$\left\langle x \left| \frac{\hat{p}^2}{2m} \right| x' \right\rangle = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \langle x|p\rangle \frac{p^2}{2m} \langle p|x'\rangle \quad . \tag{1.9}$$

Since $\langle x|p\rangle$ is simply a plane wave

$$\langle x|p\rangle = e^{ipx} \tag{1.10}$$

we have

$$\begin{aligned} \left\langle x \left| \frac{\hat{p}^2}{2m} \right| x' \right\rangle &= \int_{-\infty}^{\infty} \frac{dp}{2\pi} \frac{p^2}{2m} e^{ip(x-x')} \\ &= -\frac{1}{2m} \frac{\partial^2}{\partial x^2} \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ip(x-x')} \\ &= -\frac{1}{2m} \frac{\partial^2}{\partial x^2} \delta(x-x') \quad . \end{aligned} \tag{1.11}$$

Substitution back into Eq. 1.3 yields

$$\begin{aligned} & i\frac{\partial}{\partial t} \langle x|\psi(t)\rangle = i\frac{\partial}{\partial t}\psi(x,t) \\ & = \left(-\frac{1}{2m} \frac{\partial^2}{\partial x^2} + V(x)\right) \int_{-\infty}^{\infty} dx' \, \delta(x-x') \langle x'|\psi(t)\rangle \\ & = H(x)\psi(x,t) \end{aligned} \tag{1.12}$$

which is the usual version of the Schrödinger equation, where

$$H(x) = -\frac{1}{2m} \frac{\partial^2}{\partial x^2} + V(x) \tag{1.13}$$

provides the representation of the operator $\hat{H}$ in coordinate space. For a free particle this reduces to the simple form

$$H_0(x) = -\frac{1}{2m} \frac{\partial^2}{\partial x^2} \quad . \tag{1.14}$$

Time Development Operator

An alternative formulation of this problem is in terms of the time development operator $\hat{U}(t,t')$ defined via

$$\hat{U}(t,t')|\psi(t')\rangle = \begin{cases} |\psi(t)\rangle & t \geq t' \\ 0 & t < t' \end{cases} \tag{1.15}$$

with the boundary condition

$$\lim_{t \to t'^+} \hat{U}(t,t') = \mathbf{1} \quad . \tag{1.16}$$

For the case of a free particle, obeying

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}_0|\psi(t)\rangle \tag{1.17}$$

the solution for $\hat{U}^{(0)}(t,0)$ is

$$\hat{U}^{(0)}(t,0) = \theta(t) \exp\left(-i\hat{H}_0 t\right) \quad , \tag{1.18}$$

where

$$\theta(t) = \begin{cases} 1 & t > 0 \\ 0 & t < 0 \end{cases} \tag{1.19}$$

is the usual theta function. For example, if

$$\psi(x,0) = \frac{1}{(2\pi\sigma^2)^{1/4}} \exp\left(-\frac{(x-a)^2}{4\sigma^2}\right) \tag{1.20}$$

we find

$$\begin{aligned} \psi(x,t) &=< x|\hat{U}^{(0)}(t,0)|\psi(0) >= \int_{-\infty}^{\infty} dx' < x|\hat{U}^{(0)}(t,0)|x' >< x'|\psi(0) > \\ &= e^{-iH_0(x)t}\psi(x,0) = e^{-iH_0(x)t}\frac{1}{(2\pi\sigma^2)^{1/4}} \exp\left(-\frac{(x-a)^2}{4\sigma^2}\right) \\ &= \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{it}{2m}\right)^n \frac{\partial^{2n}}{\partial x^{2n}} \exp\left(-\frac{(x-a)^2}{4\sigma^2}\right) \frac{1}{(2\pi\sigma^2)^{1/4}} \quad . \end{aligned} \tag{1.21}$$

Although one could straightforwardly evaluate this power series, it is easier to note the identity [Bl 68]

$$\frac{\partial^2}{\partial x^2}\frac{1}{\sqrt{\rho}} \exp\left(-\frac{(x-a)^2}{4\rho}\right) = \frac{\partial}{\partial \rho}\ \frac{1}{\sqrt{\rho}} \exp\left(-\frac{(x-a)^2}{4\rho}\right) \quad . \tag{1.22}$$

Then using

$$\exp\left(\alpha\frac{\partial}{\partial z}\right) f(z) = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!}\ \frac{\partial^n}{\partial z^n} f(z) = f(z+\alpha) \tag{1.23}$$

we find

$$\psi(x,t) = \left(\frac{\sigma^2}{2\pi}\right)^{1/4} \frac{1}{\left(\sigma^2 + i\frac{t}{2m}\right)^{1/2}} \exp\left(-\frac{(x-a)^2}{4\left(\sigma^2 + i\frac{t}{2m}\right)}\right) \quad . \tag{1.24}$$

We note that

$$|\psi(x,t)|^2 = \frac{1}{\sqrt{2\pi}\,\sigma(t)} \exp\left(-\frac{(x-a)^2}{2\sigma^2(t)}\right) \quad \text{with} \quad \sigma(t) = \left(\sigma^2 + \frac{t^2}{4m^2\sigma^2}\right)^{1/2} \tag{1.25}$$

which obviously exhibits the canonical spreading experienced by such a wavepacket.

We can equivalently perform the above calculation in momentum space, where the time development operator has the simple form

$$\left\langle p \left| \hat{U}^{(0)}(t,t') \right| p' \right\rangle =< p| \exp(-i\hat{p}^2(t-t')/2m)|p' > \theta(t-t')$$

$$= \exp -i\frac{p^2}{2m}(t-t') < p|p' > \theta(t-t') = \exp -i\frac{p^2}{2m}(t-t')2\pi\delta(p-p')\theta(t-t') \ . \quad (1.26)$$

If

$$\langle x|\psi(0)\rangle = \frac{1}{(2\pi\sigma^2)^{1/4}} \exp\left(-\frac{(x-a)^2}{4\sigma^2}\right) \quad (1.27)$$

we have

$$\begin{aligned}\langle p|\psi(0)\rangle &= \int_{-\infty}^{\infty} dx \ \langle p|x\rangle \langle x|\psi(0)\rangle \\ &= \int_{-\infty}^{\infty} dx \, e^{-ipx} \frac{1}{(2\pi\sigma^2)^{1/4}} \exp\left(-\frac{(x-a)^2}{4\sigma^2}\right) \\ &= \left(8\pi\sigma^2\right)^{1/4} \exp\left(-\sigma^2 p^2\right) \exp\left(-ipa\right) \quad .\end{aligned} \quad (1.28)$$

Then

$$\begin{aligned}\langle p|\psi(t)\rangle &= \int_{-\infty}^{\infty} \frac{dp'}{2\pi} < p|\hat{U}^{(0)}(t,0)|p' >< p'|\psi(0) > \\ &= \left(8\pi\sigma^2\right)^{1/4} \exp\left(-\sigma^2 p^2 - ipa - i\frac{p^2}{2m}t\right)\theta(t) \quad .\end{aligned} \quad (1.29)$$

We can return to coordinate space via

$$\begin{aligned}\langle x|\psi(t)\rangle &= \int_{-\infty}^{\infty} \frac{dp}{2\pi} \langle x|p\rangle \langle p|\psi(t)\rangle \\ &= \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ipx} \left(8\pi\sigma^2\right)^{1/4} \exp\left(-\sigma^2 p^2 - ipa - i\frac{p^2}{2m}t\right)\theta(t) \\ &= \left(\frac{\sigma^2}{2\pi}\right)^{1/4} \frac{1}{\left(\sigma^2 + i\frac{t}{2m}\right)^{1/2}} \exp -\frac{(x-a)^2}{4\left(\sigma^2 + i\frac{t}{2m}\right)}\theta(t)\end{aligned} \quad (1.30)$$

which agrees precisely with Eq. 1.24 found via coordinate space methods.

