Introduction to Quantum Mechanics: Problem Set 2

1 (Textbook 2.1) Consider the wave packet $\psi(x) \equiv \Psi(x, t=0)$ given by

$$\psi(x) = Ce^{ip_0x/\hbar}e^{-|x|/(2\Delta x)}$$

where C is a normalisation constant.

- (a) Normalise $\psi(x)$ to unity.
- (b) Obtain the corresponding momentum space wave function $\phi(p_x)$ and verify that it is normalised to unity according to (2.44)
- (c) Suggest a reasonable definition of the width Δp_x of the momentum distribution an show that $\Delta x \Delta p_x \geq \hbar$.

Solution:

(a) To normalize the wavefunction we have to find C such that

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, \mathrm{d}x = 1$$

Plugging in the definition for $\psi(x)$ we get

$$\int_{-\infty}^{\infty} \left| C e^{ip_0 x/\hbar} e^{-|x|/(2\Delta x)} \right|^2 dx$$
$$\int_{-\infty}^{\infty} \left| C \right|^2 \left| e^{ip_0 x/\hbar} \right|^2 \left| e^{-|x|/(2\Delta x)} \right|^2 dx$$

The magnitude squared of the imaginary exponential is 1 and the magnitude squared of the real exponential can be obtained by simply squaring it (it is its own complex conjugate), so the integral is now

$$|C|^2 \int_{-\infty}^{\infty} e^{-|x|/(\Delta x)} \mathrm{d}x$$

We can get rid of the absolute value sign by splitting the integral into two parts, one with x running over all negative numbers where

|x| = -x and the other with x running over all positive numbers where |x| = x

$$|C|^{2} \left[\int_{-\infty}^{0} e^{x/(\Delta x)} dx + \int_{0}^{\infty} e^{-x/(\Delta x)} dx \right]$$

$$= |C|^{2} \left[\Delta x e^{x/\Delta x} \Big|_{x=-\infty}^{x=0} + (-\Delta x) e^{-x/\Delta x} \Big|_{x=0}^{x=\infty} \right]$$

$$= |C|^{2} \left[\Delta x (1-0) - \Delta x (0-1) \right]$$

$$= 2\Delta x |C|^{2}$$

And if that is equal to 1 then $|C|^2$ must equal $1/(2\Delta x)$. So $|C| = 1/\sqrt{2\Delta x}$. The phase of C is not specified, but by convention it is usually taken to be 0 so that C is a real number. So $C = 1/\sqrt{2\Delta x}$.

(b) $\phi(p_x)$ is the Fourier Transform of $\psi(x)$, and can be obtained from it using equation (2.41) in the book.

$$\phi(p_x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ip_x x/\hbar} \psi(x) \, \mathrm{d}x$$

Before calculating the Fourier Transform it's always a good idea to see what we can predict about it generally by inspection and application of the Fourier Transform properties. One property is the shift property which I didn't cover in tutorial but you can read about at

 $http://en.wikipedia.org/wiki/Fourier_transform\#Properties$

Multiplication by the phasor $e^{ip_0x/\hbar}$ shifts the center of the Fourier transform from $p_x = 0$ to $p_x = p_0$. Also

$$\Re \left[\psi(x)\right] = \frac{1}{\sqrt{2\Delta x}} e^{-|x|/(2\Delta x)} \cos p_0 x$$
$$\Im \left[\psi(x)\right] = \frac{1}{\sqrt{2\Delta x}} e^{-|x|/(2\Delta x)} \sin p_0 x$$

The real part of $\psi(x)$ is even and the imaginary part is odd, so we expect the Fourier transform to be purely real.

Let's explicitly evaluate the integral and we'll look for these properties in the result. We have

