# Quantum Mechanics I - PSet 5

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**Note:** In previous problem sheets we used the following Fourier transform

$$\phi(p) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \psi(x) e^{-i\frac{p}{\hbar}x} dx, \tag{1.1}$$

instead of the more common quantum mechanics normalization

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \psi(x) e^{-i\frac{p}{\hbar}x} dx. \tag{1.2}$$

The latter leads to a normalized wavefunction in momentum space while the former does not.

## Exercise 1

- (a) Let's start by normalizing the (spatial) wavefunction

$$\begin{aligned} 1 &= \int_{\mathbb{R}} \psi^*(x)\psi(x)dx = N^2 \int_{\mathbb{R}} e^{-\frac{x^2}{a^2}} dx \\ &= |N|^2 a\sqrt{\pi}. \end{aligned} \tag{1.3}$$

Thus, taking $N \in \mathbb{R}_+$, we have

$$N = \frac{1}{\sqrt{a}\pi^{1/4}}. \tag{1.4}$$

Since $(\Delta Q)^2 = \langle \hat{Q}^2 \rangle - \langle \hat{Q} \rangle^2$, we compute (using the given integrals and the Gaussian integral)

$$\begin{aligned} \langle \hat{x} \rangle &= N^2 \int_{\mathbb{R}} x \exp\left(-\frac{x^2}{a^2}\right) dx = -N^2 \left(\frac{a^2}{2}\right) \int_{\mathbb{R}} \left(\frac{-2x}{a^2}\right) \exp\left(-\frac{x^2}{a^2}\right) dx \\ &= -N^2 \left(\frac{a^2}{2}\right) \exp\left(-\frac{x^2}{a^2}\right) \Big|_{-\infty}^{\infty} = 0, \end{aligned} \tag{1.5}$$

and

$$\langle \hat{x}^2 \rangle = N^2 \int_{\mathbb{R}} x^2 \exp\left(-\frac{x^2}{a^2}\right) dx = \frac{N^2 a^3 \sqrt{\pi}}{2} = \frac{a^2}{2}. \tag{1.6}$$

Therefore,

$$\Delta x = \sqrt{\frac{a^2}{2}} = \frac{a}{\sqrt{2}}. \tag{1.7}$$

For momentum, we have

$$\begin{aligned} \langle \hat{p} \rangle &= \frac{iN^2\hbar}{a^2} \int_{\mathbb{R}} \exp\left(-\frac{x^2}{2a^2}\right) x \exp\left(-\frac{x^2}{2a^2}\right) dx = \\ &= \frac{iN^2\hbar}{a^2} \int_{\mathbb{R}} x \exp\left(-\frac{x^2}{a^2}\right) dx = 0, \end{aligned} \tag{1.8}$$

by the same reason as before, and

$$\begin{aligned}
\langle \hat{p}^2 \rangle &= -N^2\hbar^2 \int_{\mathbb{R}} \exp\left(-\frac{x^2}{2a^2}\right) \frac{d}{dx}\left[\left(-\frac{x}{a^2}\exp\left(-\frac{x^2}{2a^2}\right)\right)\right] dx \\
&= \frac{N^2\hbar^2}{a^2} \int_{\mathbb{R}} \left[\exp\left(-\frac{x^2}{a^2}\right) - \frac{x^2}{a^4}\exp\left(-\frac{x^2}{a^2}\right)\right] dx \\
&= \frac{N^2\hbar^2}{a^2}\left[a\sqrt{\pi} - \frac{\sqrt{\pi}}{2a}\right] = \frac{N^2\hbar^2\sqrt{\pi}}{2a} \\
&= \frac{\hbar^2}{2a^2},
\end{aligned} \tag{1.9}$$

and thus

$$\Delta p = \frac{\hbar}{a\sqrt{2}}. \tag{1.10}$$

Finally, we confirm that

$$\Delta x \Delta p = \frac{\hbar}{a\sqrt{2}} \frac{a}{\sqrt{2}} = \frac{\hbar}{2}, \tag{1.11}$$

concluding that a Gaussian wavefunction minimizes Heisenberg's uncertainty product.

**Remark 1.1.** *Not quite sure how we can avoid computing $N$.*

- (b) By Fourier transform, we have

$$\begin{aligned}
\phi(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \psi(x) e^{-i\frac{p}{\hbar}x} dx = \frac{N}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} e^{-\frac{x^2}{2a^2}} e^{-i\frac{p}{\hbar}x} dx \\
&= \frac{N}{\sqrt{2\pi}} \left(\sqrt{2\pi} a \exp\left(-\frac{a^2p^2}{2\hbar^2}\right)\right) \\
&= \frac{\sqrt{a}}{\pi^{1/4}\sqrt{\hbar}} \exp\left(-\frac{a^2}{2\hbar^2}p^2\right).
\end{aligned} \tag{1.12}$$

Parseval's identity states the following

$$\int_{\mathbb{R}} |\psi(x)|^2 dx = \int_{\mathbb{R}} |\phi(p)|^2 dp. \tag{1.13}$$