I.2 THE PROPAGATOR

One can evaluate the co-ordinate space matrix element of the time development operator by transforming to momentum space and back again.

$$\begin{aligned}D_F^{(0)}(x',t;x,0) &\equiv < x'|\hat{U}^{(0)}(t,0)|x >= \left\langle x' \left| e^{-i\hat{H}_0 t} \right| x \right\rangle \theta(t) \\ &= \theta(t) \int_{-\infty}^{\infty} \frac{dp}{2\pi} \langle x'|p\rangle \, e^{-i\frac{p^2}{2m}t} \langle p|x\rangle = \theta(t) \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ip(x'-x) - i\frac{p^2}{2m}t} \\ &= \theta(t)\sqrt{\frac{m}{2\pi i t}} \exp i\frac{m(x'-x)^2}{2t} \ .\end{aligned} \quad (2.1)$$

D_F is usually called the "propagator," as it gives the amplitude for a particle produced at position x at time 0 to "propagate" to position x' at time t.

Just as a check we can verify that this form of the propagator does indeed generate the time development of the freely moving Gaussian wavefunction

$$\begin{aligned}\psi(x',t) &= \int_{-\infty}^{\infty} dx\, D_F^{(0)}(x',t;x,0)\psi(x,0) \\ &= \int_{-\infty}^{\infty} dx \sqrt{\frac{m}{2\pi i t}} \exp \frac{im(x'-x)^2}{2t} \frac{1}{(2\pi\sigma^2)^{1/4}} \exp\left(-\frac{(x-a)^2}{4\sigma^2}\right) \\ &= \left(\frac{\sigma^2}{2\pi}\right)^{1/4} \exp\left(-\frac{(x'-a)^2}{4\left(\sigma^2+i\frac{t}{2m}\right)}\right) \frac{1}{\left(\sigma^2+i\frac{t}{2m}\right)^{1/2}}\end{aligned} \tag{2.2}$$

in complete agreement with expression derived in sect. I.1.

Path Integrals and the Propagator

Before going further, it is useful to note an alternative way by which the propagator can be calculated—the Feynman path integral [FeH 65]

$$D_F(x',t;x,0) = \int \mathcal{D}\left[x(t)\right] \exp \frac{iS\left[x(t)\right]}{\hbar} \tag{2.3}$$

where the notation is that the integral represents a sum over *all* paths $x(t)$ connecting the initial and final spacetime points — $x, 0$ and x', t respectively. For each path there is a weighting factor given by $\exp \frac{iS}{\hbar}$ where $S = \int dt L[x(t)]$ is the classical action associated with that path. The path integration can be carried out by dividing the time interval $0 - t$ into n slices of width ϵ. This provides a set of times t_i spaced a distance ϵ apart between the values 0 and t. At each time t_i we select a point x_i. A path is constructed by connecting all possible x_i points so selected by straight lines as shown in Figure I.1 and the path integral is written (setting $\hbar = 1$) as

$$D_F(x',t;x,0) = \lim_{n\to\infty} \frac{1}{A^n} \prod_{i=1}^{n-1} \left(\int_{-\infty}^{\infty} dx_i\right) \exp iS^{(0)} \tag{2.4}$$

where A is a normalization constant which defines the measure— note that there is one factor of A for each straight line segment. In the limit as $\epsilon \to 0$ we can evaluate the action for each line segment in the infinitesimal approximation. For the free particle we have

$$\begin{aligned}S^{(0)} &= \int_0^t dt' L\left(x(t'), \dot{x}(t'), t'\right) = \int_0^t dt' \frac{1}{2} m \dot{x}^2(t') \\ &= \sum_{i=1}^{n} \frac{1}{2} m \frac{(x_i - x_{i-1})^2}{\epsilon} \quad \text{with} \quad x_0 = x \quad \text{and} \quad x_n = x'\end{aligned}$$

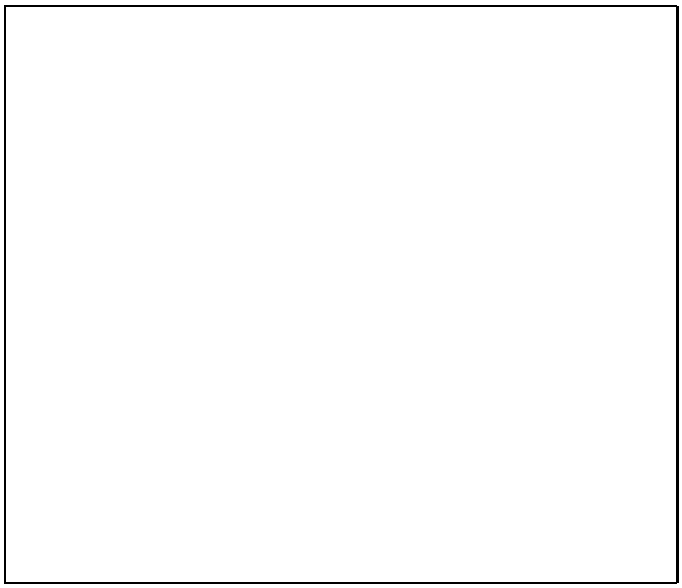

Fig. I.1: A particular time slice used in calculation of the propagator.

The integrations may be performed sequentially

$$\begin{aligned}
&\int_{-\infty}^{\infty} dx_1 \exp i\frac{m}{2\epsilon}\left((x_1-x_0)^2+(x_2-x_1)^2\right) = \sqrt{\frac{2\pi i\epsilon}{2m}}\exp i\frac{m}{2\cdot 2\epsilon}(x_2-x_0)^2 \\
&\int_{-\infty}^{\infty} dx_2 \exp i\frac{m}{2\epsilon}\left(\frac{1}{2}(x_2-x_0)^2+(x_3-x_2)^2\right) = \sqrt{\frac{2\pi i\epsilon\cdot 2}{3m}}\exp i\frac{m}{3\cdot 2\epsilon}(x_3-x_0)^2 \\
&\quad\vdots \\
&\int_{-\infty}^{\infty} dx_{n-1} \exp i\frac{m}{2\epsilon}\left(\frac{1}{n-1}(x_{n-1}-x_0)^2+(x_n-x_{n-1})^2\right) \\
&\quad = \sqrt{\frac{2\pi i\epsilon(n-1)}{nm}}\exp i\frac{m}{n\cdot 2\epsilon}(x_n-x_0)^2
\end{aligned} \tag{2.5}$$

yielding

$$D_F^{(0)}(x',t;x,0) = \left(\frac{2\pi i\epsilon}{m}\right)^{(n-1)/2}\frac{1}{A^n}\,\frac{1}{\sqrt{n}}\exp i\frac{m}{2n\epsilon}(x'-x)^2 \tag{2.6}$$

