

10. For the momentum and total energy to be measured simultaneously, the operators  $\hat{p}$  and  $\hat{H}$

must commute. In 1D we have  $\hat{p} = -i\hbar \frac{d}{dx}$  and  $\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$ . The commutator is

$$[\hat{p}, \hat{H}] = \frac{i\hbar^3}{2m} \left( \frac{d}{dx} \frac{d^2}{dx^2} - \frac{d^2}{dx^2} \frac{d}{dx} \right) - i\hbar \left( \frac{d}{dx} V(x) - V(x) \frac{d}{dx} \right). \text{ The first bracket is zero. If we apply}$$

the second bracket to an arbitrary function  $f(x)$  we get

$$\frac{d}{dx} (V(x)f(x)) - V(x) \frac{d}{dx} f(x) = \frac{dV}{dx} f(x). \text{ Therefore } [\hat{p}, \hat{H}] = -i\hbar \frac{dV}{dx}. \hat{p} \text{ and } \hat{H} \text{ commute}$$

only if  $\frac{dV}{dx} = 0$ , ie if  $V(x)$  is constant.

11. For this question, we make extensive use of the useful integrals.

$$\langle \hat{x} \rangle = \frac{2}{a} \int_0^a dx x \sin^2 \left( \frac{\pi x}{a} \right) = \frac{a}{2} \text{ (ie the average position of the particle is the centre of the well)}$$

$$\langle \hat{x}^2 \rangle = \frac{2}{a} \int_0^a dx x^2 \sin^2 \left( \frac{\pi x}{a} \right) = \frac{a^2 (2\pi^2 - 3)}{6\pi^2}$$

$$\langle \hat{p}_x \rangle = -\frac{2i\hbar}{a} \int_0^a dx \sin \left( \frac{\pi x}{a} \right) \frac{d}{dx} \sin \left( \frac{\pi x}{a} \right) = -\frac{2i\pi\hbar}{a^2} \int_0^a dx \sin \left( \frac{\pi x}{a} \right) \cos \left( \frac{\pi x}{a} \right) = 0$$

$$\langle \hat{p}_x^2 \rangle = -\frac{2\hbar^2}{a} \int_0^a dx \sin \left( \frac{\pi x}{a} \right) \frac{d^2}{dx^2} \sin \left( \frac{\pi x}{a} \right) = \frac{2\pi^2\hbar^2}{a^3} \int_0^a dx \sin \left( \frac{\pi x}{a} \right) \sin \left( \frac{\pi x}{a} \right) = \frac{\pi^2\hbar^2}{a^2}$$

$$\text{From the lecture notes, } \Delta A^2 = \int \psi^* \left( \hat{A} - \langle \hat{A} \rangle \right)^2 \psi = \int \psi^* \left( \hat{A}^2 - 2\langle \hat{A} \rangle \hat{A} + \langle \hat{A} \rangle^2 \right) \psi = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2.$$

Using this, we find  $\Delta x^2 = a^2 \left( \frac{1}{12} - \frac{1}{2\pi^2} \right)$ , so  $\Delta x = 0.18a$ . We also find  $\Delta p_x^2 = \frac{\pi^2\hbar^2}{a^2}$ , so

$\Delta p_x = 3.14 \frac{\hbar}{a}$ . This gives  $\Delta x \Delta p_x = 0.57\hbar$ , which is consistent with the uncertainty principle.