We have

$$\int_{\mathbb{R}} |\phi(p)|^2 dp = \frac{a}{\sqrt{\pi}\hbar} \int_{\mathbb{R}} \exp\left(-\frac{a^2}{\hbar^2}p^2\right) = \frac{a}{\sqrt{\pi}\hbar}\sqrt{\frac{\pi\hbar^2}{a^2}} = 1, \tag{1.14}$$

confirming the identity. We now recalculate $\Delta p$ using momentum space. Again

$$\langle \hat{p} \rangle = \frac{\sqrt{a}}{\pi^{1/4}\sqrt{\hbar}} \int_{\mathbb{R}} p \exp\left(-\frac{a^2}{\hbar^2}p^2\right) dp = 0, \tag{1.15}$$

by the same reasons as above, and

$$\begin{aligned}
\langle \hat{p}^2 \rangle &= \frac{a}{\sqrt{\pi}\hbar} \int_{\mathbb{R}} p^2 \exp\left(-\frac{a^2}{\hbar^2}p^2\right) dp = \frac{a}{\sqrt{\pi}\hbar}\left(\frac{\hbar^2}{2a^2}\sqrt{\frac{\pi\hbar^2}{a^2}}\right) \\
&= \frac{\hbar^2}{2a^2},
\end{aligned} \tag{1.16}$$

confirming what we obtained before, i.e.

$$\Delta p = \frac{\hbar}{a\sqrt{2}}. \tag{1.17}$$

# Exercise 2

Let us start by proving the given relation, i.e.

$$\Re\left(\frac{1}{z}\right) = \frac{\Re(z)}{|z|^2}. \tag{1.18}$$

$$\Re\left(\frac{1}{z}\right) = \Re\left(\frac{z^*}{zz^*}\right) = \Re\left(\frac{z^*}{|z|^2}\right) = \frac{1}{|z|^2}\Re\left(z^*\right) = \frac{1}{|z|^2}\Re\left(z\right) = \Re\left(\frac{z}{|z|^2}\right). \tag{1.19}$$

- (a) Let's start by normalizing the (spatial) wavefunction

$$\begin{aligned} 1 &= \int_{\mathbb{R}} \psi^*(x)\psi(x)dx = N^2 \int_{\mathbb{R}} e^{-\frac{x^2}{2(\Delta^2)^*}} e^{-\frac{x^2}{2\Delta^2}} dx \\ &= |N|^2 \int_{\mathbb{R}} e^{-\frac{x^2}{2}\left(\frac{1}{(\Delta)^2}+\frac{1}{(\Delta^2)^*}\right)} dx = N^2 \int_{\mathbb{R}} e^{-\frac{x^2}{2}\left(2\frac{\Re(\Delta^2)}{|\Delta|^4}\right)} dx \\ &= |N|^2 \int_{\mathbb{R}} e^{-\left(\frac{\Re(\Delta^2)}{|\Delta|^4}\right)x^2} dx \\ &= |N|^2|\Delta|^2\sqrt{\frac{\pi}{\Re(\Delta^2)}}. \end{aligned} \tag{1.20}$$

Thus, taking $N \in \mathbb{R}_+$, we have

$$N = \frac{(\Re(\Delta^2))^{1/4}}{|\Delta|\pi^{1/4}}. \tag{1.21}$$

**Remark 1.2.** *As a sanity check, if $\Delta \in \mathbb{R}$ we recover the previous normalization, i.e.*

$$N = \frac{1}{\sqrt{\Delta}\pi^{1/4}}. \tag{1.22}$$

We have

$$\begin{aligned} \langle \hat{x} \rangle &= N^2 \int_{\mathbb{R}} x \exp\left(-\frac{1}{2}\frac{x^2}{(\Delta^2)^*}\right) \exp\left(-\frac{1}{2}\frac{x^2}{(\Delta^2)}\right)dx \\ &= N^2 \int_{\mathbb{R}} x e^{-\left(\frac{\Re(\Delta^2)}{|\Delta|^4}\right)x^2} dx = 0, \end{aligned} \tag{1.23}$$

by the same computations as in exercise 1. We now have

$$\begin{aligned} \langle \hat{x}^2 \rangle &= N^2 \int_{\mathbb{R}} x^2 \exp\left(-\frac{1}{2}\frac{x^2}{(\Delta^2)^*}\right) \exp\left(-\frac{1}{2}\frac{x^2}{(\Delta^2)}\right)dx \\ &= N^2 \int_{\mathbb{R}} x^2 e^{-\left(\frac{\Re(\Delta^2)}{|\Delta|^4}\right)x^2} dx \\ &= N^2 \frac{|\Delta|^4}{2\Re(\Delta^2)}\sqrt{\frac{\pi|\Delta|^4}{\Re(\Delta^2)}} \\ &= \frac{\sqrt{\Re(\Delta^2)}}{|\Delta|^2\sqrt{\pi}} \frac{|\Delta|^4}{2\Re(\Delta^2)}\sqrt{\frac{\pi|\Delta|^4}{\Re(\Delta^2)}} \\ &= \frac{|\Delta|^4}{2\Re(\Delta^2)}. \end{aligned} \tag{1.24}$$

**Remark 1.3.** *Again, as a sanity check, if $\Delta \in \mathbb{R}$ we recover the previous result, i.e.*

$$\langle \hat{x}^2 \rangle = \frac{\Delta^2}{2}. \tag{1.25}$$

We conclude then that

$$\Delta x = \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2} = \frac{|\Delta|^2}{\sqrt{2\Re(\Delta^2)}}. \tag{1.26}$$