The constant A may be determined by use of the completeness condition

$$\begin{aligned}
\psi(x',t) &= \int_{-\infty}^{\infty} dx < x'|\hat{U}^{(0)}(t,0)|x >< x|\psi(0) > \\
&= \int_{-\infty}^{\infty} dx D_F^{(0)}(x',t;x,0)\psi(x,0) \quad .
\end{aligned} \tag{2.7}$$

If we pick $t = \epsilon <<< 1$ then

$$\psi(x', \epsilon) \cong \int_{-\infty}^{\infty} dx \frac{1}{A} \exp i \frac{m(x'-x)^2}{2\epsilon} \psi(x, 0) + \dots \quad . \tag{2.8}$$

Since ϵ is small, the exponential will rapidly oscillate and thereby wash out the integral unless $x \cong x'$. Thus, we can write

$$\begin{aligned} \psi(x', \epsilon) &\cong \psi(x', 0) \frac{1}{A} \int_{-\infty}^{\infty} dx \ \exp i \frac{m(x'-x)^2}{2\epsilon} + \dots \\ &= \psi(x', 0) \frac{1}{A} \sqrt{\frac{2\pi i \epsilon}{m}} + \dots \quad . \end{aligned} \tag{2.9}$$

Hence in order to have the correct behavior as $\epsilon \to 0$ we must pick

$$A = \sqrt{\frac{2\pi i \epsilon}{m}} \tag{2.10}$$

so that the free propagator becomes, using $t = n\epsilon$

$$D_F^{(0)}(x', t; x, 0) = \sqrt{\frac{m}{2\pi i n \epsilon}} \exp \frac{im}{2n\epsilon} (x'-x)^2 = \sqrt{\frac{m}{2\pi i t}} \exp \frac{im(x'-x)^2}{2t} \tag{2.11}$$

in complete agreement with the expression derived via more conventional means (*cf.* Eq. 2.1).

The reason that the propagator can be written as a path integral can be understood by using the completeness relation

$$\mathbf{1} = \int_{-\infty}^{\infty} dx_i \ |x_i\rangle\langle x_i| \quad . \tag{2.12}$$

For later use, we shall give the derivation here for the general case involving interaction with a potential $V(\hat{x})$. Starting with the definition

$$D_F(x_f, t_f; x_i, t_i) = \left\langle x_f \left| \exp -i\hat{H}(t_f - t_i) \right| x_i \right\rangle \theta(t_f - t_i) \tag{2.13}$$

and breaking the time interval $t_f - t_i$ (assumed to be positive) into n discrete steps of size

$$\epsilon = \frac{t_f - t_i}{n} \tag{2.14}$$

we can write

$$\begin{aligned} D_F(x_f, t_f; x_i, t_i) = \int_{-\infty}^{\infty} dx_1 \dots dx_{n-1} \left\langle x_n \left| e^{-i\epsilon\hat{H}} \right| x_{n-1} \right\rangle \\ \cdot \left\langle x_{n-1} \left| e^{-i\epsilon\hat{H}} \right| x_{n-2} \right\rangle \dots \left\langle x_1 \left| e^{-i\epsilon\hat{H}} \right| x_0 \right\rangle \quad . \end{aligned} \tag{2.15}$$

In the limit of large n the time slices become infinitesimal and

$$\begin{aligned}\left\langle x_\ell \left| e^{-i\epsilon\hat{H}} \right| x_{\ell-1} \right\rangle &= \left\langle x_\ell \left| \exp -i\epsilon \left(\frac{\hat{p}^2}{2m} + V(\hat{x}) \right) \right| x_{\ell-1} \right\rangle \\ &\approx \exp -i\epsilon V(x_\ell) \left\langle x_\ell \left| e^{-i\epsilon\frac{\hat{p}^2}{2m}} \right| x_{\ell-1} \right\rangle + \mathcal{O}(\epsilon^2) \quad .\end{aligned} \tag{2.16}$$

Introducing a complete set of momentum states, we have

$$\begin{aligned}\left\langle x_\ell \left| e^{-i\epsilon\frac{\hat{p}^2}{2m}} \right| x_{\ell-1} \right\rangle &= \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ip(x_\ell - x_{\ell-1})} e^{-i\epsilon\frac{p^2}{2m}} \\ &= \sqrt{\frac{m}{2\pi i\epsilon}} \exp i\frac{m}{2\epsilon}(x_\ell - x_{\ell-1})^2\end{aligned} \tag{2.17}$$

and, taking the continuum limit, we find the path integral prescription

$$\begin{aligned}D_F(x_f, t_f; x_i, t_i) &= \lim_{n\to\infty} \left(\frac{m}{2\pi i\epsilon}\right)^{\frac{n}{2}} \int_{-\infty}^{\infty} dx_{n-1} \ldots dx_1 \\ &\quad \times \exp i \sum_{\ell=1}^{n} \left(m\frac{(x_\ell - x_{\ell-1})^2}{2\epsilon} - \epsilon V(x_\ell) \right) \\ &= \int \mathcal{D}[x(t)] \exp iS[x(t)]\end{aligned} \tag{2.18}$$

where

$$S[(t)] = \int_{t_1}^{t_2} dt \left(\frac{1}{2} m\dot{x}^2(t) - V(x(t)) \right) \tag{2.19}$$

is the classical action.

Classical Connection

Perhaps the most peculiar and fascinating aspect of this prescription is that *all* paths connecting the spacetime endpoints must be included in the summation. This appears to be in total contradiction with the classical mechanics result that a particle traverses a well-defined trajectory. The resolution of this apparent paradox may be found by explicitly restoring the dependence on $\hbar$ and noting that the path integral prescription is given by

$$\sum_{x(t)} \exp iS[x(t)]/\hbar \tag{2.20}$$

Classical physics results as $\hbar \to 0$, and in this limit a slight change in the path $x(t)$ produces a huge change in phase and hence little or no contribution to the path summation except for trajectories $\bar{x}(t)$ for which the action is stationary—*i.e.*, Hamilton's principle

$$\left. \frac{\delta S[x(t)]}{\delta x} \right|_{x(t)=\bar{x}(t)} = 0 \quad . \tag{2.21}$$

In order to find such a path we take

$$0 = S\left[\bar{x}(t) + \delta x(t)\right] - S\left[\bar{x}(t)\right]$$

$$= \int_0^t dt' \left[\frac{m}{2}\left(\dot{\bar{x}}(t') + \delta\dot{x}(t')\right)^2 - \frac{m}{2}(\dot{\bar{x}}(t'))^2 - V(\bar{x}(t') + \delta x(t')) + V(\bar{x}(t'))\right]$$

$$= \int_0^t dt' \left(m\dot{\bar{x}}(t')\delta\dot{x}(t') - V'(\bar{x}(t'))\delta x(t')\right) + \mathcal{O}((\delta x)^2) \quad . \tag{2.22}$$

integrate by parts and use the feature that the endpoints of the path are fixed, *i.e.*, $\delta x(0) = \delta x(t) = 0$. Then

$$0 = -\int_0^t dt'(m\ddot{\bar{x}}(t') + V'(\bar{x}(t')))\delta x(t') \quad . \tag{2.23}$$

so that the trajectory which satisfies the stationary phase condition for arbitrary $\delta x(t')$ must obey

$$m\ddot{\bar{x}} + V'(\bar{x}) = 0 \tag{2.24}$$

which is just the classical mechanics prescription for the motion of a freely moving particle, *i.e.*, $\bar{x}(t) = x_{\rm cl}(t)$. In the limit $\hbar \to 0$ the classical trajectory represents the *only* path contributing to the path integral and the paradox is resolved.