$$\begin{split} \phi\left(p_{x}\right) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ip_{x}x/\hbar} \frac{1}{\sqrt{2\Delta x}} e^{ip_{0}x/\hbar} e^{-|x|/(2\Delta x)} \mathrm{d}x \\ &= \frac{1}{2\sqrt{\pi\hbar\Delta x}} \int_{-\infty}^{0} e^{[\hbar/(2\Delta x) + i(-p_{x} + p_{0})]x/\hbar} \mathrm{d}x + \frac{1}{2\sqrt{\pi\hbar\Delta x}} \int_{0}^{\infty} e^{[-\hbar/(2\Delta x) + i(-p_{x} + p_{0})]x/\hbar} \mathrm{d}x \\ &= \frac{1}{2\sqrt{\pi\hbar\Delta x}} \left[\frac{\hbar}{\hbar/(2\Delta x) + i(-p_{x} + p_{0})} e^{[\hbar/(2\Delta x) + i(-p_{x} + p_{0})]x/\hbar} \Big|_{-\infty}^{0} + \frac{\hbar}{-\hbar/(2\Delta x) + i(-p_{x} + p_{0})} e^{[-\hbar/(2\Delta x) + i(-p_{x} + p_{0})]x/\hbar} \Big|_{0}^{\infty} \right] \\ &= \frac{1}{2} \sqrt{\frac{\hbar}{\pi\Delta x}} \left[\frac{1}{\hbar/(2\Delta x) + i(-p_{x} + p_{0})} (1 - 0) + \frac{1}{-\hbar/(2\Delta x) + i(-p_{x} + p_{0})} (1 - 0) \right] \\ &= \frac{1}{2} \sqrt{\frac{\hbar}{\pi\Delta x}} \left[\frac{1}{\hbar/(2\Delta x) + i(-p_{x} + p_{0})} - \frac{1}{-\hbar/(2\Delta x) + i(-p_{x} + p_{0})} \right] \\ &= \frac{1}{2} \sqrt{\frac{\hbar}{\pi\Delta x}} \left[\frac{-\hbar/(2\Delta x) + i(-p_{x} + p_{0}) - (\hbar/(2\Delta x) - i(-p_{x} + p_{0}))}{(\hbar/(2\Delta x) + i(-p_{x} + p_{0})) (-\hbar/(2\Delta x) + i(-p_{x} + p_{0}))} \right] \\ &= \frac{1}{2} \sqrt{\frac{\hbar}{\pi\Delta x}} \left[\frac{-\hbar/(2\Delta x) + i(-p_{x} + p_{0}) - (\hbar/(2\Delta x) + i(-p_{x} + p_{0}))}{(\hbar/(2\Delta x) + i(-p_{x} + p_{0}))} \right] \\ &= \frac{1}{2} \sqrt{\frac{\hbar}{\pi\Delta x}} \left[\frac{1}{-\hbar^{2}/(4\Delta x^{2}) - (-p_{x} + p_{0})^{2}} \right] \\ &= \frac{1}{2} \sqrt{\frac{\hbar^{3}}{\Delta x^{3\pi}}} \left[\frac{1}{\hbar^{2}/(4\Delta x^{2}) + (-p_{x} + p_{0})^{2}} \right] \end{split}$$

So the Fourier transform is real, and furthermore its real part is symmetric about the centre at p_x as can be seen in figure on the next page.

Now to verify that it is normalized. If it is still normalized then

$$\int_{-\infty}^{\infty} \left| \phi \left(p_x \right) \right|^2 \mathrm{d}p_x = 1$$

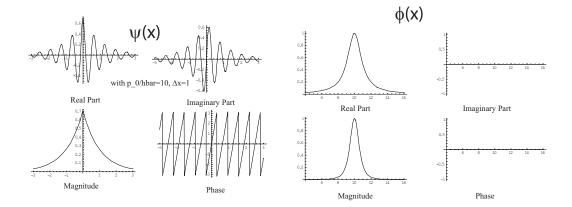
Let's see if it's true.

$$\int_{-\infty}^{\infty} |\phi(p_x)|^2 dp_x =$$

$$\int_{-\infty}^{\infty} \left| \frac{1}{2} \sqrt{\frac{\hbar^3}{\Delta x^3 \pi}} \left[\frac{1}{\hbar^2 / (4\Delta x^2) + (-p_x + p_0)^2} \right] \right|^2 dp_x$$

Since the function is real, $|\phi(p_x)|^2 = \phi(p_x)^2$.

$$\frac{\hbar^3}{4\Delta x^3 \pi} \int_{-\infty}^{\infty} \frac{1}{\left(\hbar^2 / (4\Delta x^2) + (-p_x + p_0)^2\right)^2} dp_x$$



We can start by making a change of variables $u = -p_x + p_0$, $du = -dp_x$. u goes to $-\infty$ when p_x goes to ∞ and to ∞ when p_x goes to $-\infty$.