For the momentum, we have

$$\begin{aligned} \langle \hat{p} \rangle &= -N^2 \frac{\hbar}{i} \int_{\mathbb{R}} \exp\left(-\frac{1}{2}\frac{x^2}{(\Delta^2)^*}\right)\left(\frac{x}{\Delta^2}\right)\exp\left(-\frac{1}{2}\frac{x^2}{(\Delta^2)}\right)dx \\ &= -N^2 \frac{\hbar}{i\Delta^2} \int_{\mathbb{R}} x e^{-\left(\frac{\Re(\Delta^2)}{|\Delta|^4}\right)x^2} dx = 0, \end{aligned} \tag{1.27}$$

as before. We now compute

$$\begin{aligned} \langle \hat{p}^2 \rangle &= N^2\hbar^2 \int_{\mathbb{R}} \exp\left(-\frac{1}{2}\frac{x^2}{(\Delta^2)^*}\right)\frac{d}{dx}\left[\left(\frac{x}{\Delta^2}\right)\exp\left(-\frac{1}{2}\frac{x^2}{(\Delta^2)}\right)\right]dx \\ &= N^2\hbar^2 \int_{\mathbb{R}} \exp\left(-\frac{1}{2}\frac{x^2}{(\Delta^2)^*}\right)\left[\frac{1}{\Delta^2} - \frac{x^2}{\Delta^4}\right]\exp\left(-\frac{1}{2}\frac{x^2}{(\Delta^2)}\right)dx \\ &= N^2\hbar^2 \left[\frac{1}{\Delta^2}\int_{\mathbb{R}} e^{-\left(\frac{\Re(\Delta^2)}{|\Delta|^4}\right)x^2}dx - \frac{1}{\Delta^4}\int_{\mathbb{R}} x^2 e^{-\left(\frac{\Re(\Delta^2)}{|\Delta|^4}\right)x^2}dx\right] \\ &= \frac{N^2\hbar^2}{\Delta^2}\sqrt{\frac{\pi|\Delta|^4}{\Re(\Delta^2)}} - \frac{N^2\hbar^2}{\Delta^4}\frac{|\Delta|^4}{2\Re(\Delta^2)}\sqrt{\frac{\pi|\Delta|^4}{\Re(\Delta^2)}} \\ &= \frac{\sqrt{\Re(\Delta^2)}}{|\Delta|^2\sqrt{\pi}}\frac{\hbar^2}{\Delta^2}\left(\sqrt{\frac{\pi|\Delta|^4}{\Re(\Delta^2)}}\right) - \frac{\sqrt{\Re(\Delta^2)}}{|\Delta|^2\sqrt{\pi}}\frac{\hbar^2|\Delta|^4}{2\Re(\Delta^2)\Delta^4}\sqrt{\frac{\pi|\Delta|^4}{\Re(\Delta^2)}} \\ &= \frac{\hbar^2}{\Delta^2} - \frac{\hbar^2|\Delta|^4}{2\Re(\Delta^2)\Delta^4}. \end{aligned} \tag{1.28}$$

**Remark 1.4.** *Again, we can check that taking $\Delta \in \mathbb{R}$ recovers the result of exercise 1, i.e.*

$$\frac{\hbar^2}{2\Delta^2}. \tag{1.29}$$

This is a complex value, if we let $\Delta = |\Delta|e^{i\phi_\Delta}$ and take the real part one obtains

$$\frac{1}{\Delta^2} = \frac{e^{-2i\phi_\Delta}}{|\Delta|^2}, \quad \Re(\Delta^2) = |\Delta|^2\cos(2\phi_\Delta). \tag{1.30}$$

Therefore

$$\langle \hat{p}^2 \rangle = \frac{\hbar^2 e^{-2i\phi_\Delta}}{|\Delta|^2}\left(1 - \frac{e^{-2i\phi_\Delta}}{2\cos(2\phi_\Delta)}\right), \tag{1.31}$$

and

$$\Re(\langle p^2 \rangle) = \frac{\hbar^2}{|\Delta|^2}\Re\left\{e^{-2i\phi_\Delta}\left(1 - \frac{e^{-2i\phi_\Delta}}{2\cos(2\phi_\Delta)}\right)\right\} = \frac{\hbar^2}{2\,\Re(\Delta^2)}. \tag{1.32}$$

Thus

$$\Delta p = \sqrt{\Re(\langle p^2 \rangle)} = \frac{\hbar}{\sqrt{2\Re(\Delta^2)}}. \tag{1.33}$$

- (b) By Fourier transform, we have

$$\begin{aligned} \phi(p) &= \frac{N}{\sqrt{2\pi\hbar}}\int_{\mathbb{R}} \psi(x) e^{-i\frac{p}{\hbar}x}dx = \frac{N}{\sqrt{2\pi\hbar}}\int_{\mathbb{R}} e^{-\frac{x^2}{2\Delta^2} - i\frac{p}{\hbar}x}dx \\ &= \frac{N}{\sqrt{2\pi\hbar}}\sqrt{2\pi}\Delta\exp\left(-\frac{2\Delta^2 p^2}{4\hbar^2}\right) \\ &= \frac{(\Re(\Delta^2))^{1/4}}{|\Delta|\pi^{1/4}}\frac{\Delta}{\sqrt{\hbar}}\exp\left(-\frac{\Delta^2 p^2}{2\hbar^2}\right). \end{aligned} \tag{1.34}$$