One can also get a feel for the meaning of the propagator by noting that since

$$\begin{aligned}\langle x|\psi(t)\rangle &= \left\langle x \left| e^{-i\hat{H}_0 t} \right| \psi(0)\right\rangle = \int_{-\infty}^{\infty} dx' \left\langle x \left| e^{-i\hat{H}_o t} \right| x'\right\rangle \langle x'|\psi(0)\rangle \\ &= \int_{-\infty}^{\infty} dx'\, D_F^{(0)}(x,t;x',0)\, \langle x'|\psi(0)\rangle\end{aligned} \quad . \tag{2.25}$$

if we take

$$\langle x'|\psi(0)\rangle = \delta(x') \tag{2.26}$$

so that at $t = 0$ the particle is located precisely at the origin, then

$$D_F^{(0)}(x,t;0,0) = \sqrt{\frac{m}{2\pi i t}} \exp\frac{imx^2}{2t} = \langle x|\psi(t)\rangle \quad . \tag{2.27}$$

That is to say, $D_F^{(0)}(x,t;0,0)$ is just the Schrödinger wavefunction of a freely moving particle which started at the origin at time zero. If we look at a specific location x_0, t_0 we would say classically that if a particle is observed at this point then it must have momentum

$$p_{\rm cl} = mv_0 = m\frac{x_0}{t_0} \tag{2.28}$$

and energy

$$E_{\rm cl} = \frac{1}{2}mv_0^2 = \frac{1}{2}m\frac{x_0^2}{t_0^2} \quad . \tag{2.29}$$

Examining the variation of the phase of the wavefunction in the vicinity of x_0, t_0, we find

$$\begin{aligned}\langle x|\psi(t)\rangle &= \sqrt{\frac{m}{2\pi i t}}\exp i\frac{mx^2}{2t} \\ &= \sqrt{\frac{m}{2\pi i t}}\exp i\frac{m}{2}\left(\frac{x_0^2}{t_0} + (x-x_0)\frac{\partial}{\partial x}\left.\frac{x^2}{t}\right|_{x=x_0} + (t-t_0)\frac{\partial}{\partial t}\left.\frac{x^2}{t}\right|_{t=t_0} + \ldots\right) \\ &= \sqrt{\frac{m}{2\pi i t}}\exp i\frac{m}{2}\left(\frac{x_0^2}{t_0} + 2\frac{x_0}{t_0}(x-x_0) - \frac{x_0^2}{t_0^2}(t-t_0) + \ldots\right) \quad .\end{aligned} \tag{2.30}$$

Thus in the vicinity of this point we can write

$$\langle x|\psi(t)\rangle \approx \sqrt{\frac{m}{2\pi i t}}\exp\left(ip_{\rm cl}x - iE_{\rm cl}t\right) \tag{2.31}$$

so that both the wavelength associated with the particle

$$\lambda = \frac{2\pi}{p_{\rm cl}} \tag{2.32}$$

and the corresponding frequency

$$\nu = \frac{E_{\rm cl}}{2\pi} \tag{2.33}$$

are given by the usual quantum mechanical relations.

Finally, the probability that the particle is located between x and $x + dx$ at time t is

$$P(x, x+dx) = |<x|\psi(t)>|^2 dx = \frac{m\,dx}{2\pi t} \tag{2.34}$$

and is independent of x. All momenta then are equally likely at $t = 0$, as would be expected from the momentum space representation of the co-ordinate space wavefunction

$$\delta(x) = \int \frac{dp}{2\pi} e^{ipx} \tag{2.35}$$

and the momentum density is $\frac{dp}{2\pi}$ with $dp = \frac{m dx}{t}$. We conclude that all our intuitive notions are satisfied by the propagator, Eq. 2.27.

Frequency Space Representation

Before moving on to the more interesting case of motion in the presence of a potential, it is important to note that the time development operator is often used in Fourier transform or frequency space form rather than in its time representation. Before examining this result, however, it is useful to prove a simple mathematical identity. Consider the integral

$$I(a) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \frac{i}{\omega - a + i\epsilon} \quad . \tag{2.36}$$

If $t > 0$ the contour can be closed in the lower half plane by means of a large semicircle (*cf.* Figure I.2)

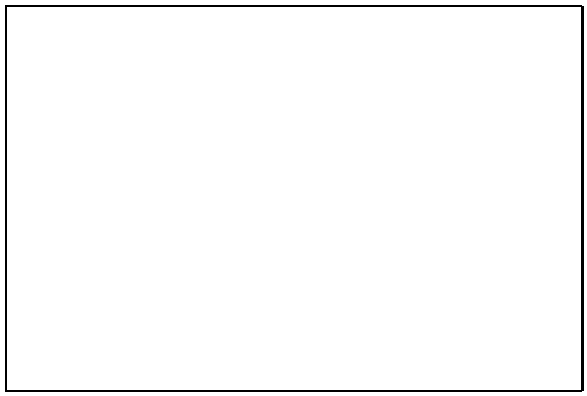

Fig. I.2: When $t > 0$ the contour is closed by means of a large semicircle in the lower half plane.

which contributes nothing to the integral because of the exponential damping introduced by the factor $e^{-(\mathrm{Im}\omega)t}$. The integral can then be evaluated by means of the residue theorem [MaW 64]. There exists a single pole at $\omega = a - i\epsilon$ and the integral is found to be

$$I(a) = -2\pi i \times \frac{i}{2\pi} e^{-iat} = e^{-iat} \qquad t > 0 \quad . \tag{2.37}$$

On the other hand, if $t < 0$ exponential damping of the semicircular contribution demands that we close the contour in the upper half plane. In this case there is no singularity so

$$I(a) = 0 \qquad t < 0 \quad . \tag{2.38}$$

We have in general then

$$I(a) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \frac{i}{\omega - a + i\epsilon} = \theta(t) e^{-iat} \quad , \tag{2.39}$$

so that, replacing a by the operator $\hat{H}_0$, an alternative way to represent the free time development operator is

$$\hat{U}^{(0)}(t,0) = e^{-i\hat{H}_o t}\theta(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \frac{i}{\omega - \hat{H}_0 + i\epsilon} \tag{2.40}$$

i.e., $\hat{U}^{(0)}(t,0)$ can be written as a Fourier transform with

$$\hat{U}^{(0)}(\omega) = \frac{i}{\omega - \hat{H}_0 + i\epsilon} \quad . \tag{2.41}$$