$$\frac{\hbar^3}{4\Delta x^3 \pi} \int_{-\infty}^{-\infty} \frac{1}{(1/(4\Delta x^2) + u^2)^2} (-du)$$
$$= \frac{\hbar^3}{4\Delta x^3 \pi} \int_{-\infty}^{\infty} \frac{1}{(1/(4\Delta x^2) + u^2)^2} du$$

If you don't recognize this integral you can look it up in an integral table like the one at http://www.sosmath.com/tables/tables.html or use Mathematica or Maple to evaluate it. In the tables we find that

$$\int \frac{1}{(a^2 + x^2)^2} dx = \frac{x}{2a^2(x^2 + a^2)} + \frac{1}{a^3} \tan^{-1} \frac{x}{a}$$

To put our integral into this form we can substitute x = u and $a = \hbar/(2\Delta x)$ to obtain

$$\frac{\hbar^3}{4\Delta x^3\pi} \left[\frac{u}{2\left(1/\left(4\Delta x^2\right)\right)\left(u^2 + \hbar^2/\left(4\Delta x^2\right)\right)} + \frac{4\Delta x^3}{\hbar^3} \tan^{-1} \left(\frac{2\Delta xu}{\hbar}\right) \right]_{u=-\infty}^{u=-\infty}$$

The first term goes asymptotically to zero as 1/u as u goes to $\pm \infty$, so it can be neglected. Using $\tan^{-1} \pm \infty = \pm \pi/2$,

$$\frac{\hbar^3}{4\Delta x^3 \pi} \left[\frac{4\Delta x^3}{\hbar^3} \left(\frac{\pi}{2} - \left(-\frac{\pi}{2} \right) \right) \right]$$
= 1

So the Fourier transform is indeed normalized.

(c) There are many different definitions of the 'width' of a function. Most of them give the distance from the center of the function where the function falls of to some fraction of its central value. One of the most common such measures is the full-width at half-maximum or FWHM

that measures the full width of the function when it has fallen to half of its peak value. Since $\phi(p_x)$ can in general be complex we should specify that we mean the magnitude $|\phi(p_x)|$ falls to half its central value although for this particular function ϕ is real, so $|\phi(p_x)| = \phi(p_x)$. The function is peaked at $p_x = p_0$ where

$$\phi(p_0) = \frac{1}{2} \sqrt{\frac{\hbar^3}{\Delta x^3 \pi}} \left[\frac{1}{\hbar^2 / (4\Delta x^2) + (-p_x + p_0)^2} \right]$$
$$= \frac{1}{2} \sqrt{\frac{\hbar^3}{\Delta x^3 \pi}} \left[\frac{1}{\hbar^2 / (4\Delta x^2)} \right]$$
$$= 2\sqrt{\frac{\Delta x}{\hbar \pi}}$$

To find the FWHM we find for what value of p_x the function is equal to $\sqrt{\frac{\Delta x}{\hbar \pi}}$

$$\frac{1}{2}\sqrt{\frac{\hbar^3}{\Delta x^3\pi}} \left[\frac{1}{\hbar^2/(4\Delta x^2) + (-p_x + p_0)^2} \right] = \sqrt{\frac{\Delta x}{\hbar\pi}}$$

$$\frac{1}{2}\sqrt{\frac{\hbar^3}{\Delta x^3\pi}} \left[\frac{\frac{4\Delta x^2}{\hbar^2}}{1 + \frac{4\Delta x^2}{\hbar^2}(-p_x + p_0)^2} \right] = \sqrt{\frac{\Delta x}{\hbar\pi}}$$

$$\frac{1}{1 + \frac{4\Delta x^2}{\hbar^2}(-p_x + p_0)^2} = \frac{1}{2}$$

in order to get this we require that

$$\frac{4\Delta x^2}{\hbar^2}(-p_x + p_0)^2 = 1$$
$$(-p_x + p_0)^2 = \frac{\hbar^2}{4\Delta x^2}$$
$$p_x = p_0 \pm \frac{\hbar}{2\Delta x}$$

So we can define $(\Delta p_x)_{\text{FWHM}} \equiv \frac{\hbar}{\Delta x}$ and $(\Delta p_x)_{\text{FWHM}} \Delta x = \hbar$, as expected from the uncertainty principle.

Other reasonable definitions of the width are equally valid. As long as they are reasonable $\Delta x \Delta p_x$ will be within an order of magnitude of \hbar .