Parseval's identity states the following

$$\int_{\mathbb{R}} |\psi(x)|^2 dx = \int_{\mathbb{R}} |\phi(p)|^2 dp, \tag{1.35}$$

and we have

$$\begin{aligned}
\int_{\mathbb{R}} |\phi(p)|^2 dp &= \frac{|\Delta|^2 \sqrt{\Re(\Delta^2)}}{|\Delta|^2 \sqrt{\pi}\hbar} \int_{\mathbb{R}} \exp\left(-\frac{(\Delta^2)^* p^2}{2\hbar^2}\right) \exp\left(-\frac{(\Delta^2) p^2}{2\hbar^2}\right) dx \\
&= \frac{\sqrt{\Re(\Delta^2)}}{\sqrt{\pi}\hbar} \int_{\mathbb{R}} \exp\left(-\frac{p^2 \Re(\Delta^2)}{\hbar^2}\right) dx \\
&= \frac{\sqrt{\Re(\Delta^2)}}{\sqrt{\pi}\hbar} \sqrt{\frac{\pi \hbar^2}{\Re(\Delta^2)}} \\
&= 1.
\end{aligned} \tag{1.36}$$

We now recalculate $\Delta p$ in momentum space, we have

$$\begin{aligned}
\langle \hat{p} \rangle &= \frac{\sqrt{\Re(\Delta^2)}}{|\Delta|^2 \sqrt{\pi}} \frac{|\Delta|^2}{\hbar} \int_{\mathbb{R}} \exp\left(-\frac{(\Delta^2)^* p^2}{2\hbar^2}\right) p \exp\left(-\frac{\Delta^2 p^2}{2\hbar}\right) dp \\
&= \frac{\sqrt{\Re(\Delta^2)}}{\hbar \sqrt{\pi}} \int_{\mathbb{R}} p \exp\left(-\frac{p^2 \Re(\Delta^2)}{\hbar^2}\right) dp \\
&= 0,
\end{aligned} \tag{1.37}$$

since it is an odd integral as before, we also have

$$\begin{aligned}
\langle \hat{p}^2 \rangle &= \frac{\sqrt{\Re(\Delta^2)}}{\hbar \sqrt{\pi}} \int_{\mathbb{R}} p^2 \exp\left(-\frac{p^2 \Re(\Delta^2)}{\hbar^2}\right) dp \\
&= \frac{\sqrt{\Re(\Delta^2)}}{\hbar \sqrt{\pi}} \frac{\hbar^2}{2\Re(\Delta^2)} \hbar \sqrt{\frac{\pi}{\Re(\Delta^2)}} \\
&= \frac{\hbar^2}{2\Re(\Delta^2)},
\end{aligned} \tag{1.38}$$

as before. Thus

$$\Delta p = \sqrt{\langle p^2 \rangle} = \frac{\hbar}{\sqrt{2\Re(\Delta^2)}}. \tag{1.39}$$

- (c) Parameterize $\Delta$ by the real phase $\phi_\Delta$, i.e.

$$\Delta = |\Delta| e^{i\phi_\Delta}. \tag{1.40}$$

We have then

$$\begin{aligned}
\Delta x \Delta p &= \frac{|\Delta|^2}{\sqrt{2\Re(\Delta^2)}} \frac{\hbar}{\sqrt{2\Re(\Delta^2)}} \\
&= \frac{\hbar}{2\cos(2\phi_\Delta)}.
\end{aligned} \tag{1.41}$$

If $\phi_\Delta = 0$ then $\Delta \in \mathbb{R}$ and we have

$$\Delta x \Delta p = \frac{\hbar}{2}, \tag{1.42}$$

as in exercise 1. This results are valid for $\Re(\Delta^2) > 0$, and therefore $\Delta_\phi \in (-\frac{\pi}{4}, \frac{\pi}{4}) \pmod{2\pi}$. Thus, our expression is not valid for $\phi_\Delta = \pi/4$ and in fact

$$\lim_{\phi_\Delta \to \pi/4} \Delta x \Delta p = \lim_{y \to 0^+} \frac{\hbar}{y} = \infty, \tag{1.43}$$

so $\Delta x \Delta p$ diverges.

- (d) From exercise 3 in problems set 4, the time evolution of the given Gaussian wave-packet is

$$\Psi(x,t) = \frac{1}{\pi^{1/4}\sqrt{\Delta}} \sqrt{\frac{1}{1+\frac{i\hbar t}{m\Delta^2}}} \exp\left(-\frac{x^2}{2\Delta^2(1+\frac{i\hbar t}{m\Delta^2})}\right). \tag{1.44}$$

In momentum space, it is given by

$$\Phi(x,t) = \frac{(\Re(\Delta^2))^{1/4}}{|\Delta|\pi^{1/4}} \frac{\Delta}{\sqrt{\hbar}} \exp\left(-\frac{\Delta^2 p^2}{2\hbar^2} - i\frac{p^2}{2m\hbar}t\right). \tag{1.45}$$

At $t=0$ we simply recover our starting time-independent wavefunctions, thus, we must have exactly the same $\Delta p.$ as before, i.e.