Other Representations

It is often useful to represent $\hat{U}^{(0)}(\omega)$ in terms either of its momentum space

$$\left\langle p \left| \hat{U}^{(0)}(\omega) \right| p' \right\rangle = 2\pi\delta(p - p') \frac{i}{\omega - \frac{p^2}{2m} + i\epsilon} \tag{2.42}$$

or coordinate space matrix elements

$$\left\langle x \left| \hat{U}^{(0)}(\omega) \right| x' \right\rangle = \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ip(x-x')} \frac{i}{\omega - \frac{p^2}{2m} + i\epsilon} \quad . \tag{2.43}$$

Defining

$$\omega = \frac{p_0^2}{2m} \tag{2.44}$$

we can explicitly evaluate the latter

$$\begin{aligned} < x|\hat{U}^{(0)}(\omega)|x' > &= \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ip(x-x')} \frac{i}{\omega - \frac{p^2}{2m} + i\epsilon} \\ &= -\int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ip(x-x')} \frac{2mi}{p^2 - p_0^2 - i\epsilon} \\ &= -2m \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ip(x-x')} \frac{i}{(p - p_0 - i\epsilon)(p + p_0 + i\epsilon)} \quad . \end{aligned} \tag{2.45}$$

If $x - x' > 0$ we close the contour in the upper half plane and pick up the pole at $p_0 + i\epsilon$, yielding

$$< x|\hat{U}^{(0)}(\omega)|x' >= 2\pi i \times \frac{-2mi}{2\pi} \times \frac{1}{2p_0} e^{ip_0(x-x')} = \frac{m}{p_0} e^{ip_0(x-x')} \quad , \tag{2.46}$$

while if $x - x' < 0$ we must close the contour in the lower half plane and pick up the pole at $-p_0 - i\epsilon$, yielding

$$< x|\hat{U}^{(0)}(\omega)x' >= -2\pi i \times \frac{-2mi}{2\pi} \times \frac{1}{-2p_0} e^{-ip_o(x-x')} = \frac{m}{p_0} e^{-ip_0(x-x')} \quad . \tag{2.47}$$

The general result can be written as

$$< x|\hat{U}^{(0)}(\omega)|x' >= \frac{m}{p_0} e^{ip_0|x-x'|} \tag{2.48}$$

and will be useful later.

I.3 HARMONIC OSCILLATOR PROPAGATOR

Having examined the form of the free propagator in the previous section, we now consider motion under the influence of a potential $V(\hat{x})$. In this case the time development operator becomes (hereafter assuming $t > 0$)

$$\hat{U}(t,0) = e^{-i\hat{H}t} = e^{-i(\hat{H}_0 + V(\hat{x}))t} \tag{3.1}$$

which has the coordinate space representation

$$D_F(x',t;x,0) = \left\langle x' \left| e^{-i(\hat{H}_0+V(\hat{x}))t} \right| x \right\rangle \quad . \tag{3.2}$$

Provided that the Hamiltonian can be solved exactly to yield eigenvalues and eigenfunctions

$$\hat{H}|\phi_n\rangle = E_n|\phi_n\rangle \qquad n = 0,1,2,\ldots \tag{3.3}$$

we can find an exact representation of the propagator

$$\begin{aligned} D_F(x',t;x,0) &= \sum_n \langle x'|\phi_n\rangle\, e^{-iE_n t}\, \langle \phi_n|x\rangle \\ &= \sum_n \phi_n(x')\phi_n^*(x) e^{-iE_n t} \quad . \end{aligned} \tag{3.4}$$

(Note that the free particle propagator is of this form since

$$\begin{aligned} D_F(x',t;x,0) &= \sum_p \langle x'|p\rangle\, e^{-i\frac{p^2}{2m}t}\, \langle p|x\rangle \\ &= \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ip(x'-x) - i\frac{p^2}{2m}t} \end{aligned} \tag{3.5}$$

as before.) That Eq. 3.4 generates the time development of an arbitrary wavefunction is clear since, assuming $t > 0$

$$\begin{aligned} \psi(x,t) &= \int_{-\infty}^{\infty} dx < x'|e^{-i\hat{H}t}|x >< x|\psi(0) > \\ &= \int_{-\infty}^{\infty} dx\, D_F(x',t;x,0)\psi(x,0) = \sum_n \phi_n(x') e^{-iE_n t} c_n \end{aligned} \tag{3.6}$$

where

$$c_n = \int_{-\infty}^{\infty} dx\, \phi_n^*(x)\psi(x,0) \quad . \tag{3.7}$$

is the projection of the initial state wavefunction $\psi(x,0)$ onto eigenstate $\phi_n(x)$. Eq. 3.6 then is simply the usual expansion of the wavefunction at later time t in terms of eigenstates of the Hamiltonian.

For soluble problems the propagator can generally be given simply and in closed form, and below we shall show how this is done for the case of the harmonic oscillator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \quad . \tag{3.8}$$

However, before deriving the explicit form it is useful to review the solution of the harmonic oscillator problem using the technique due to Dirac [Di 58].

Harmonic Oscillator Review

We begin by defining the so called "creation" and "annihilation" operators

$$\hat{a} = \sqrt{\frac{m\omega}{2}}\hat{x} + \frac{i\hat{p}}{\sqrt{2m\omega}} \qquad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2}}\hat{x} - \frac{i\hat{p}}{\sqrt{2m\omega}} \quad . \tag{3.9}$$

Then defining the "number operator" $\hat{N} \equiv \hat{a}^\dagger\hat{a}$ we find

$$\begin{aligned} \hat{N} &= \frac{\hat{p}^2}{2m\omega} + \frac{1}{2}m\omega\hat{x}^2 + \frac{i}{2}[\hat{x},\hat{p}] \\ &= \frac{\hat{H}}{\omega} - \frac{1}{2} \end{aligned} \tag{3.10}$$

or

$$\hat{H} = \omega\left(\hat{N} + \frac{1}{2}\right) \quad . \tag{3.11}$$

Now look for eigenstates $|n\rangle$ such that

$$\hat{N}|n\rangle = n|n\rangle \quad . \tag{3.12}$$

We can determine the properties of the eigenvalues n as follows. Since $\hat{N}$ is hermitian—

$$\hat{N}^\dagger = \left(\hat{a}^\dagger\hat{a}\right)^\dagger = \hat{a}^\dagger\hat{a} = \hat{N} \tag{3.13}$$

—we have

$$n = \left\langle n|\hat{N}|n\right\rangle = \left\langle n|\hat{N}^\dagger|n\right\rangle^* = \left\langle n|\hat{N}|n\right\rangle^* = n^* \quad . \tag{3.14}$$

i.e., n is real. Also n is non-negative since it can be written as the inner product of a state with itself.

$$n = \left\langle n|\hat{N}|n\right\rangle = \langle n|\hat{a}^\dagger\hat{a}|n\rangle = \left(\langle n|\hat{a}^\dagger\right)\hat{a}|n\rangle \geq 0 \quad . \tag{3.15}$$

