P1.4 At time $t=0$, a particle is represented by the wavefunction

$$\Psi(x,0) = \begin{cases} A\left(\frac{x}{a}\right), & 0 \le x \le a \\ A\left(\frac{b-x}{b-a}\right) & a \le x \le b \\ 0 & \text{otherwise} \end{cases}$$

where A, a, and b are positive constants.

(a) Normalize Ψ (Find A in terms of a and b) ✓

(b) Sketch $\Psi(x,0)$ as a function of x ✓

(c) Where is the particle most likely to be found at $t=0$? ✓

(d) What is the probability of finding the particle to the left of a? ✓
Check your result in the limiting cases $b=a$ ✓ and $b=2a$ ✓

(e) What is the expectation value of x? ✓

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integrals over other intervals yield 0

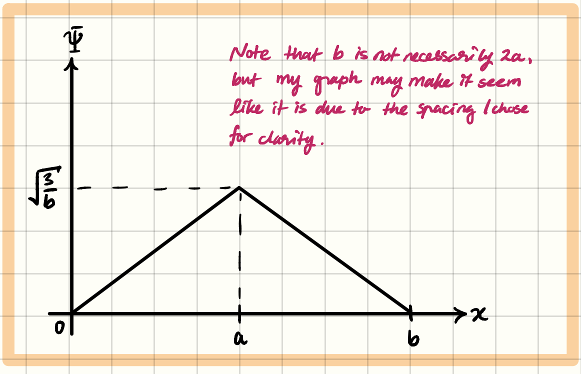
(a) $$\int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx = 1 \implies \int_0^a A^2 \frac{x^2}{a^2} dx + \int_a^b A^2 \left(\frac{b-x}{b-a}\right)^2 dx = 1$$

$$\implies \frac{A^2}{a^2}\left(\frac{x^3}{3}\Big|_0^a\right) + \frac{A^2}{(b-a)^2}\int_a^b (b^2 - 2bx + x^2)\,dx = \frac{1}{3}A^2 a + \frac{A^2}{(b-a)^2}\left(b^2 x - bx^2 + \frac{x^3}{3}\right)\Big|_a^b = 1$$

$$\implies A^2\left[\frac{1}{3}a + \frac{1}{\cancel{(b-a)^2}}\Big(\cancel{b^3} - \cancel{b^3} + \overbrace{\frac{b^3}{3} - b^2 a + ba^2 - \frac{a^3}{3}}^{\frac{1}{3}(b-a)^{\cancel{3}}}\Big)\right] = A^2\left(\cancel{\tfrac{1}{3}}a + \frac{1}{3}b - \cancel{\tfrac{1}{3}}a\right) = 1$$

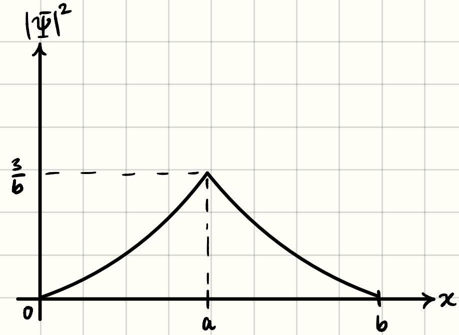
$$\implies \boxed{A = \sqrt{\frac{b}{3}}}$$

(b) $$\Psi(x,0) = \begin{cases} \sqrt{\frac{3}{b}}\left(\frac{x}{a}\right) & 0 \le x \le a \\ \sqrt{\frac{3}{b}}\left(\frac{b-x}{b-a}\right) & a \le x \le b \\ 0 & \text{otherwise} \end{cases}$$



(c) We can guess from the graph for $|\Psi|^2$ below that it will be $x = a$.

$$|\Psi(x,0)|^2 \begin{cases} \frac{3}{b}\left(\frac{x}{a}\right)^2 & 0 \le x \le a \\ \frac{3}{b}\left(\frac{b-x}{b-a}\right)^2 & a \le x \le b \\ 0 & \text{otherwise} \end{cases}$$