$$\Delta p = \frac{\hbar}{\sqrt{2\Re(\Delta^2)}}. \tag{1.46}$$

The time dependent complex "constant" equivalent to $\Delta^2$ in $\Psi(x,t)$ now reads

$$\Delta^2 \left(1 + \frac{i\hbar t}{m\Delta^2}\right). \tag{1.47}$$

We now compute $\Delta p(t)$ in momentum space. For $\langle \hat{p} \rangle$ we still end up with an odd integral and therefore $\langle \hat{p} \rangle = 0$. We now compute

$$\begin{aligned} \langle \hat{p}^2 \rangle &= \frac{\sqrt{\Re(\Delta^2)}}{\hbar\sqrt{\pi}} \int_{\mathbb{R}} \exp\left(-\frac{(\Delta^2)^* p^2}{2\hbar^2} + i\frac{p^2}{2m\hbar}t\right) p^2 \exp\left(-\frac{\Delta^2 p^2}{2\hbar^2} - i\frac{p^2}{2m\hbar}t\right) dp \\ &= \frac{\sqrt{\Re(\Delta^2)}}{\hbar\sqrt{\pi}} \int_{\mathbb{R}} p^2 \exp\left(-\frac{p^2\Re(\Delta^2)}{\hbar^2}\right) dp \\ &= \frac{\hbar^2}{2\Re(\Delta^2)}, \end{aligned} \tag{1.48}$$

which shows that $\Delta p(0) = \Delta p(t)$, for all time $t$. We conclude that for a Gaussian wave-packet, the position uncertainty grows with time, while the momentum uncertainty stays fixed.

# Exercise 3

In this problem we consider a square well with infinite potential barriers together with a particle of mass $m$ free to move in the range $x \in [0,a]$. The potential is given by

$$V(x) = \begin{cases} \infty, & x \leq 0, x \geq a, \\ 0, & 0 \leq x \leq a. \end{cases} \tag{1.49}$$

The solution to this system Schrödinger's equation is

$$\Psi_n(x,t) = N \sin\left(\frac{n\pi}{a}x\right) e^{-i\phi_n(t)}, \quad x \in [0,a], \tag{1.50}$$

for $n \in \mathbb{N}$ with $\Psi_n(x,t) = 0$ for $x < 0$ or $x > a$.

- (a) Substituting in Schrödinger's equation we obtain

$$\hbar\dot{\phi}_n N \sin\left(\frac{n\pi}{a}x\right) e^{-i\phi_n(t)} = N\frac{\hbar^2}{2m}\left(\frac{n^2\pi^2}{a^2}\right) \sin\left(\frac{n\pi}{a}x\right) e^{-i\phi_n(t)}, \tag{1.51}$$

obtaining

$$\dot{\phi}_n = \frac{\hbar n^2 \pi^2}{2ma^2}, \tag{1.52}$$

and thus

$$\phi_n(t) = \frac{\hbar n^2 \pi^2}{2ma^2} t + C, \tag{1.53}$$

for $C \in \mathbb{R}$. Using the normalization condition to compute $N \in \mathbb{R}$ we have

$$1 = N^2 \int_0^a \sin^2\left(\frac{n\pi}{a} x\right) dx, \tag{1.54}$$

leading to

$$N = \sqrt{\frac{2}{a}}. \tag{1.55}$$

- (b) We have

$$\begin{aligned} \langle \hat{x} \rangle &= \frac{2}{a} \int_0^a x \sin^2\left(\frac{n\pi}{a} x\right) dx \\ &= \frac{1}{a} \int_0^a x - x\cos\left(\frac{2n\pi}{a} x\right) dx \\ &= \frac{a}{2} - \frac{1}{2n\pi} \sin\left(\frac{2n\pi}{a} x\right)\Big|_0^a \\ &= \frac{a}{2}, \end{aligned} \tag{1.56}$$

where we used the trigonometric relation

$$\sin^2(x) = \frac{1 - \cos(2x)}{2}. \tag{1.57}$$

We now compute

$$\begin{aligned} \langle \hat{x}^2 \rangle &= \frac{2}{a} \int_0^a x^2 \sin^2\left(\frac{n\pi}{a} x\right) dx \\ &= \frac{1}{a} \int_0^a x^2 - x^2 \cos\left(\frac{2n\pi}{a} x\right) dx \\ &= \frac{a^2}{3} - \frac{1}{a}\left( x^2 \frac{a}{2n\pi} \sin\left(\frac{2n\pi}{a} x\right)\Big|_0^a - \int_0^a x \frac{a}{n\pi} \sin\left(\frac{2n\pi}{a} x\right) dx \right) \\ &= \frac{a^2}{3} + \frac{1}{a}\left( -x \frac{a^2}{2n^2\pi^2} \cos\left(\frac{2n\pi}{a} x\right)\Big|_0^a + \int_0^a \frac{a^2}{2n^2\pi^2} \cos\left(\frac{2n\pi}{a} x\right) dx \right) \\ &= \frac{a^2}{3} - \frac{a^2}{2n^2\pi^2} + \frac{a^2}{2n^2\pi^2} \sin\left(\frac{2n\pi}{a} x\right)\Big|_0^a \\ &= \frac{a^2}{3} - \frac{a^2}{2n^2\pi^2}. \end{aligned} \tag{1.58}$$

Therefore

$$\begin{aligned} \Delta x = \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2} &= \sqrt{\frac{a^2}{3} - \frac{a^2}{2n^2\pi^2} - \frac{a^2}{4}} \\ &= a\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}}. \end{aligned} \tag{1.59}$$