Commutation relations are easily found

$$\left[\hat{a},\hat{a}^\dagger\right] = \frac{1}{2}\left(i\left[\hat{p},\hat{x}\right] - i\left[\hat{x},\hat{p}\right]\right) = 1 \quad . \tag{3.16}$$

Also

$$\begin{aligned} [\hat{N},\hat{a}] &= \hat{a}^\dagger\hat{a}\hat{a} - \hat{a}\hat{a}^\dagger\hat{a} = [\hat{a}^\dagger,\hat{a}]\hat{a} = -\hat{a} \\ [\hat{N},\hat{a}^\dagger] &= \hat{a}^\dagger\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}^\dagger\hat{a} = \hat{a}^\dagger[\hat{a},\hat{a}^\dagger] = \hat{a}^\dagger \quad . \end{aligned} \tag{3.17}$$

The state $\hat{a}|n\rangle$ is an eigenstate of $\hat{N}$ with eigenvalue $n-1$, since

$$\hat{N}\hat{a}|n\rangle = (\hat{a}\hat{N} - \hat{a})|n\rangle = (n-1)\hat{a}|n\rangle \quad . \tag{3.18}$$

The normalization of this state $\hat{a}|n>$ is given by

$$\left(\langle n|\hat{a}^\dagger\right)\hat{a}|n\rangle = \left\langle n|\hat{N}|n\right\rangle = n \tag{3.19}$$

so that

$$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle \quad . \tag{3.20}$$

Similarly, operating repeatedly with $\hat{a}$ we can lower the eigenvalue even further

$$\hat{a}^m|n\rangle = \sqrt{n(n-1)\ldots(n-m+1)}\,|n-m\rangle \quad . \tag{3.21}$$

¿From Eq. 3.15, however, negative eigenvalues are not permitted, so we must eventually reach a state $|1\rangle$ such that

$$\hat{N}|1\rangle = |1\rangle \tag{3.22}$$

and

$$\hat{a}|1\rangle = |0\rangle \quad \text{with} \quad \hat{N}|0\rangle = \hat{a}|0\rangle = 0 \quad . \tag{3.23}$$

We conclude that the eigenvalue n must be an integer—$n = 0, 1, 2, \ldots$. Likewise, we can increase the eigenvalues by utilizing the adjoint operator $\hat{a}^\dagger$

$$\hat{N}\hat{a}^\dagger|n\rangle = \left(\hat{a}^\dagger\hat{N} + \hat{a}^\dagger\right)|n\rangle = (n+1)\hat{a}^\dagger|n\rangle \tag{3.24}$$

with the normalization condition

$$\begin{aligned}(\langle n|\hat{a})\,\hat{a}^\dagger|n\rangle &= \langle n|\hat{a}\hat{a}^\dagger|n\rangle \\ &= \left\langle n|\hat{N} + [\hat{a},\hat{a}^\dagger]|n\right\rangle = n+1 \quad .\end{aligned} \tag{3.25}$$

Application of $\hat{a}^\dagger$ then yields

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}\;|n+1\rangle \quad . \tag{3.26}$$

Starting with the lowest energy (ground) state $|0>$ we find

$$\left(\hat{a}^\dagger\right)^n|0\rangle = \sqrt{n(n-1)\ldots 1}\,|n\rangle \quad . \tag{3.27}$$

so that an arbitrary state $|n\rangle$ can be written as

$$|n\rangle = \frac{1}{\sqrt{n!}}\left(\hat{a}^\dagger\right)^n|0\rangle \quad . \tag{3.28}$$

The energy of the eigenstate $|n>$ is given by

$$\hat{H}|n\rangle = \omega\left(\hat{N} + \frac{1}{2}\right)|n\rangle = \omega\left(n + \frac{1}{2}\right)|n\rangle \quad . \tag{3.29}$$

as expected.

Thus far we have been dealing with the eigenstates in an abstract—ket—representation. In order to make connection with the usual Schrödinger wavefunction, we take the coordinate space projection of the equation $\hat{a}|0\rangle = 0$, namely

$$\begin{aligned}0 = \langle x|\hat{a}|0\rangle &= \left\langle x\left|\sqrt{\frac{m\omega}{2}}\hat{x} + i\frac{\hat{p}}{\sqrt{2m\omega}}\right|0\right\rangle \\ &= \left(\sqrt{\frac{m\omega}{2}}x + \frac{1}{\sqrt{2m\omega}}\,\frac{d}{dx}\right)\langle x|0\rangle = \frac{1}{\sqrt{2m\omega}}\left(\frac{d}{dx} + m\omega x\right)\langle x|0\rangle \quad .\end{aligned} \tag{3.30}$$

The solution to this differential equation yields the familiar ground state wavefunction

$$\langle x|0\rangle = \left(\frac{m\omega}{\pi}\right)^{1/4} \exp\left(-\frac{1}{2}m\omega x^2\right) \quad . \tag{3.31}$$

Excited state wavefunctions may be generated by repeated applications of $\hat{a}^\dagger$. For the first excited state, we find

$$\begin{aligned} \langle x|1\rangle = \langle x|\hat{a}^\dagger|0\rangle &= \left\langle x \left| \sqrt{\frac{m\omega}{2}}\hat{x} - i\frac{\hat{p}}{\sqrt{2m\omega}} \right| 0 \right\rangle \\ &= -\frac{1}{\sqrt{2m\omega}}\left(\frac{d}{dx} - m\omega x\right)\langle x|0\rangle = \sqrt{2m\omega}\, x\, \langle x|0\rangle \quad , \end{aligned} \tag{3.32}$$

and one can generate the wavefunction of an arbitrary excited state via

$$\begin{aligned} \langle x|n\rangle &= \frac{1}{\sqrt{n!}} < x|(\hat{a}^\dagger)^n|0 >= \frac{(-)^n}{\sqrt{n!}(2m\omega)^{\frac{n}{2}}}(\frac{d}{dx} - m\omega x)^n < x|0 > \\ &= \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{m\omega}\, x\right)\langle x|0\rangle \quad . \end{aligned} \tag{3.33}$$

where $H_n(x)$ represents the Hermite polynomial of order n.

Harmonic Oscillator Propagator

We now return to the problem of the harmonic oscillator propagator. There exist a number of techniques by which this result may be obtained. For example, Itzykson and Zuber [ItZ 80] use a traditional time slice procedure in order to yield the closed form

$$D_F(x', t; x, 0) = \sqrt{\frac{m\omega}{2\pi i \sin\omega t}} \exp i\frac{m\omega}{2}\left[\left(x'^2 + x^2\right)\operatorname{ctn}\omega t - 2x'x\csc\omega t\right] \quad . \tag{3.34}$$

(Note that Eq. 3.34 reduces to the free propagator result in the limit $\omega \to 0$.) However this procedure, while straightforward, is also lengthy and cumbersome. An alternate way to obtain the same result is by use of the Feynman path integral

$$D_F(x', t; x, 0) = \int \mathcal{D}\left[x(t)\right] \exp iS\left[x(t)\right] \quad , \tag{3.35}$$

but with the arbitrary trajectory $x(t)$ characterized in terms of its deviation $\delta x(t)$ from the classical path $x_{\rm cl}(t)$, which satisfies

$$\begin{aligned} \ddot{x}_{\rm cl}(t) &= -\omega^2 x_{\rm cl}(t) \\ x_{\rm cl}(0) &= x \\ x_{\rm cl}(t) &= x' \end{aligned} \tag{3.36}$$