12. a) The probability of measuring both  $E_1 = \frac{\hbar^2 \pi^2}{2ma^2}$  and  $E_2 = \frac{4\hbar^2 \pi^2}{2ma^2}$  is  $\frac{1}{2}$ .

b)  $\psi(x, t) = \frac{1}{\sqrt{2}} \phi_1(x) \exp(-iE_1 t / \hbar) + \frac{1}{\sqrt{2}} \phi_2(x) \exp(-iE_2 t / \hbar)$  with  $\phi_1(x)$  and  $\phi_2(x)$  given in the question, and  $E_1$  and  $E_2$  given above.

c) We want to calculate  $\langle \hat{H} \rangle = \int_0^a dx \psi^*(x, t) \hat{H} \psi(x, t)$ . Because  $\phi_1(x)$  and  $\phi_2(x)$  are energy eigenfunctions  $\hat{H} \psi(x, t) = \frac{E_1}{\sqrt{2}} \phi_1(x) \exp(-iE_1 t / \hbar) + \frac{E_2}{\sqrt{2}} \phi_2(x) \exp(-iE_2 t / \hbar)$ . Because  $\phi_1(x)$  and  $\phi_2(x)$  are normalised and orthogonal to each other, the integrals are easy and we find  $\langle \hat{H} \rangle = \frac{E_1}{2} + \frac{E_2}{2}$ . Note that this is independent of time, and is consistent with the result found in part a).

d) We want to calculate  $\langle \hat{x} \rangle = \int_0^a dx \psi^*(x, t) x \psi(x, t)$ . The algebra is messy, but we eventually find

$$\langle \hat{x} \rangle = \frac{1}{a} \int_0^a dx x \sin^2\left(\frac{\pi x}{a}\right) + \frac{1}{a} \int_0^a dx x \sin^2\left(\frac{2\pi x}{a}\right) + \frac{2}{a} \cos\left(\frac{(E_1 - E_2)t}{\hbar}\right) \int_0^a dx x \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{2\pi x}{a}\right).$$

Using the useful integrals, we find  $\langle \hat{x} \rangle = \frac{a}{2} - \frac{16a}{9\pi^2} \cos\left(\frac{(E_1 - E_2)t}{\hbar}\right)$ . Note how the average position of the particle oscillates about the centre of the well (ie  $a/2$ ), with a frequency determined by the difference in the energy levels of  $\phi_1(x)$  and  $\phi_2(x)$ .

13. a) We want to calculate  $c(k) = \frac{1}{2\pi} \sqrt{\frac{2}{a}} \int_0^a dx \sin\left(\frac{\pi x}{a}\right) \exp(-ikx)$ . The useful integrals give

$$c(k) = \frac{1}{2\pi} \sqrt{\frac{2}{a}} \frac{\pi a (1 + \exp(-ika))}{\pi^2 - k^2 a^2}.$$

b) We find that  $|c(k)|^2 \propto \frac{\cos^2\left(\frac{ka}{2}\right)}{(\pi^2 - k^2 a^2)^2}$ . This is symmetrical about  $k = 0$ , so we are equally

likely to measure positive and negative momenta. This is consistent with  $\langle \hat{p}_x \rangle = 0$  in question

11.  $|c(k)|^2$  is strongly peaked for  $k = \pm \frac{\pi}{a}$ . Given that  $p = \hbar k$ , this is consistent with

$$\langle \hat{p}_x^2 \rangle = \frac{\pi^2 \hbar^2}{a^2} \text{ in question 11.}$$

14. From the lecture notes, we know that the width of a Gaussian wavepacket varies with time as

$$\Delta x(t) = \sqrt{\frac{1}{2a} + \frac{\hbar^2 a t^2}{2m^2}}. \text{ At } t = 0, \Delta x = \sqrt{\frac{1}{2a}} = 1 \text{ \AA}.$$

a) We need  $\frac{\hbar^2 a t^2}{2m^2} = \frac{3}{2a}$ , ie  $t = \frac{\sqrt{3}m}{\hbar a}$ . Putting in the numbers gives  $t \approx 3 \times 10^{-16} \text{ s}$ .

b) The second term under the square root in  $\Delta x(t)$  dominates in this case, so  $\Delta x = \frac{\hbar t \sqrt{a}}{\sqrt{2}m}$ .

Putting in the numbers gives  $\Delta x \approx 6 \times 10^5 \text{ m}$ .