PROPAGATOR FOR A GAUSSIAN WAVE PACKET FOR THE FREE PARTICLE

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.1, Exercise 5.1.3.

The propagator for the free particle is

$$U(t)=\int_{-\infty}^{\infty}e^{-ip^{2}t/2m\hbar}|p\rangle\langle p|\,dp \tag{1}$$

We can find its matrix elements in position space by using the position space form of the momentum

$$\langle x|p\rangle=\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar} \tag{2}$$

Taking the matrix element of 1 we have

$$\begin{aligned}
U\left(x,t;x'\right) &= \left\langle x\left|U(t)\right|x'\right\rangle &(3)\\
&=\int\langle x|p\rangle\left\langle p\left|x'\right.\right\rangle e^{-ip^{2}t/2m\hbar}dp &(4)\\
&=\frac{1}{2\pi\hbar}\int e^{ip(x-x')/\hbar}e^{-ip^{2}t/2m\hbar}dp &(5)\\
&=\sqrt{\frac{m}{2\pi\hbar it}}e^{im(x-x')^{2}/2\hbar t} &(6)
\end{aligned}$$

The final integral can be done by combining the exponents in the third line, completing the square and using the standard formula for Gaussian integrals. We won't go through that here, as our main goal is to explore the evolution of an initial wave packet using the propagator. Given 6, we can in principle find the wave function for all future times given an initial wave function, by using the propagator:

$$\psi(x,t)=\int U\left(x,t;x'\right)\psi\left(x',0\right)dx' \tag{7}$$

Here, we're assuming that the initial time is $t=0$. Shankar uses the standard example where the initial wave packet is a Gaussian:

$$\psi\left(x',0\right)=e^{ip_0x'/\hbar}\frac{e^{-x'^2/2\Delta^2}}{\left(\pi\Delta^2\right)^{1/4}} \tag{8}$$

This is a wave packet distributed symmetrically about the origin, so that $\langle X\rangle=0$, and with mean momentum given by $\langle P\rangle=p_0$. By plugging this and 6 into 7, we can work out the time-dependent version of the wave packet, which Shankar gives as

(9)

$$\psi(x,t)=\left[\sqrt{\pi}\left(\Delta+\frac{i\hbar t}{m\Delta}\right)\right]^{-1/2}\exp\left[\frac{-\left(x-p_0t/m\right)^2}{2\Delta^2\left(1+i\hbar t/m\Delta^2\right)}\right]\exp\left[\frac{ip_0}{\hbar}\left(x-\frac{p_0t}{2m}\right)\right]$$

Again, we won't go through the derivation of this result as it involves a messy calculation with Gaussian integrals again. The main problem we want to solve here is to use our alternative form of the propagator in terms of the Hamiltonian:

$$U(t)=e^{-iHt/\hbar} \tag{10}$$

For the free particle

$$H=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \tag{11}$$

so if we expand $U(t)$ as a power series, we have

$$U(t)=\sum_{s=0}^{\infty}\frac{1}{s!}\left(\frac{i\hbar t}{2m}\right)^s\frac{d^{2s}}{dx^{2s}} \tag{12}$$

To see how we can use this form to generate the time-dependent wave function, we'll consider a special case of 8 with $p_0=0$ and $\Delta=1$, so that

$$\psi_0(x) = \frac{e^{-x^2/2}}{\pi^{1/4}} \tag{13}$$

$$= \frac{1}{\pi^{1/4}}\sum_{n=0}^{\infty}\frac{(-1)^n x^{2n}}{2^n n!} \tag{14}$$

We therefore need to apply one power series 12 to the other 14. This is best done by examining a few specific terms and then generalizing to the main result. To save writing, we'll work with the following

$$\alpha \equiv \frac{i\hbar t}{m} \tag{15}$$

$$\psi_\pi(x) \equiv \pi^{1/4}\psi_0(x) \tag{16}$$

The $s=0$ term in 12 is just 1, so we'll look at the $s=1$ term and apply it to 14:

$$\frac{\alpha}{2}\frac{d^2}{dx^2}\left[\sum_{n=0}^{\infty}\frac{(-1)^n x^{2n}}{2^n n!}\right] = \frac{\alpha}{2}\sum_{n=1}^{\infty}\frac{(-1)^n (2n)(2n-1)x^{2n-2}}{2^n n!} \tag{17}$$

$$= \frac{\alpha}{2}\sum_{n=1}^{\infty}\frac{(-1)^n (2n)!x^{2n-2}}{2^n n!(2n-2)!} \tag{18}$$

We can simplify this by using an identity involving factorials:

$$\frac{(2n)!}{n!} = \frac{(2n)(2n-1)(2n-2)(2n-3)\ldots(2)(1)}{n(n-1)(n-2)\ldots(2)(1)} \tag{19}$$

$$= \frac{2^n[n(n-1)(n-2)\ldots(2)(1)][(2n-1)(2n-3)\ldots(3)(1)]}{n!} \tag{20}$$

$$= \frac{2^n n!(2n-1)!!}{n!} \tag{21}$$

$$= 2^n(2n-1)!! \tag{22}$$

The 'double factorial' notation is defined as

$$(2n-1)!! \equiv (2n-1)(2n-3)\ldots(3)(1) \tag{23}$$

That is, it's the product of every other term from n down to 1. Using this result, we can write 18 as

$$\frac{\alpha}{2}\sum_{n=1}^{\infty}\frac{(-1)^n (2n)!x^{2n-2}}{2^n n!(2n-2)!} = \alpha\sum_{n=1}^{\infty}\frac{(-1)^n (2n-1)!!x^{2n-2}}{2(2n-2)!} \tag{24}$$

Now look at the $s=2$ term from 12.

