

## Quantum Mechanics - Sheet 2

1. Recall the result referred to as “conservation of probability”:

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0 \quad (1)$$

This equation applies to *any* wavefunction that satisfies the Schrödinger equation, even if it is not normalisable.

*Exercise:* Why is this called conservation of probability? By integrating (1) between  $\pm\infty$ , derive a condition under which a normalised wavefunction remains normalised for all time. Can you find a (normalised) wavefunction that violates this condition? What is the corresponding potential,  $V$ ?

Normally,  $\rho(x, t) = |\Psi(x, t)|^2$ , but for a stationary state wavefunction

$$\begin{aligned} \Psi(x, t) &= \psi(x)e^{-iEt/\hbar}, \\ \rho &= |\psi(x)|^2. \end{aligned}$$

Equation (1) then implies that  $\frac{\partial j}{\partial x} = 0$ .

If the “large- $|x|$ ” behaviour of  $\psi$  is

$$\psi(x) = \begin{cases} e^{ikx} + Ae^{-ikx}, & x \ll 0 \\ Be^{ikx}, & x \gg 0 \end{cases}$$

then, using the definition  $j = \frac{\hbar}{m}\text{Im}(\psi^*\psi')$ ,

$$\begin{aligned} j(x) &= \frac{\hbar}{m}\text{Im} \begin{cases} (e^{ikx} + A^*e^{-ikx})ik(e^{ikx} - Ae^{-ikx}), & x \ll 0 \\ B^*e^{ikx}ikBe^{ikx}, & x \gg 0 \end{cases} \\ &= \frac{\hbar k}{m}\text{Re} \begin{cases} (1 - |A|^2) + A^*e^{2ikx} - Ae^{-2ikx}, & x \ll 0 \\ |B|^2, & x \gg 0 \end{cases} \\ &= \frac{\hbar k}{m} \begin{cases} 1 - |A|^2, & x \ll 0 \\ |B|^2, & x \gg 0 \end{cases} \end{aligned}$$

So the probability current is constant for both large positive and large negative  $x$ . Since  $j$  is independent of  $x$ , we must have

$$1 - |A|^2 = |B|^2. \quad (2)$$

This is an instance of conservation of probability. The stationary state  $\psi(x) = Be^{ikx}$  corresponds to a wavefunction  $\Psi(x, t) = Be^{i(kx - Et/\hbar)}$  - i.e. a wave travelling to the right. Similarly, the state  $\psi(x) = e^{ikx} + Ae^{-ikx}$  represents a superposition of right and left propagating waves. If we interpret the scattering state  $\psi$  as a beam of particles, then  $|A|^2$  is the proportion that are reflected and  $|B|^2$  is the proportion that are transmitted. Another way to say this is that  $|A|^2$  is the probability that any given particle will be reflected, and  $|B|^2$  is the complementary transmission probability. Equation (2) then says that all particles are either reflected or transmitted.

2. We have

$$V(x) = \begin{cases} 0, & x < 0 \\ U_0, & 0 < x < a, \\ 0, & x > a \end{cases}$$

so we need to solve

$$\psi'' = -\frac{2m}{\hbar^2} \begin{cases} E\psi, & x < 0 \\ (E - U_0)\psi, & 0 < x < a. \\ E\psi, & x > a \end{cases}$$

We are interested in the energy range  $0 < E < U_0$ , so we can define

$$k^2 = \frac{2mE}{\hbar^2}, \quad \text{and} \quad l^2 = \frac{2m(U_0 - E)}{\hbar^2}.$$

The scattering solution is then

$$\psi(x) = \begin{cases} e^{ikx} + Ae^{-ikx}, & x < 0 \\ \alpha e^{lx} + \beta e^{-lx}, & 0 < x < a. \\ Be^{ikx}, & x > a \end{cases}$$