2 (Textbook 2.13) A beam of monoenergetic electrons is used to raise atoms to an excited state in a Franck-Hertz experiment. If this excited state has a lifetime of 10^{-9} s, calculate the spread in energy of the inelastically scattered electrons.

Solution: The time-energy uncertainty relation $\Delta E \Delta t \geq \hbar$ gives a lower bound on the uncertainty in energy that will show up experimentally as a spread in the energy $\Delta E \geq \hbar/\Delta t$. Using the excited state lifetime as the time uncertainty,

$$\Delta E \ge \frac{\hbar}{\Delta t}$$

$$\Delta E \ge \frac{1.055 \times 10^{-34} J \cdot s}{10^{-9} s}$$

$$\Delta E \ge 1.055 \times 10^{-25} J$$

$$\Delta E \ge 3.4 \times 10^{-7} eV$$

So the spread is very small, less than a millionth of an electron volt, but this is still a realistic number.

3 Nuclei, typically of size 10^{-14} m, emit electrons with energies in the range 1-10 MeV. Show that electrons of these energies can't be contained in the nucleus. (Hint: Use the uncertainty relation)

Solution: Assume that the electrons are free. This is a good assumption since 1-10 MeV is far more energy than the binding energy holding the electron to the atom. In this case we can obtain a range of momenta corresponding to this range of energies. Since the energy range is not small compared to the electron rest mass-energy of 511 KeV we need to use the relativistic expressions for energy.

$$E = \sqrt{m^2c^4 + p^2c^2}$$

$$E^2 = m^2c^4 + p^2c^2$$

$$p = \sqrt{E^2/c^2 - m^2c^2}$$

When E = 1 MeV,

$$p_1 = \sqrt{\frac{\left[(10^6 eV)(1.602 \times 10^{-19} J/eV) \right]^2}{\left[3 \times 10^8 m/s \right]^2} - \left[9.11 \times 10^{-31} kg \right]^2 \left[3 \times 10^8 m/s \right]^2}$$

$$p = 4.59 \times 10^{-22} kg \cdot m/s$$

When E = 10 MeV,

$$p_{10} = \sqrt{\frac{\left[(10^7 eV)(1.602 \times 10^{-19} J/eV) \right]^2}{\left[3 \times 10^8 m/s \right]^2} - \left[9.11 \times 10^{-31} kg \right]^2 \left[3 \times 10^8 m/s \right]^2}$$

$$p = 5.33 \times 10^{-21} kg \cdot m/s$$

Subtracting these two gives us a range for the uncertainty in the momentum.

$$\Delta p = p_{10} - p_1 = 4.87 \times 10^{-21} kg \cdot m/s$$

The Heisenberg uncertainty principle gives us a lower bound on the position uncertainty of the electrons corresponding to this degree of momentum uncertainty.

$$\Delta x \ge \frac{\hbar}{\Delta p}$$

$$\Delta x \ge \frac{1.055 \times 10^{-34} J \cdot s}{4.87 \times 10^{-21} kg \cdot m/s}$$

$$\Delta x \ge 2.2 \times 10^{-14} m$$

4 Consider the following wave function:

$$\psi(x) = Nxe^{-\alpha x} \qquad x > 0$$

$$= 0 \qquad x < 0$$

- (a) Find N.
- (b) Where does the probability $|\psi(x)|$ peak?
- (c) What is the probability of finding the particle between 0 and $1/\alpha$?
- (d) Find $\phi(p)$.

Solution:

(a) Normalization proceeds as in the first question. We require that

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, \mathrm{d}x = 1$$

Plugging in the definition for $\psi(x)$ and reducing the range of the integral to be 0 to ∞ since $\psi(x) = 0$ for x < 0 we get

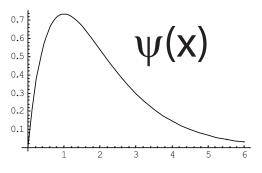
$$\int_0^\infty |Nxe^{-\alpha x}|^2 dx$$
$$= |N|^2 \int_0^\infty x^2 e^{-2\alpha x} dx$$