- (c) We have

$$
\begin{aligned}
\langle \hat{p} \rangle &= \int_0^a \Psi_n^*(x,0)\,(-i\hbar)\frac{\partial}{\partial x}\Psi_n(x,0)\,dx \\
&= -i\hbar\frac{2}{a}\frac{n\pi}{a}\int_0^a \sin\left(\frac{n\pi x}{a}\right)\cos\left(\frac{n\pi x}{a}\right)dx \\
&= -i\hbar\frac{n\pi}{a^2}\int_0^a \sin\left(\frac{2n\pi x}{a}\right)dx \\
&= \frac{i\hbar}{2a}\cos\left(\frac{2n\pi x}{a}\right)\Big|_0^a \\
&= 0.
\end{aligned}
\tag{1.60}
$$

We further have

$$
\begin{aligned}
\langle \hat{p}^2 \rangle &= \int_0^a \Psi_n^*(x)\,(-\hbar^2)\frac{\partial^2}{\partial x^2}\Psi_n(x)\,dx \\
&= \hbar^2\left(\frac{n\pi}{a}\right)^2\int_0^a |\Psi_n(x)|^2 dx \\
&= \hbar^2\left(\frac{n\pi}{a}\right)^2.
\end{aligned}
\tag{1.61}
$$

Thus

$$
\Delta p = \sqrt{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2} = \frac{\hbar n\pi}{a}. \tag{1.62}
$$

- (d) We have

$$
\Delta x \Delta p = \hbar n\pi\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}}. \tag{1.63}
$$

For $n = 1$ we have

$$
(\Delta x \Delta p)_{n=1} \approx 0.568\hbar > \hbar/2. \tag{1.64}
$$

and

$$
(\Delta x \Delta p)_{n=2} \approx 1.67\hbar > \hbar/2. \tag{1.65}
$$

- (e) Because the wavefunction is factorized, each $\Psi_n$ represents a stationary state. As we have seen, stationary states have time-independent expectation values.

# Exercise 4

Consider the potential

$$
V(x) = \begin{cases} 0, & \text{for } x > 0, \\ \infty, & \text{for } x \leq 0. \end{cases} \tag{1.66}
$$

We want to find the stationary states (which are eigenstates of the Hamiltonian operator) and their corresponding energies, keeping in mind these states will not be normalizable. We consider

$$
\Psi(x,t) = \psi(x)\varphi(t), \tag{1.67}
$$

and substitute it in Schrödinger's equation. We have then

$$
i\hbar\varphi'(t)\psi(x) = -\frac{\hbar^2}{2m}\psi''(x)\varphi(t), \tag{1.68}
$$

and therefore

$$i\hbar\frac{\varphi'(t)}{\varphi(t)} = -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)}. \tag{1.69}$$

Since this is to hold for all $x$ and all $t$, we must have

$$i\hbar\frac{\varphi'(t)}{\varphi(t)} = -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} = E, \tag{1.70}$$

for some constant $E \in \mathbb{R}$ (as seen in class this needs to be real). Thus, we have

$$\int_0^t i\hbar\frac{\varphi'(t')}{\varphi(t')}dt' = Et, \tag{1.71}$$

then

$$\ln\varphi(t) - \ln\varphi(0) = \frac{E}{\hbar i}t, \tag{1.72}$$

where we require $\varphi(0) > 0$, and we obtain

$$\varphi(t) = Ce^{-i\frac{E}{\hbar}t}, \tag{1.73}$$

for some $C \in \mathbb{C}$ in general, absorbing all constants. The TISE is given by

$$-\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} = E, \tag{1.74}$$

or equivalently

$$\psi''(x) = -\frac{2mE}{\hbar^2}\psi(x). \tag{1.75}$$

The general solution is given by

$$\psi(x) = Ae^{i\frac{\sqrt{2mE}}{\hbar}x} + Be^{-i\frac{\sqrt{2mE}}{\hbar}x}, \tag{1.76}$$

with $A, B \in \mathbb{C}$. Since $\psi(0) = 0$, by continuity, we have $A = -B$ and therefore

$$\psi(x) = Ae^{i\frac{\sqrt{2mE}}{\hbar}x} - Ae^{-i\frac{\sqrt{2mE}}{\hbar}x} = 2iA\sin(kx), \tag{1.77}$$

where $k = \sqrt{2mE}/\hbar$. Thus, we have $E = k^2\hbar^2/(2m)$. Thus, with only a single barrier, there are no extra conditions imposed on $E$. In particular, the energy is not discretized as in the two barriers case.

**Remark 1.5.** *If we try to normalize the state we get*

$$1 = 4|A|^2\int_0^{+\infty}\sin^2(kx)dx, \tag{1.78}$$

*however the integral diverges.*

**Remark 1.6.** *We can actually look at this case by considering the starting case with barriers at* $x = 0$ *and* $x = a$ *and then take* $\lim a \to \infty$*. We had*

$$E_n = \frac{\hbar^2\pi^2n^2}{2ma^2}. \tag{1.79}$$

*As $a$ becomes very large, the separation between energy levels becomes very small. In the limit, the separation shrinks to zero and we get a continuous spectrum.*

## Exercise 5

Consider the potential

$$V(x) = \begin{cases} 0, & \text{for } x \leq 0, \\ V_0, & \text{for } x > 0. \end{cases} \tag{1.80}$$

We want to find the stationary states which exist for $0 < E < V_0$. We consider simply the TISE since the equation affecting time does not change. For $x \leq 0$ we have

$$-\frac{\hbar^2}{2m}\psi_a''(x) = E\psi_a(x), \tag{1.81}$$

While for $x > 0$ we have

$$-\frac{\hbar^2}{2m}\psi_b''(x) = (E - V_0)\psi_b(x), \tag{1.82}$$

and such that $\psi_a(0) = \psi_b(0)$ and $\psi_a'(0) = \psi_b'(0)$.