(Note that this is precisely an example of the scattering state in Question 1.) Applying continuity of  $\psi$  and  $\psi'$  at  $x = 0$  and  $x = a$ , we obtain four equations relating the amplitudes  $A, B, \alpha, \beta$ :

$$\begin{aligned} 1 + A &= \alpha + \beta \\ ik(1 - A) &= l(\alpha - \beta) \\ \alpha e^{la} + \beta e^{-la} &= Be^{ika} \\ l(\alpha e^{la} - \beta e^{-la}) &= ikBe^{ika}. \end{aligned}$$

Hence

$$A = \frac{(l^2 + k^2)(e^{la} - e^{-la})}{(l + ik)^2 e^{-la} - (l - ik)^2 e^{la}}, \quad B = \frac{4ikle^{-ika}}{(l + ik)^2 e^{-la} - (l - ik)^2 e^{la}}.$$

But  $E = U_0/2 \Rightarrow k = l$ . Therefore

$$A = -i \tanh ka \quad \text{and} \quad B = e^{-ika} \operatorname{sech} ka.$$

So  $\mathbb{P}(\text{Transmission}) = \operatorname{sech}^2 ka$ .

*Exercise:* Plot  $\mathbb{P}$  against  $ka$ . What happens in the limit of large barrier height ( $U_0 \rightarrow \infty$ ) or width ( $a \rightarrow \infty$ )? This is called the ‘classical limit’. Why?

3. On sheet 1, we had  $A^\dagger A \psi = (\epsilon + 1)\psi$ , where

$$A = \frac{d}{dx} + \tanh x, \quad A^\dagger = -\frac{d}{dx} + \tanh x.$$

So if  $\psi(x) = e^{ikx}(\tanh x - ik)$ , then

$$\begin{aligned} A\psi &= (k^2 + 1)e^{ikx} \\ A^\dagger A\psi &= (k^2 + 1)\psi \end{aligned}$$

i.e. energy  $\epsilon = k^2$ .

For  $x \ll 0$ , we have  $\psi(x) \sim (-1 - ik)e^{ikx}$ .

For  $x \gg 0$ , we have  $\psi(x) \sim (1 - ik)e^{ikx}$ .

So  $\psi$  represents an incident wave of amplitude  $(-1 - ik)$  and a transmitted wave of amplitude  $(1 - ik)$ . So the transmission probability is

$$\frac{|+1 - ik|^2}{|-1 - ik|^2} = \frac{1 + k^2}{1 + k^2} = 1.$$

If we now suppose  $k$  is complex then we may write  $k = k_r + ik_i$ . The (scaled) energy of the wavefunction is now

$$\epsilon = (k_r^2 - k_i^2) + 2ik_r k_i.$$

We also have

$$\begin{aligned} \psi(x) &\sim (-1 + k_i - ik_r)e^{ik_r x - k_i x}, & x \ll 0 \\ \psi(x) &\sim (+1 + k_i - ik_r)e^{ik_r x - k_i x}, & x \gg 0 \end{aligned}$$

For  $k_r > 0$  we may therefore still regard  $\psi(x)$  as a rightward propagating wave. The wave grows in size if  $k_i < 0$  and shrinks if  $k_i > 0$ . However, if we take one of the limits  $k \rightarrow \pm i$ , then  $\psi$  remains bounded  $\forall x$ . We also see that the energy  $\epsilon$  is real in this limit. In fact,  $\psi(x) = \pm \text{sech}(x)$  for  $k = \pm i$ , which is exactly the ground state wavefunction we found on sheet 1.

Assuming it still makes sense to talk about transmission amplitude for complex  $k$ , we have

$$T = \frac{1 - ik}{-1 - ik} = \frac{k + i}{k - i} \quad \text{if } k_r > 0.$$

We say that  $T$  has a ‘simple pole’ at  $k = i$ , and a ‘simple zero’ at  $k = -i$ .