(d) $$P(x \le a) = \int_0^a \frac{3}{b}\left(\frac{x}{a}\right)^2 dx = \frac{\cancel{3}}{a^2 b}\frac{x^3}{\cancel{3}}\Big|_0^a = \frac{a}{b}$$

Check for $b = a \longrightarrow P(x \le a) = 1$

Check for $b = 2a \longrightarrow P(x \le a) = \frac{1}{2}$

(e) $$\langle x \rangle = \int_{-\infty}^{\infty} x|\Psi|^2 dx = \int_0^a \frac{3}{b}\frac{x^3}{a^2} dx + \int_a^b \frac{3}{b} x \left(\frac{b-x}{b-a}\right)^2 dx$$

$$= \frac{3}{a^2 b}\frac{a^4}{4} + \frac{3}{b(b-a)^2}\int_a^b x(b-x)^2 dx$$

$u = x - b$, $du = dx$

$$= \frac{3}{4}\frac{a^2}{b} + \frac{3}{b(b-a)^2}\int_{x=a}^{x=b}(u+b)u^2 du = \frac{3}{4}\cdot\frac{a^2}{b} + \frac{3}{b(b-a)^2}\int_{x=a}^{x=b} u^3 + bu^2 du$$

$$= \frac{3}{4}\cdot\frac{a^2}{b} + \frac{3}{b(b-a)^2}\left(\frac{u^4}{4} + b\frac{u^3}{3}\Big|_{x=a}^{x=b}\right. = \frac{3a^2}{4b} + \frac{3}{b(b-a)^2}\cdot\left(\frac{(x-b)^4}{4} + \frac{b(x-b)^3}{3}\Big|_a^b\right.$$

$$= \frac{3a^2}{4b} + \frac{\cancel{3}}{b\cancel{(b-a)^2}}\cdot\frac{(b-a)^{\cancel{3}}(b+3a)}{\cancel{12}\ 4}$$

$$= \frac{\cancel{3a^2} + b^2 + 2ab - \cancel{3a^2}}{4b}$$

$$= \frac{b+2a}{4}$$

P1.9 A particle of mass m has the wave function

$$\Psi(x,t) = Ae^{-a\left[\frac{mx^2}{\hbar} + it\right]}$$

where A and a are positive real constants

(a) Find A. ✓

(b) For what potential energy function, V(x), is this a solution to the Schrödinger equation? ✓

(c) Calculate the expectation values of x, x^2, p, and p^2. ✓ ✓ ✓ ✓

(d) Find σ_x and σ_p. ✓ Is their product consistent with the uncertainty principle? ✓

(a) $$\int_{-\infty}^{\infty} |\Psi(x,t)|^2\, dx = 1 \implies \int_{-\infty}^{\infty} \Psi\Psi^*\, dx = 1$$

$n=0 \rightarrow \sqrt{\pi}\,\frac{2(0)!}{(0)!}\left(\frac{a}{2}\right)^{2(0)+1}$

$$\implies \int_{-\infty}^{\infty} A^2 e^{-2a\frac{mx^2}{\hbar}} \cancel{e^{-ait}}\, \cancel{e^{ait}}\, dx = A^2 \int_{-\infty}^{\infty} e^{-\overbrace{\left(\frac{2am}{\hbar}\right)}^{1/a^2}x^2}\, dx = 2A^2 \int_0^{\infty} e^{-\frac{x^2}{a^2}}\, dx = 1$$

$$\implies \cancel{2}A^2\sqrt{\pi}\cdot\sqrt{\frac{\hbar}{2am}}\cdot\frac{1}{\cancel{2}} = A^2\sqrt{\frac{\pi\hbar}{2am}} = 1 \implies A = \left(\frac{2am}{\pi\hbar}\right)^{1/4}$$