(25)
$$\frac{1}{2!}\frac{\alpha^2}{2^2}\frac{d^4}{dx^4}\left[\sum_{n=0}^{\infty}\frac{(-1)^n x^{2n}}{2^n n!}\right]=\frac{1}{2!}\frac{\alpha^2}{2^2}\sum_{n=2}^{\infty}\frac{(-1)^n(2n)(2n-1)(2n-2)(2n-3)x^{2n-4}}{2^n n!}$$

$$=\frac{1}{2!}\frac{\alpha^2}{2^2}\sum_{n=2}^{\infty}\frac{(-1)^n(2n)!x^{2n-4}}{2^n n!(2n-4)!} \tag{26}$$

$$=\frac{\alpha^2}{2^2 2!}\sum_{n=2}^{\infty}\frac{(-1)^n(2n-1)!!x^{2n-4}}{(2n-4)!} \tag{27}$$

We can see the pattern for the general term for arbitrary s from 12 (we could prove it by induction, but hopefully the pattern is fairly obvious):

$$\frac{1}{s!}\frac{\alpha^s}{2^s}\frac{d^{2s}}{dx^{2s}}\left[\sum_{n=0}^{\infty}\frac{(-1)^n x^{2n}}{2^n n!}\right]=\frac{1}{s!}\frac{\alpha^s}{2^s}\sum_{n=s}^{\infty}\frac{(-1)^n(2n)!x^{2n-2s}}{2^n n!(2n-2s)!} \tag{28}$$

$$=\frac{\alpha^s}{2^s s!}\sum_{n=s}^{\infty}\frac{(-1)^n(2n-1)!!x^{2n-2s}}{(2n-2s)!} \tag{29}$$

Now we can collect terms for each power of x. The constant term (for x^0) is the first term from each series for each value of s, so we have, using the general term 29 and taking the first term where $n=s$:

$$\sum_{s=0}^{\infty}\frac{(-1)^s\alpha^s(2s-1)!!}{2^s s!}=1-\frac{\alpha}{2}+\frac{\alpha^2}{2!}\frac{3}{2}\frac{1}{2}-\frac{\alpha^3}{3!}\frac{5}{2}\frac{3}{2}\frac{1}{2}+\ldots \tag{30}$$

[The $(2s-1)!!$ factor is 1 when $s=0$ as we can see from the result 22.] The series on the RHS is the Taylor expansion of $(1+\alpha)^{-1/2}$, as can be verified using tables.

In general, to get the coefficient of x^{2r} (only even powers of x occur in the series), we take the term where $n=s+r$ from 29 and sum over s. This gives

$$\sum_{s=0}^{\infty}\frac{\alpha^s}{2^s s!}\frac{(-1)^{s+r}(2s+2r-1)!!}{(2r)!}=\frac{(-1)^r}{2^r r!}\sum_{s=0}^{\infty}\frac{\alpha^s}{2^s s!}\frac{(-1)^s(2s+2r-1)!!}{(2r-1)!!} \tag{31}$$

where we used 22 to get the RHS. Expanding the sum gives

$$\sum_{s=0}^{\infty}\frac{\alpha^s}{2^s s!}\frac{(-1)^s(2s+2r-1)!!}{(2r-1)!!}=1-\alpha\frac{2r+1}{2}+\frac{\alpha^2}{2!}\left(\frac{2r+3}{2}\right)\left(\frac{2r+1}{2}\right)-\ldots \tag{32}$$

$$=1-\alpha\left(r+\frac{1}{2}\right)+\frac{\alpha^2}{2!}\left(r+\frac{3}{2}\right)\left(r+\frac{1}{2}\right)-\ldots \tag{33}$$

$$=(1+\alpha)^{-r-\frac{1}{2}} \tag{34}$$

where again we've used a standard series from tables (given by Shankar in the problem) to get the last line. Combining this with 31, we see that the coefficient of x^{2r} is

$$\frac{(-1)^r}{2^r r!}(1+\alpha)^{-r-\frac{1}{2}} \tag{35}$$

Thus the time-dependent wave function can be written as a single series as:

$$\psi(x,t)=U(t)\,\psi(x,0) \tag{36}$$

$$=e^{-iHt/\hbar}\psi(x,0) \tag{37}$$

$$=\frac{1}{\pi^{1/4}}\sum_{r=0}^{\infty}\frac{(-1)^r}{2^r r!}(1+\alpha)^{-r-\frac{1}{2}}x^{2r} \tag{38}$$

$$=\frac{1}{\pi^{1/4}\sqrt{1+\alpha}}\sum_{r=0}^{\infty}\frac{(-1)^r}{2^r(1+\alpha)^r r!}x^{2r} \tag{39}$$

$$=\frac{1}{\pi^{1/4}\sqrt{1+\alpha}}\exp\left[\frac{-x^2}{2(1+\alpha)}\right] \tag{40}$$

$$=\frac{1}{\pi^{1/4}\sqrt{1+i\hbar t/m}}\exp\left[\frac{-x^2}{2(1+i\hbar t/m)}\right] \tag{41}$$

This agrees with 9 when $p_0=0$ and $\Delta=1$, though it does take a fair bit of work!