4. There are two ways to tackle this question:

- Method 1 - Without using operators

We need to solve

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi$$

Define  $y = \left(\frac{m\omega}{\hbar}\right)^{1/2} x$ ,  $\alpha = \frac{2E}{\hbar\omega}$ , so

$$\frac{d^2\psi}{dy^2} - y^2\psi = -\alpha\psi.$$

So we expect  $\psi = H(y)e^{-y^2/2}$ , where  $H(y)$  is bounded as  $|y| \rightarrow \infty$ . Then  $H$  satisfies

$$H'' - 2yH' + (\alpha - 1)H = 0.$$

So if  $H(y) = \sum h_m y^m$  then

$$h_{m+2} = \frac{2m + 1 - \alpha}{(m + 1)(m + 2)}. \quad (3)$$

To ensure  $\psi$  is bounded, we require  $\alpha = \alpha_n \equiv 2n + 1$  for some integer  $n$ . Thus  $E_n = \frac{1}{2}\hbar\omega\alpha_n = (n + \frac{1}{2})\hbar\omega$ .

We can now use the recursion relation (3) to obtain the first three energy states, which are  $\chi_0 \propto e^{-y^2/2}$ ,  $\chi_1 \propto ye^{-y^2/2}$  and  $\chi_2 \propto (1 - 2y^2)e^{-y^2/2}$ . (These can all be normalised, but I won't do it here.) We see from (3) that  $\chi_n$  is even/odd if  $n$  is even/odd. Since  $\int_{-\infty}^{+\infty} (\text{even}) \times (\text{odd}) dx = 0$  (assuming the integral is defined), we see that the even states are orthogonal to the odd ones. We can also check explicitly that  $\chi_0$  is orthogonal to  $\chi_2$ . We know this must be the case because  $H$  is Hermitian, so energy eigenstates of different energy are *always* orthogonal - see lecture notes.)

- Method 2 - With operators

(We'll be using some results from Question 5 here. You may want to have a look at that question first.)

Define  $A = p - im\omega x$ . Then

$$\begin{aligned} A^\dagger A &= p^2 + im\omega[x, p] + m^2\omega^2 x^2 \\ &= p^2 - m\hbar\omega + m^2\omega^2 x^2 \end{aligned}$$

So  $A^\dagger A\psi = 2m(E - \frac{1}{2}\hbar\omega)\psi$ .

Referring back to Question 8 of Sheet 1, we find that the base state is the solution of  $A\psi = 0$ , which we may easily show to be  $\chi_0 \propto e^{-\frac{m\omega}{2\hbar}x^2}$ . However, we also find that the commutator  $[A, A^\dagger] = 2m\hbar\omega$ , and so if  $A^\dagger A\psi = \mu\psi$  then

$$\begin{aligned} A^\dagger A(A^\dagger\psi) &= A^\dagger[A, A^\dagger]\psi + A^\dagger(A^\dagger A\psi) \\ &= (2m\hbar\omega + \mu)(A^\dagger\psi), \end{aligned}$$

so  $(A^\dagger\psi)$  is also an energy eigenstate with eigenvalue  $(\mu + 2m\hbar\omega)$ . Similarly, we may show that  $(A\psi)$  is an eigenstate with eigenvalue  $(\mu - 2m\hbar\omega)$ . In fact, we have the following theorem:

*Theorem:* Suppose we have an operator with the following properties:

(a) The Schrödinger Equation may be written in the form

$$A^\dagger A\psi = \mu(E)\psi.$$

(b) The commutator of  $A$  and its Hermitian conjugate is

$$[A, A^\dagger] = \lambda,$$

where  $\lambda \neq 0$  is a constant.

Then the base state  $\chi_0$  satisfies  $A\chi_0 = 0$  and the remaining *normalised* eigenstates satisfy  $\chi_n = \frac{1}{\sqrt{n\lambda}}A^\dagger\chi_{n-1}$ , and have eigenvalue  $n\lambda$ .

*Exercise:* Prove this theorem. You'll need to explain why there aren't any *other* eigenstates than those listed above.