Then

$$D_F(x', t; x, 0) = \int \mathcal{D}\left[\delta x(t)\right] \exp iS\left[x_{\rm cl}(t) + \delta x(t)\right] \quad . \tag{3.37}$$

where

$$S\left[x_{\rm cl}(t)+\delta x(t)\right]=S[x_{\rm cl}(t)]+2\int_0^t dt'\frac{1}{2}m\left(\dot{x}_{\rm cl}(t')\delta\dot{x}(t')-\omega^2 x_{\rm cl}(t')\delta x(t')\right)$$
$$+\int_0^t dt'\frac{1}{2}m\left((\delta\dot{x}(t'))^2-\omega^2(\delta x(t'))^2\right)\quad . \tag{3.38}$$

Integrating the term linear in δx by parts, we find

$$\int_0^t dt' m\left(\dot{x}_{\rm cl}(t')\delta\dot{x}(t')-\omega^2 x_{\rm cl}(t')\delta x(t')\right)=-\int_0^t dt' m\delta x(t')\left(\ddot{x}_{\rm cl}(t')+\omega^2 x_{\rm cl}(t')\right)=0 \tag{3.39}$$

where we have used the classical equation of motion and the fixed endpoint constraint—$\delta x(t)=\delta x(0)=0$. We have then

$$S[x(t)]=S[x_{\rm cl}(t)]+S[\delta x(t)] \tag{3.40}$$

and

$$D_F(x',t;x,0)=\int[\mathcal{D}\delta x(t)]\exp iS[x(t)]=\exp iS[x_{\rm cl}]\times D_F(0,t;0,0) \tag{3.41}$$

i.e., the phase of the exponential is simply the action for the classical path! Writing

$$x_{\rm cl}(t)=A\sin(\omega t+\phi) \tag{3.42}$$

we require the boundary conditions

$$\begin{aligned} x_{\rm cl}(0)&=A\sin\phi=x\\ x_{\rm cl}(t)&=A\sin(\omega t+\phi)=x'\quad , \end{aligned} \tag{3.43}$$

and the action is found to be

$$\begin{aligned} S[x_{\rm cl}(t)]&=\frac{1}{2}m\int_0^t dt'\left(\dot{x}_{\rm cl}^2(t')-\omega^2 x_{\rm cl}^2(t')\right)\\ &=\frac{1}{2}mA^2\omega^2\int_0^t dt'\left(\cos^2(\omega t'+\phi)-\sin^2(\omega t'+\phi)\right)\\ &=\frac{1}{2}mA^2\omega^2\int_0^t dt'\cos(2\omega t'+2\phi)=\frac{m\omega}{4}A^2\left(\sin(2\omega t+2\phi)-\sin 2\phi\right)\quad . \end{aligned} \tag{3.44}$$

We must now eliminate A,ϕ in favor of x,x'. Noting that

$$\frac{x}{x'}=\frac{\sin\phi}{\sin(\omega t+\phi)}=\frac{\sin\phi}{\sin\omega t\cos\phi+\cos\omega t\sin\phi} \tag{3.45}$$

and solving for $\cos\phi$ we have

$$A\cos\phi=\frac{x'}{\sin\omega t}-\frac{x\cos\omega t}{\sin\omega t}\quad . \tag{3.46}$$

Thus

$$A^2 \sin 2\phi = 2A\cos\phi \cdot A\sin\phi = 2x\left(\frac{x'}{\sin\omega t} - \frac{x\cos\omega t}{\sin\omega t}\right)$$
$$A^2\sin(2\omega t + 2\phi) = 2A^2\sin(\omega t+\phi)\cos(\omega t+\phi) = 2x'A(\cos\omega t\cos\phi - \sin\omega t\sin\phi)$$
$$= 2x'\left(\cos\omega t\left(\frac{x'}{\sin\omega t} - \frac{x\cos\omega t}{\sin\omega t}\right) - x\sin\omega t\right) = 2x'\left(\frac{x'\cos\omega t}{\sin\omega t} - \frac{x}{\sin\omega t}\right) \tag{3.47}$$

and

$$S[x_{\rm cl}(t)] = \frac{m\omega}{2}\left[\left(x^2 + x'^2\right)\,\mathrm{ctn}\,\omega t - 2xx'\csc\omega t\right] \quad . \tag{3.48}$$

The time dependent prefactor $D_F(0,t;0,0)$ can be evaluated either via standard path integral techniques or via a shortcut. We first demonstrate the latter. Using the completeness property

$$\begin{aligned}\left\langle x'\left|e^{-i\hat{H}t}\right|x\right\rangle &= \left\langle x'\left|e^{-i\hat{H}(t-t_1)}e^{-i\hat{H}t_1}\right|x\right\rangle \\ &= \int_{-\infty}^{\infty} dx''\left\langle x'\left|e^{-i\hat{H}(t-t_1)}\right|x''\right\rangle\left\langle x''\left|e^{-i\hat{H}t_1}\right|x\right\rangle \quad .\end{aligned} \tag{3.49}$$

Defining

$$D_F(0,t;0,0) \equiv J(t) \tag{3.50}$$

we have, combining Eqs. 3.34 and 3.49

$$\begin{aligned}&J(t)\exp i\frac{m\omega}{2}\left[\left(x^2+x'^2\right)\,\mathrm{ctn}\,\omega t - 2xx'\csc\omega t\right] \\ &= J(t-t_1)J(t_1)\int_{-\infty}^{\infty} dx''\exp\frac{im\omega}{2}\left[\left(x'^2+x''^2\right)\,\mathrm{ctn}\,\omega(t-t_1)\right. \\ &\left.-2x'x''\csc\omega(t-t_1)\right]\exp\frac{im\omega}{2}\left[\left(x^2+x''^2\right)\,\mathrm{ctn}\,\omega t_1 - 2xx''\csc\omega t_1\right] \quad .\end{aligned} \tag{3.51}$$

To simplify things pick $x = x' = 0$. Then

$$\begin{aligned}\frac{J(t)}{J(t-t_1)J(t_1)} &= \int_{-\infty}^{\infty} dx''\exp i\frac{m\omega}{2}\left(\mathrm{ctn}\,\omega(t-t_1) + \mathrm{ctn}\,\omega t_1\right)x''^2 \\ &= \sqrt{\frac{2\pi i}{m\omega}\frac{1}{\mathrm{ctn}\,\omega(t-t_1) + \mathrm{ctn}\,\omega t_1}} = \sqrt{\frac{2\pi i}{m\omega}\frac{\sin\omega(t-t_1)\sin\omega t_1}{\sin\omega t}}\end{aligned} \tag{3.52}$$

whose solution is

$$J(t) = \sqrt{\frac{m\omega}{2\pi i\sin\omega t}} \quad . \tag{3.53}$$

in agreement with Eq. 3.34.