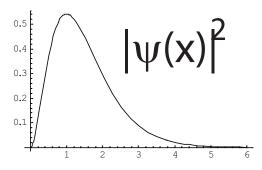
Making a change of variables to $u=2\alpha x,\ x=u/(2\alpha),\ \mathrm{d} x=\mathrm{d} u/(2\alpha),\ u\to\infty$ when $x\to\infty$ and $u\to0$ when $x\to0$,

$$\int_0^\infty |Nxe^{\alpha x}|^2 dx$$

$$= |N|^2 \int_0^\infty \frac{u^2}{4\alpha^2} e^{-u} \frac{du}{2\alpha}$$

$$= \frac{|N|^2}{8\alpha^3} \int_0^\infty u^2 e^{-u} du$$





With $\alpha=1$

This integral can be looked up in a table, solved with Mathematica or Maple or evaluated with integration by parts. We'll do the latter. Setting $t = u^2$, dt = 2udu and $ds = e^{-u}du$, $s = -e^{-u}$,

$$\int_0^\infty u^2 e^{-u} du$$

$$= -u^2 e^{-u} \Big|_{u=0}^{u=\infty} + 2 \int_0^\infty u e^{-u}$$

$$= 2 \int_0^\infty u e^{-u} du$$

Setting t = u, dt = du and $ds = e^{-u}du$, $s = -e^{-u}$,

$$\int_0^\infty u^2 e^{-2u} du$$

$$= 2 \left[u e^{-u} \Big|_{u=0}^{u=\infty} + \int_0^\infty e^{-u} du \right]$$

$$= 2 \left[-e^{-u} \Big|_0^\infty \right]$$

$$= 2$$

So

$$1 = \frac{|N|^2}{8\alpha^3} \int_0^\infty u^2 e^{-u} du$$
$$1 = \frac{|N|^2}{4\alpha^3}$$

Which means that $|N|=2\alpha^{3/2}$. Again we'll follow convention and keep the phase as zero so that N is real and say $N=2\alpha^{3/2}$. So finally

$$\psi(x) = 2\alpha^{3/2}xe^{-\alpha x}$$

(b) We can find extrema in the probability by setting the derivative

of $|\psi(x)|^2$ with respect to x to zero and solving for x.

$$\frac{\mathrm{d}|\psi(x)|^2}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}x} 4\alpha^3 x^2 e^{-2\alpha x}$$
$$= 4\alpha^3 \left(2xe^{-2\alpha x} + x^2(-2\alpha)e^{-2\alpha x}\right)$$

Setting this equal to zero,

$$4\alpha^{3} \left(2xe^{-2\alpha x} - 2x^{2}\alpha e^{-2\alpha x}\right) = 0$$
$$8\alpha^{3}xe^{-2\alpha x}(1 - x\alpha) = 0$$
$$x = \left\{\frac{1}{\alpha}, 0\right\}$$

If we plot the function (see figure), we see that the solution at $x = \frac{1}{\alpha}$ is the maximum.

(c) The probability of finding the particle between zero and $1/\alpha$ is given by the integral of the absolute square of the wavefunction over that integral. Note that we expect the probability to just be a number so there shouldn't be any α 's in the answer. We'll use the same change of variables as in part (a).

$$P(x \in \{0, 1/\alpha\}) = 4\alpha^3 \int_0^{1/\alpha} x^2 e^{-2\alpha x} dx$$
$$= 4\alpha^3 \int_0^2 \frac{u^2}{4\alpha^2} e^{-u} \frac{du}{2\alpha}$$
$$= \frac{1}{2} \int_0^2 u^2 e^{-u} du$$

This is indeed just a number, so we're doing well. Integrating by parts with $t=u^2$, $\mathrm{d}t=2u\mathrm{d}u$, $\mathrm{d}s=e^{-u}\mathrm{d}u$, $s=-e^{-u}$

$$P(x \in \{0, 1/\alpha\}) = \frac{1}{2} \left[-u^2 e^{-u} \Big|_{u=0}^{u=2} + 2 \int_0^2 u e^{-u} du \right]$$
$$= \frac{1}{2} \left[-4e^{-2} + 2 \int_0^2 u e^{-u} du \right]$$