So we have a formula for the eigenstates of the 1D harmonic oscillator:  $\chi_n \propto (A^\dagger)^n\chi_0$ . (You should check that this formula reproduces the same  $\chi_1$  and  $\chi_2$  we found previously.) We can use this formula to show that *all* energy states are orthogonal:

$$\begin{aligned} (\chi_n, \chi_{n+m}) &\propto (\chi_n, (A^\dagger)^m\chi_n) \\ &= (A^m\chi_n, \chi_n) \\ &\propto (\chi_{n-m}, \chi_n). \end{aligned}$$

Repeat this procedure until we're left with  $(\chi_n, \chi_{n+m})$ , where  $m > n$ . Then

$$\begin{aligned} (\chi_n, \chi_{n+m}) &\propto (\chi_n, (A^\dagger)^m\chi_n) \\ &= (A^{n+1}\chi_n, (A^\dagger)^{m-n-1}\chi_n) \\ &\propto (0, \chi_{m-1}) = 0 \end{aligned}$$

*Exercise:* Prove that (unfortunately) it's only possible to find an operator  $A$  with properties (4a) and (4b) if the potential is quadratic. So the harmonic oscillator is essentially the only system that can be solved in this way. However, the oscillator is of great importance to quantum physics; Dirac showed it does a very good job of describing a single boson particle.

5. We say an operator  $A$  has the Hermitian conjugate  $A^\dagger$  if  $(A\psi, \phi) = (\psi, A^\dagger\phi)$  for all pairs of normalisable wavefunctions  $\psi, \phi$ . If  $A = A^\dagger$ , then  $A$  is *Hermitian*. But then

$$\begin{aligned} \langle A \rangle_\psi &= (\psi, A\psi) \\ &= (A\psi, \psi) \quad \text{because } A \text{ is Hermitian} \\ &= (\psi, A\psi)^* \\ &= \langle A \rangle_\psi^*. \end{aligned}$$

So  $A$  has real expectation (and real eigenvalues).

There are three important rules for Hermitian conjugates:

- (a)  $\lambda^\dagger = \lambda^*$  for any constant  $\lambda$
- (b)  $(A + B)^\dagger = A^\dagger + B^\dagger$
- (c)  $(AB)^\dagger = B^\dagger A^\dagger$

*Exercise:* Prove these rules using properties of the bracket notation  $(\cdot, \cdot)$ .

So, for *any* two operators  $A_1$  and  $A_2$ , we find

$$\begin{aligned} \{i[A_1, A_2]\}^\dagger &= -i[A_1, A_2]^\dagger \quad \text{by (5a)} \\ &= -i[(A_1A_2)^\dagger - (A_2A_1)^\dagger] \quad \text{by (5b)} \\ &= -i[A_2^\dagger A_1^\dagger - A_1^\dagger A_2^\dagger] \quad \text{by (5c)} \\ &= i[A_1^\dagger, A_2^\dagger]. \end{aligned}$$

So, if  $A_1$  and  $A_2$  are Hermitian, then so is  $i[A_1, A_2]$ .

6. How do we go about solving the *time-dependent* Schrödinger Equation, supposing we have the initial wavefunction? The solution is to write the initial function as a superposition of energy eigenstates. We know exactly how each of these evolves individually, and the initial superposition evolves just as a superposition of these time-dependent states. This question involves applying this process to a particular potential; we begin by finding the energy eigenstates:

For  $x < 0$  and  $x > a$ , we must have  $\psi = 0$ , since the potential is infinite. Even though there is an infinite discontinuity in the potential at  $x = 0$  and  $x = a$ , we still expect the wavefunction to be continuous, so  $\psi(0) = \psi(a) = 0$ .

For  $0 < x < a$ , we need to solve  $-\frac{\hbar^2}{2m}\psi'' = E\psi$ . To get solutions, we need  $E > 0$ , so we may find  $k > 0$  s.t.  $k^2 = 2mE/\hbar^2$  and solve

$$\psi'' + k^2\psi = 0.$$

The normalised eigenstates are

$$\psi_n(x, t) = (2/a)^{1/2} \sin(k_n x) e^{-iE_n t/\hbar},$$

where  $k_n = n\pi/a$  and  $E_n = \hbar^2 k_n^2 / 2m = (n\pi\hbar)^2 / 2ma^2$ .