- (a) as before, the general solution is given by

$$\psi_a(x) = A_1 e^{i\frac{\sqrt{2mE}}{\hbar}x} + B_1 e^{-i\frac{\sqrt{2mE}}{\hbar}x}. \tag{1.83}$$

- (b) Here, we get

$$\psi_b(x) = A_2 e^{i\frac{\sqrt{2m(E-V_0)}}{\hbar}x} + B_2 e^{-i\frac{\sqrt{2m(E-V_0)}}{\hbar}x}, \tag{1.84}$$

  or equivalently

$$\psi_b(x) = A_2 e^{-kx} + B_2 e^{kx}, \tag{1.85}$$

  where

$$k = \frac{\sqrt{2m(V_0 - E)}}{\hbar}. \tag{1.86}$$

  The continuity conditions give us $A_1 + B_1 = A_2 + B_2$ and

$$iA_1\frac{\sqrt{2mE}}{\hbar} - iB_1\frac{\sqrt{2mE}}{\hbar} = -kA_2 + kB_2. \tag{1.87}$$

Since we have 4 unknowns and only two equations relating them, **we most impose some extra physical conditions**. The problem is a scattering model of a free particle coming from the left and encountering a potential barrier.

Imposing decay at infinity, in the region $x > 0$, we must have $B_2 = 0$. The incident wave $\psi_a$ we consider as follows

$$\psi_a(x) = e^{i\frac{\sqrt{2mE}}{\hbar}x} + Re^{-i\frac{\sqrt{2mE}}{\hbar}x}, \tag{1.88}$$

where we consider the incident magnitude to be 1 (by convention) and $R$ corresponds to the reflected portion (or reflection coefficient).

**Remark 1.7.** *By looking at the phase we can check that $e^{ikx}$ is the part moving to the right, i.e. from $\varphi = kx - \omega t$ and $\varphi = C$, where $C$ is a constant, we have $x = (\omega/k)t + C$, which increases in time.*

We have then, by the continuity conditions, that

$$\begin{cases} 1+R = A_2, \\ i(1-R)\frac{\sqrt{2mE}}{\hbar} = -kA_2, \end{cases} \tag{1.89}$$

and thus

$$i(R-1)\frac{\sqrt{2mE}}{\hbar} = k(1+R) \tag{1.90}$$

$$R\left(i\frac{\sqrt{2mE}}{\hbar} - k\right) = i\frac{\sqrt{2mE}}{\hbar} + k \tag{1.91}$$

$$R = \frac{i\sqrt{2mE} + k\hbar}{i\sqrt{2mE} - k\hbar}. \tag{1.92}$$

To make it clearer we can write

$$R = \frac{ik_1 + k_2}{ik_1 - k_2}, \tag{1.93}$$

where $k_1 = \sqrt{2mE}/\hbar$ and $k_2 = \sqrt{2m(V_0 - E)}/\hbar$. Thus, our wave function is given by

$$\psi(x) = \begin{cases} e^{ik_1x} + \frac{ik_1+k_2}{ik_1-k_2}e^{-ik_1x}, & \text{for } x < 0 \\ \frac{2ik_1}{ik_1-k_2}e^{-k_2x}, & \text{for } x \geq 0. \end{cases} \tag{1.94}$$

Thus, we have a stationary state for each value of the energy satisfying $0 < E < V_0$.

# Exercise 6

Consider a particle of mass $m$ moving through the potential

$$V(x) = \begin{cases} \infty, & \text{for } x < 0, \\ -V_0, & \text{for } 0 < x < a, \\ 0, & \text{for } x > a. \end{cases} \tag{1.95}$$

We want to find the stationary states which exist for $-V_0 < E < 0$. We consider again the TISE and the solutions we found in exercise 5, i.e.

- ($x > a$) Because $E < 0$ the solution in this region is given by

  $$\psi_a(x) = A'e^{-kx}, \tag{1.96}$$

  $A' \in \mathbb{C}$, where we now define (unlike the previous exercise)

  $$k = \frac{\sqrt{2m|E|}}{\hbar}. \tag{1.97}$$

  For convenience when matching boundary conditions we let

  $$\psi_a(x) = Ae^{-k(x-a)}, \tag{1.98}$$

  for $A \in \mathbb{C}$.

- $(0 < x < a)$ Because $E + V_0 > 0$, the solution in this region is given by

$$\psi_b(x) = Be^{-i\kappa x} + Ce^{i\kappa x} \tag{1.99}$$

where we now define

$$\kappa = \frac{\sqrt{2m(V_0 - |E|)}}{\hbar}. \tag{1.100}$$

The boundary conditions we need to satisfy are (assuming continuity)

- $\psi_b(x=0) = 0$, forces $B = -C$, and thus

$$\psi_b(x) = Be^{-i\kappa x} - Be^{i\kappa x} = 2iB\sin(\kappa x) =: D\sin(\kappa x), \tag{1.101}$$

where $D \in \mathbb{C}$.