Integrating by parts again, with t = u, dt = du, $ds = e^{-u}du$, $s = -e^{-u}$,

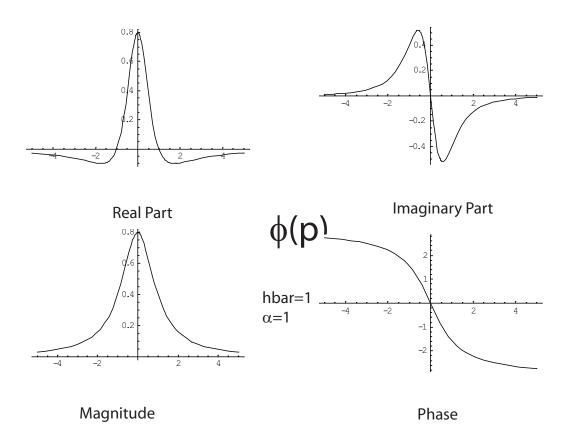
$$P(x \in \{0, 1/\alpha\}) = -2e^{-2} + -ue^{-u}\Big|_{u=0}^{u=2} + \int_{0}^{2} e^{-u} du$$

$$= -2e^{-2} - 2e^{-2} + \left[-e^{-u}\right]_{u=0}^{u=2}$$

$$= -4e^{-2} + (-e^{-2} + 1)$$

$$= 1 - 5e^{-2}$$

$$\approx 0.323$$



So the probability of finding the particle between x=0 and $x=\alpha$ is 32%.

(d) To find $\phi(p)$ we do the same thing we did in question 1. Again, before starting we'll try to use the Fourier transform properties to know what to expect. The $\psi(x)$ is neither even nor odd, but it is real, so $\phi(p)$ should have an even real part and an odd imaginary part. Also the width of $\psi(x)$ is $1/\alpha$, so the width of $\phi(p)$ should be on the order of $\hbar\alpha$.

Applying equation (2.41) from the textbook we have

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \psi(x) dx$$
$$= \frac{1}{\sqrt{2\pi\hbar}} \int_{0}^{\infty} e^{-ipx/\hbar} 2\alpha^{3/2} x e^{-\alpha x} dx$$
$$= \sqrt{\frac{2\alpha^{3}}{\pi\hbar}} \int_{0}^{\infty} e^{[-ip/\hbar - \alpha]x} x dx$$

Integrating by parts with t=x, $\mathrm{d}t=\mathrm{d}x$ and $\mathrm{d}s=e^{[-ip/\hbar-\alpha]x}\mathrm{d}x$, $s=\frac{e^{[-ip/\hbar-\alpha]x}}{-ip/\hbar-\alpha}$,

$$\phi\left(p\right) = \sqrt{\frac{2\alpha^{3}}{\pi\hbar}} \left[\frac{xe^{[-ip/\hbar - \alpha]x}}{-ip/\hbar - \alpha} \right]_{0}^{\infty} - \sqrt{\frac{2\alpha^{3}}{\pi\hbar}} \frac{1}{-ip/\hbar - \alpha} \int_{0}^{\infty} e^{[-ip/\hbar - \alpha]x} dx$$

The first term vanishes at both limits. At infinity because the exponential goes to zero (or at least the real exponential does - the imaginary part is non-zero but finite so when it gets multiplied by zero it goes to zero), and at 0 because of the x term. So we have

$$\phi(p) = -\sqrt{\frac{2\alpha^3}{\pi\hbar}} \frac{1}{(-ip/\hbar - \alpha)^2} \left[e^{[-ip/\hbar - \alpha]x} \right]_0^{\infty}$$

$$= \sqrt{\frac{2\alpha^3}{\pi\hbar}} \frac{1}{(-ip/\hbar - \alpha)^2}$$

$$= \sqrt{\frac{2\alpha^3}{\pi\hbar}} \frac{1}{(ip/\hbar + \alpha)^2}$$

$$= \sqrt{\frac{2\alpha^3}{\pi\hbar}} \frac{(ip/\hbar - \alpha)(ip/\hbar - \alpha)}{(ip/\hbar + \alpha)(ip/\hbar - \alpha)(ip/\hbar + \alpha)(ip/\hbar - \alpha)}$$

$$= \sqrt{\frac{2\alpha^3}{\pi\hbar}} \frac{(\alpha - ip/\hbar)^2}{(\alpha^2 + p^2/\hbar^2)^2}$$

$$= \sqrt{\frac{2\alpha^3}{\pi\hbar}} \frac{(\alpha^2 - p^2/\hbar^2) - 2i\alpha p/\hbar}{(\alpha^2 + p^2/\hbar^2)^2}$$

So, as expected the real part is even in p and the imaginary part is odd in p.