The general solution of the Schrödinger Equation may be written as a linear superposition of these eigenstates. Since the states are sine functions, such a superposition is in fact just a Fourier series.

If  $\psi(x, 0) = Cx(a - x)$  then

$$\begin{aligned} \|\psi(x, 0)\|^2 &= 1 \\ \Rightarrow \int_0^a C^2 x^2 (a - x)^2 dx &= 1 \\ \Rightarrow C &= \left(\frac{30}{a^5}\right)^{1/2}. \end{aligned}$$

We wish to write  $\psi(x, 0) = \sum_{n=1}^{\infty} b_n \psi_n(x, 0)$ . But then

$$\begin{aligned} (\psi_m(x, 0), \psi(x, 0)) &= \sum_{n=1}^{\infty} b_n (\psi_m(x, 0), \psi_n(x, 0)) \\ &= b_m \|\psi_m(x, 0)\|^2 = b_m. \end{aligned}$$

So

$$\begin{aligned} b_m &= (\psi_m(x, 0), \psi(x, 0)) \\ &= (2/a)^{1/2} (\sin(m\pi x/a), Cx(a - x)) \\ &= (2/a)^{1/2} C \int_0^a x(a - x) \sin(m\pi x/a) dx \\ &= \frac{4\sqrt{15}}{(m\pi)^3} (1 - (-1)^m) \\ \text{So } \phi(x, 0) &= \sum_{n \text{ odd}} \frac{8Ca^2}{(n\pi)^3} \sin(k_n x) \\ \therefore \phi(x, t) &= \sum_{n \text{ odd}} \frac{8Ca^2}{(n\pi)^3} \sin(k_n x) e^{-iE_n t/\hbar}. \end{aligned}$$

Since  $\psi(x, 0)$  contains no components of  $\psi_n$  for  $n$  even, nor does  $\psi(x, t)$ . So the probability of measuring the energy to be  $E_n$  is zero for even  $n$ . In general, the probability of measuring the energy

to be  $E_n$  at time  $t > 0$  is

$$\begin{aligned}
 \mathbb{P}(E_n) &= |(\psi_n(x, t), \psi(x, t))|^2. \\
 \text{But } \psi(x, t) &= \sum_m b_m \psi_m(x, t), \\
 \text{so } \mathbb{P}(E_n) &= \left| \sum_m (\psi_n(x, t), b_m \psi_m(x, t)) \right|^2 \\
 &= |b_n (\psi_n(x, t), \psi_n(x, t))|^2 \quad (\text{since states are orthogonal}) \\
 &= |b_n (\psi_n(x, 0), \psi_n(x, 0))|^2 \quad (\text{for energy eigenstates}) \\
 &= |b_n|^2.
 \end{aligned}$$

The important point is that *these probabilities do not change with time*. This is only the case for *energy* eigenstates, not for the eigenfunctions of other operators in general.

For this particular problem,  $\mathbb{P}(E_n) = |b_n|^2 = 960/(n\pi)^6$  for odd  $n$ . These probabilities are determined entirely by the co-efficients in the Fourier expansion of  $\psi(x, 0)$ ; by far the largest is  $b_1 = (960/\pi^6)^{1/2} \approx 0.999$ . This co-efficient is large simply because  $\psi(x, 0)$  “looks a lot like”  $\psi_1(x, 0) = (2/a)^{1/2} \sin(\pi x/a)$  (see Figure 1).