- $\psi_a(a) = \psi_b(a)$, forces

$$D\sin(\kappa a) = A. \tag{1.102}$$

- $\psi_a'(a) = \psi_b'(a)$ forces

$$-kA = D\kappa\cos(\kappa a). \tag{1.103}$$

Dividing the above equations we get

$$\tan(\kappa a) = -\frac{\kappa}{k} = \sqrt{\frac{2m(V_0 - |E|)}{2m|E|}}. \tag{1.104}$$

We now work with dimensionless parameters, as done in class for the finite square well, let

$$\begin{cases} \xi = \kappa a > 0, \\ \eta = ka > 0, \end{cases} \tag{1.105}$$

and define

$$z_0^2 := a^2(k^2 + \kappa^2) = \frac{2ma^2(V_0 - |E|)}{\hbar^2} + \frac{2ma^2|E|}{\hbar^2} = \frac{2mV_0a^2}{\hbar^2} = \xi^2 + \eta^2. \tag{1.106}$$

Furthermore, we have

$$\tan(\xi) = -\frac{\xi}{\eta}. \tag{1.107}$$

This two equations specify the allowed energies the system can have. The following graph shows their plot.

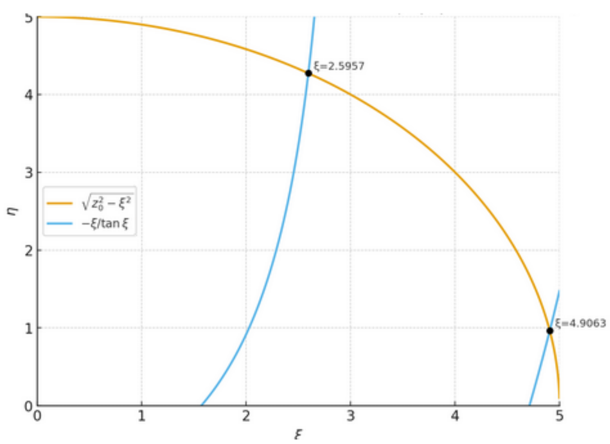


Figure 1: Plot of $\eta(\xi)$ from (1.106) and (1.107).

In **comparison** with the finite square well we notice that this potential is not symmetric (and can not be made symmetric by translation) so we are not constrained to the either even or odd solutions. Furthermore, for small enough energies, we will not have bound states. To obtain (at least) three bound states we need to check where $\eta$ becomes positive, we have

$$\eta(\xi) = -\frac{\xi}{\tan(\xi)}, \tag{1.108}$$

which transitions from negative to positive when $\xi = \frac{\pi}{2} + n\pi$, $n \in \mathbb{N}$. Therefore, we will have at least three bound states for $\xi \geq 5\pi/2$ or equivalently when $z_0 \geq 5\pi/2$.

# Exercise 7

For the finite square well we defined the following in class

$$\begin{cases} \xi^2 := \kappa a = \frac{2ma_0^2}{\hbar^2}|E|, \\ \eta^2 := ka = \frac{2ma_0^2}{\hbar^2}(V_0 - |E|), \end{cases} \tag{1.109}$$

and ultimately found the relation

$$\xi = \eta \tan(\eta). \tag{1.110}$$

If we let $|E| = 13.6eV$, with $a_0$ being the Bohr radius, we just need to find the $V_0$ which solves the last equation. Solving the equation numerically we obtain

$$V_0 \approx 23.669\, eV, \tag{1.111}$$

which agrees with the requirement that $-V_0 < E$.

# Exercise 8

Consider a real stationary state $\psi(x)$ with energy $E$ satisfying

$$-\frac{\hbar^2}{2m}\psi''(x) + [V(x) - E]\psi(x) = 0. \tag{1.112}$$

- (a) We need to prove that $E > V_{\min}(x)$ by using the fact that $\langle \hat{H} \rangle = E$. We have

$$\begin{aligned} E = \langle \hat{H} \rangle &= \int_{\mathbb{R}} \psi(x) \left( -\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) \right) dx \\ &= \int_{\mathbb{R}} \psi^2(x)V(x) + \left( \frac{\hbar^2}{2m}\psi'^2(x) \right) dx \\ &\geq \int_{\mathbb{R}} \psi^2(x)V_{min} + \left( \frac{\hbar^2}{2m}\psi'^2(x) \right) dx \\ &\geq V_{min} + \int_{\mathbb{R}} \frac{\hbar^2}{2m}\psi'^2(x)dx \\ &\geq V_{min}, \end{aligned} \tag{1.113}$$

  where we used integration by parts and assumed the state is normalized. Let $V_{min} = \inf_x V(x)$ and suppose $E = V_{min}$, then we obtain

$$0 \geq \int_{\mathbb{R}} \frac{\hbar^2}{2m}\psi'^2(x)dx, \tag{1.114}$$

and therefore $\psi'(x) = 0$. However $\psi(x)$ must be nonzero and can not be constant since in that case $\psi \notin L^2(\mathbb{R})$.

- (b) We have $V(x) - E > 0$ for all $x$ so let us assume w.l.o.g. (since it does not affect the qualitative behaviour) that $V(x)$ is constant equal to $V_0$, then we have

$$\psi''(x) = \frac{2m}{\hbar^2}(V_0 - E)\psi(x) =: \kappa^2\psi(x). \tag{1.115}$$

This leads to

$$\psi(x) = Ae^{\kappa x} + Be^{-\kappa x}, \tag{1.116}$$

which is not bounded when either $x \to \infty$ or $x \to -\infty$.