Determinant Methods and the Prefactor

A technique by which to evaluate the prefactor which is more generally useful is given below. Writing the path integral as

$$D_F(0,t_f;0,t_i) = \int \mathcal{D}\left[\delta x(t)\right] \exp iS\left[\delta x(t)\right] \tag{3.54}$$

where $\delta x(t_i) = \delta x(t_f) = 0$ and integrating by parts we find

$$\begin{aligned} S\left[\delta x(t)\right] &= \int_{t_i}^{t_f} dt \left(\frac{1}{2}m(\delta\dot{x}(t))^2 - \frac{1}{2}m\omega^2(\delta x(t))^2\right) \\ &= \int_{t_i}^{t_f} dt\frac{m}{2}\delta x(t)\left(-\frac{d^2}{dt^2} - \omega^2\right)\delta x(t) \\ &\equiv \int_{t_i}^{t_f} dt\delta x(t)\mathcal{O}\delta x(t) \quad . \end{aligned} \tag{3.55}$$

Now expand $\delta x(t)$ in terms of eigenfunctions of the operator $\mathcal{O} = -\frac{d^2}{dt^2} - \omega^2$

$$\delta x(t) = \sum_n a_n x_n(t) \tag{3.56}$$

where $x_n(t)$ satisfies

$$\mathcal{O}x_n(t) = \lambda_n x_n(t) \tag{3.57}$$

with $x_n(t_i) = x_f(t_f) = 0$ and is subject to the orthogonality condition

$$\int_{t_i}^{t_f} dt\, x_n(t)x_m(t) = \delta_{nm} \quad . \tag{3.58}$$

The sum over all possible trajectories can then be performed by summation over *all* expansion coefficients a_n

$$\begin{aligned} D_F(0,t_f;0,t_i) &= N\prod_{j=1}^{\infty}\left(\int_{-\infty}^{\infty} da_j\right)\exp i\int_{t_i}^{t_f} dt\,\delta x(t)\mathcal{O}\delta x(t) \\ &= N\prod_{j=1}^{\infty}\left(\int_{-\infty}^{\infty} da_j\right)\exp i\int_{t_i}^{t_f}\sum_{k=1}^{\infty} a_k x_k(t)\sum_{\ell=1}^{\infty} a_\ell x_\ell(t)\lambda_\ell dt \\ &= N\prod_{j=1}^{\infty}\left(\int_{-\infty}^{\infty} da_j \exp i\lambda_j a_j^2\right) \\ &\equiv N'\left(\det\mathcal{O}\right)^{-1/2} \end{aligned} \tag{3.59}$$

where N, N' are normalization coefficients and

$$\det\mathcal{O} \equiv \prod_{j=1}^{\infty}\lambda_j \tag{3.60}$$

is the product of operator eigenvalues. For the harmonic oscillator

$$\begin{aligned} x_n(t) &= \sqrt{\frac{2}{t_f - t_i}} \sin \omega_n (t - t_i) \quad , \\ \text{with} \qquad \omega_n &= \left(\frac{n\pi}{t_f - t_i} \right) \quad n = 1, 2, \ldots \end{aligned} \tag{3.61}$$

Then $\lambda_n = \omega_n^2 - \omega^2$ and the determinant can be evaluated using the identity [GrR 65]

$$\prod_{n=1}^{\infty} \left(1 - \frac{x^2}{n^2 \pi^2} \right) = \frac{\sin x}{x} \quad , \tag{3.62}$$

i.e.,

$$\begin{aligned} \det \mathcal{O} &= \prod_{n=1}^{\infty} \left(\left(\frac{n\pi}{t_f - t_i} \right)^2 - \omega^2 \right) \\ &= \text{Const.} \times \prod_{n=1}^{\infty} \left(1 - \frac{\omega^2 \left(t_f - t_i \right)^2}{n^2 \pi^2} \right) \\ &= \text{Const.} \times \frac{\sin \omega (t_f - t_i)}{\omega (t_f - t_i)} \end{aligned} \tag{3.63}$$

where the constant is independent of ω, and may be absorbed into N'. The normalization constant N' can in turn be determined by demanding that

$$\lim_{\omega \to 0} N' \left(\det \mathcal{O} \right)^{-1/2} = \left(\frac{m}{2\pi i (t_f - t_i)} \right)^{1/2} \tag{3.64}$$

i.e. that the free particle result be obtained in the limit $\omega \to 0$. Hence

$$N' \left(\det \mathcal{O} \right)^{-1/2} = D_F(0, t_f; 0, t_i) = \left(\frac{m\omega}{2\pi i \sin \omega (t_f - t_i)} \right)^{1/2} \tag{3.65}$$

which agrees with Eq. 3.53 found via the completeness property.

Wavefunction Connection

We can explicitly verify that Eq. 3.34 represents the correct form of the harmonic oscillator propagator by comparing with the sum over eigenstates, Eq. 3.4. We first examine the spectrum by taking the coordinate space trace

$$\begin{aligned} \int_{-\infty}^{\infty} dx \, D_F(x, t; x, 0) &= \sum_n e^{-iE_n t} \int_{-\infty}^{\infty} dx \, \phi_n^*(x) \phi_n(x) \\ &= \sum_n e^{-iE_n t} \quad . \end{aligned} \tag{3.66}$$

Using Eq. 3.34 we have

$$\begin{aligned}\int_{-\infty}^{\infty} dx\, D_F(x,t;x,0) &= \int_{-\infty}^{\infty} dx \sqrt{\frac{m\omega}{2\pi i \sin\omega t}} \exp(-im\omega x^2 \tan\frac{\omega t}{2}) \\ &= \sqrt{\frac{m\omega}{2\pi i \sin\omega t}} \times \sqrt{\frac{\pi}{im\omega \tan\frac{\omega t}{2}}} = \frac{1}{2i\sin\frac{\omega t}{2}} \\ &= \sum_{n=0}^{\infty} e^{-i\frac{\omega}{2}(2n+1)t} \quad .\end{aligned} \tag{3.67}$$

Thus

$$E_n = \omega(n+\frac{1}{2}) \qquad n = 0,1,2,....$$

as expected. The wavefunctions may be obtained by expansion of the propagator itself:

$$\begin{aligned}D_F(x,t;x,0) &= \sqrt{\frac{m\omega}{\pi}} e^{-i\frac{\omega t}{2}} \left(1+e^{-2i\omega t}+e^{-4i\omega t}+\ldots\right)^{1/2} \\ &\times \exp\left[-m\omega x^2\left(1-e^{-i\omega t}\right)\left(1-e^{-i\omega t}+e^{-2i\omega t}-\ldots\right)\right] \\ &= \left(\frac{m\omega}{\pi}\right)^{1/2} \exp\left(-m\omega x^2\right)\left\{e^{-i\frac{\omega t}{2}}+2m\omega x^2 e^{-i\frac{3\omega t}{2}}+\ldots\right\} \quad .\end{aligned} \tag{3.68}$$

Comparing with Eq. 3.4 we identify

$$\begin{aligned}\phi_0(x) &= \left(\frac{m\omega}{\pi}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2}\right) \\ \phi_1(x) &= \sqrt{2m\omega}\; x\phi_0(x)\end{aligned} \tag{3.69}$$

etc., as the familiar harmonic oscillator wavefunctions.