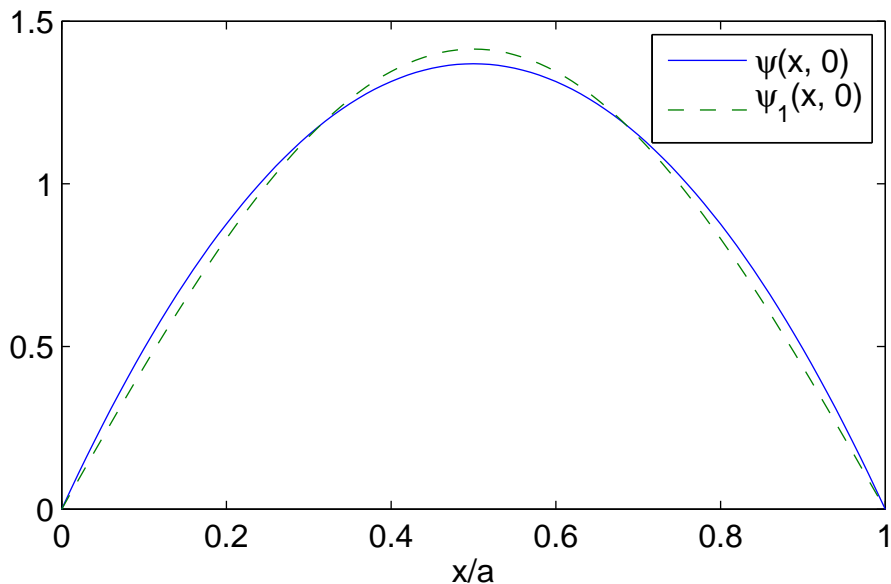


Figure 1: Comparison of the initial condition to the lowest energy eigenstate

7. Using the notation  $\langle A \rangle_n \equiv (\psi_n, A\psi_n)$ , we find

$$\begin{aligned}
 \langle x \rangle_n &= \int_0^a (2x/a) \sin^2(n\pi/a) dx \\
 &= \int_0^a (x/a)(1 - \cos(2n\pi x/a)) dx \\
 &= a/2.
 \end{aligned}$$

Also,

$$\begin{aligned}
 \langle x^2 \rangle_n &= \int_0^a (2x^2/a) \sin^2(n\pi/a) dx \\
 &= a^2(1/3 - 1/2\pi^2 n^2).
 \end{aligned}$$

Then

$$\begin{aligned}\langle (x - \langle x \rangle_n)^2 \rangle_n &= \langle x^2 \rangle_n - (\langle x \rangle_n)^2 \\ &= \frac{a^2}{12} \left( 1 - \frac{6}{\pi^2 n^2} \right).\end{aligned}$$

In the limit  $n \rightarrow \infty$ , we find  $(\Delta x)^2 \rightarrow a^2/12$ , which is precisely what we would expect for a uniform probability distribution over the interval  $[0, a]$ . So a quantum particle of high energy has the same *statistics* as a classical particle. However, if you plot the probability distribution associated with the  $n$ -th state,  $|\psi_n|^2(x)$ , you'll see that it's far from uniform, especially for large  $n$ !

8. In this question we consider a very simple quantum system: one with only two allowed energy states. As we saw in Question 6, the probability amplitudes of these states do not change with time, so to do anything interesting we have to measure some other quantity,  $S$ . The operator associated with  $S$  is defined entirely by its action on the two energy states. Since  $S\chi_1 = \chi_2$  and  $S\chi_2 = \chi_1$ , we may think of  $S$  in terms of the matrix  $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ . Finding the eigenstates of  $S$  is then equivalent to finding eigenvectors of this matrix.

The (normalised) eigenvectors are  $\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$  and  $\begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}$ , corresponding to eigenfunctions  $\phi_{\pm} = \frac{1}{\sqrt{2}}(\chi_1 \pm \chi_2)$ , with eigenvalues  $\pm 1$ . In these states, the expected energy is

$$\begin{aligned}\langle E \rangle_{\pm} &\equiv (\phi_{\pm}, H\phi_{\pm}) \\ &= \frac{1}{2}(\chi_1 \pm \chi_2, H(\chi_1 \pm \chi_2)) \\ &= \frac{1}{2}(\chi_1 \pm \chi_2, E_1\chi_1 \pm E_2\chi_2) \\ &= \frac{1}{2}(E_1 + E_2) \quad \text{since } \chi_1 \text{ and } \chi_2 \text{ are orthonormal.}\end{aligned}$$

For convenience we now define  $E \equiv (E_1 + E_2)/2$  as the expected energy of both  $S$ -eigenstates. Suppose we measure the value of  $S$  to be  $+1$  at time  $t = 0$ . Then

$$\begin{aligned}\psi(0) &= \phi_+ = \frac{1}{\sqrt{2}}(\chi_1 + \chi_2) \\ \Rightarrow \psi(t) &= \frac{1}{\sqrt{2}}(\chi_1 e^{-iE_1 t/\hbar} + \chi_2 e^{-iE_2 t/\hbar}).\end{aligned}$$

The probability of measuring  $+1$  again after time  $t$  is

$$\begin{aligned}\mathbb{P}(1) &= |(\phi_+, \psi(t))|^2 \\ \text{where } (\phi_+, \psi(t)) &= \frac{1}{2}(\chi_1 + \chi_2, \chi_1 e^{-iE_1 t/\hbar} + \chi_2 e^{-iE_2 t/\hbar}) \\ &= \frac{1}{2}(e^{-iE_1 t/\hbar} + e^{-iE_2 t/\hbar}) \\ &= e^{-iEt/\hbar} \cos\left(\frac{\Delta E}{2\hbar}t\right) \\ \text{So } \mathbb{P}(1) &= \cos^2\left(\frac{\Delta E}{2\hbar}t\right),\end{aligned}$$

which clearly vanishes at time  $t = T \equiv \frac{\pi\hbar}{\Delta E}$ . After time  $T/n$ , we have

$$\begin{aligned}A_n &= (\phi_+, \psi(T/n)) \\ &= e^{-iET/\hbar n} \cos\left(\frac{\Delta E}{2\hbar n}T\right) \\ &= 1 - \frac{iET}{2\hbar n} + O(1/n^2),\end{aligned}$$

and so

$$\begin{aligned}
 P_n &= |A_n|^{2n} \\
 &= \cos^{2n} \left( \frac{\Delta E}{2\hbar n} T \right) \\
 &= 1 - \left( \frac{\Delta E}{2\hbar} T \right)^2 \frac{1}{n} + O(1/n^2) \\
 \Rightarrow \lim_{n \rightarrow \infty} P_n &= 1
 \end{aligned}$$

9. Since  $p$  has real eigenvalues,  $p^2$  has positive eigenvalues, so we would expect  $\langle p^2 \rangle$  to be positive. Indeed, since  $p$  is Hermitian,  $\langle p^2 \rangle_\psi \equiv (\psi, p^2 \psi) = (p\psi, p\psi) = \|p\psi\|^2 \geq 0$ .

Therefore  $\langle H \rangle = \langle T \rangle + \langle U \rangle \geq \langle U \rangle$ , so a lower bound on  $\langle U \rangle$  is also a lower bound on the total energy of any eigenstate. In particular,

$$\begin{aligned}
 E_0 \equiv \langle H \rangle_{\psi_0} &\geq \langle U \rangle_{\psi_0} \\
 &= (\psi_0, U\psi_0) \\
 &= \int_{-\infty}^{+\infty} |\psi_0|^2 U(x) dx \\
 &\geq (\min_x U(x)) \int_{-\infty}^{+\infty} |\psi_0|^2 dx \\
 &= (\min_x U(x)).
 \end{aligned}$$

[In fact, the base state of a quantum system typically has energy slightly above the minimum of its potential (for example, see Question 4). The reason is the uncertainty principle: if a particle has energy just above the global minimum of its potential, then it cannot have significant kinetic energy, and so its position and momentum are both known to a high level of accuracy. But the uncertainty principle forbids this, so a quantum system must have its minimum energy state *above* the minimum of its potential. We'll make this argument more rigorous in Question 10.]

If  $H$  is a Hermitian operator and  $H\chi = E\chi$  then

$$\begin{aligned}
 \langle [H, A] \rangle_\chi &= (\chi, HA\chi) - (\chi, AH\chi) \\
 &= (H\chi, A\chi) - (\chi, A(E\chi)) \\
 &= (E^* - E)(\chi, A\chi) \\
 &= 0
 \end{aligned}$$

since the eigenvalues of a Hermitian operator are real (see Question 5).

But

$$\begin{aligned}
 [H, x] &= \frac{1}{2m} [p^2, x] + [U(x), x] \\
 &= \frac{1}{2m} p[p, x] + \frac{1}{2m} [p, x]p \\
 &= -\frac{i\hbar}{m} p.
 \end{aligned}$$

So  $\langle p \rangle = 0$  in the eigenstate  $\chi$ .

Also,

$$\begin{aligned}
 [H, xp] &= \frac{1}{2m} [p^2, xp] + [U(x), xp] \\
 &= \frac{1}{2m} [p^2, x]p + x[U, p] \\
 &= -\frac{i\hbar}{m} p^2 + i\hbar x U'(x).
 \end{aligned}$$

So  $2\langle T \rangle_\chi = \langle xU'(x) \rangle_\chi$ . If  $U(x) = kx^n$ , then  $xU'(x) = knx^n = nU(x)$ , so  $2\langle T \rangle_\chi = n\langle U \rangle_\chi$ .

But  $\langle T \rangle_\chi + \langle U \rangle_\chi = \langle H \rangle_\chi = E$ . So

$$\begin{aligned} (1 + 2/n)\langle T \rangle_\chi &= E \\ \Leftrightarrow \langle T \rangle_\chi &= \frac{n}{n+2}E. \end{aligned}$$

This is called the virial theorem because it describes the typical partition of energy in a quantum system.

10. We have already seen that the base state for the quantum harmonic oscillator has energy  $E_0 = \frac{1}{2}\hbar\omega$ . However, we can prove this result using just the uncertainty principle. In Question 7, we saw

$$\begin{aligned} (\Delta x)^2 &= \langle (x - \langle x \rangle)^2 \rangle \\ &= \langle x^2 \rangle - \langle x \rangle^2. \end{aligned}$$

Similarly,  $(\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2$ . So

$$\begin{aligned} \langle E \rangle &= \left\langle \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \right\rangle \\ &= \frac{1}{2m}\langle p^2 \rangle + \frac{1}{2}m\omega^2\langle x^2 \rangle \\ &= \frac{1}{2m}((\Delta p)^2 + \langle p \rangle^2) + \frac{1}{2}m\omega^2((\Delta x)^2 + \langle x \rangle^2). \end{aligned}$$

We need to find a lower bound for  $\langle E \rangle$ . The expression above clearly shows that  $\langle E \rangle \geq 0$ , since every term on the RHS is positive. In fact, we already proved this in Question 9.

Suppose the function that minimises  $\langle E \rangle_\chi$  is  $\chi_0$ . We can easily find functions  $\chi(x)$  for which  $\langle x \rangle_\chi$  and  $\langle p \rangle_\chi$  are both arbitrarily small; actually, both are zero if we  $\chi$  is symmetric. However, we cannot make *both*  $(\Delta x)$  and  $(\Delta p)$  arbitrarily small since we know that

$$(\Delta x)(\Delta p) \geq \frac{1}{2}\hbar.$$

Using this relation, together with the AM/GM inequality, we can find a lower bound for  $\langle E \rangle$ :

$$\begin{aligned} \langle E \rangle &= \frac{1}{2m}((\Delta p)^2 + \langle p \rangle^2) + \frac{1}{2}m\omega^2((\Delta x)^2 + \langle x \rangle^2) \\ &\geq \frac{1}{2m}(\Delta p)^2 + \frac{1}{2}m\omega^2(\Delta x)^2 \\ &\geq \omega(\Delta p)(\Delta x) \\ &\geq \frac{1}{2}\hbar\omega. \end{aligned}$$