(b) $$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi$$

$$\frac{\partial\Psi}{\partial t} = -aiAe^{-a\left[\frac{mx^2}{\hbar}+it\right]}$$

$$\frac{\partial^2\Psi}{\partial x^2} = \frac{\partial}{\partial x}\left(-\frac{2amx}{\hbar}Ae^{-a\left[\frac{mx^2}{\hbar}+it\right]}\right) = -\frac{2am}{\hbar}Ae^{-a\left[\frac{mx^2}{\hbar}+it\right]} + \frac{4a^2m^2x^2}{\hbar^2}Ae^{-a\left[\frac{mx^2}{\hbar}+it\right]}$$

$$V\cancel{\Psi} = i\hbar\Big(-ai\underbrace{\cancel{Ae^{-a\left[\frac{mx^2}{\hbar}+it\right]}}}_{\Psi}\Big) - \frac{\hbar^2}{2m}\underbrace{\cancel{Ae^{-a\left[\frac{mx^2}{\hbar}+it\right]}}}_{\Psi}\left(\frac{2am}{\hbar} - \frac{4a^2m^2x^2}{\hbar^2}\right)$$

$$V(x) = a\hbar - \frac{\hbar^2}{2m}\left(\frac{2am}{\hbar} - \frac{4a^2m^2x^2}{\hbar^2}\right) = \cancel{a\hbar} - \cancel{a\hbar} + 2a^2mx^2 = 2a^2mx^2$$

(c) $\langle x\rangle = \int_{-\infty}^{\infty} x|\Psi|^2 dx = A^2\int_{-\infty}^{\infty} \underbrace{x e^{-\left(\frac{2am}{\hbar}\right)x^2}}_{f(x)} dx = 0$

$f(-x) = -xe^{-\frac{2am}{\hbar}x^2} = -f(x) \Rightarrow$ odd

$\langle x^2\rangle = 2A^2\int_0^{\infty} x^2 e^{-\underbrace{\left(\frac{2am}{\hbar}\right)}_{1/\alpha^2}x^2} dx = 2A^2\sqrt{\pi}\,\frac{[2(1)]!}{(1)!}\left(\frac{\alpha}{2}\right)^3 = \frac{1}{2}\sqrt{\frac{2am}{\cancel{\pi}\hbar}}\cancel{\sqrt{\pi}}\cdot\left(\frac{\hbar}{2am}\right)^{3/2}$

$= \frac{\hbar}{4am}$

$\langle p\rangle = -i\hbar\int \Psi^* \frac{\partial\Psi}{\partial x}dx = -i\hbar\int_{-\infty} Ae^{-a\left(\frac{mx^2}{\hbar}-\cancel{it}\right)}\cdot\left(-\frac{2amx}{\hbar}Ae^{-a\left(\frac{mx^2}{\hbar}+\cancel{it}\right)}\right)dx$

$= +i\hbar A^2\cdot\frac{2am}{\hbar}\int_{-\infty}^{\infty} \underbrace{xe^{-2a\frac{mx^2}{\hbar}}}_{\text{odd}} dx = 0$

$\langle p^2\rangle = -\hbar^2\int\Psi^*\frac{\partial^2\Psi}{\partial x^2}dx = +\hbar^2\int_{-\infty}^{\infty} Ae^{-a\left(\frac{mx^2}{\hbar}-\cancel{it}\right)}\cdot Ae^{-a\left[\frac{mx^2}{\hbar}+\cancel{it}\right]}\left(\frac{2am}{\hbar}-\frac{4a^2m^2x^2}{\hbar^2}\right)$

$= 2\hbar^2A^2\int_0^{\infty} e^{-\frac{2amx^2}{\hbar}}\cdot\frac{2am}{\hbar}\left(1-\frac{2amx^2}{\hbar}\right)dx$

$= 2\hbar^2\sqrt{\frac{2am}{\cancel{\pi}\hbar}}\cdot\frac{2am}{\hbar}\left[\frac{\cancel{\sqrt{\pi}}}{2}\left(\frac{\hbar}{2am}\right)^{1/2} - \left(\frac{2am}{\hbar}\right)^{2/2}\cancel{\sqrt{\pi}}\,\frac{(2)!}{(1)!}\cdot\frac{1}{8}\left(\frac{\hbar}{2am}\right)^{3/2}\right]$

$= \hbar^2\,\frac{4am}{\hbar}\sqrt{\frac{2a\cancel{m}}{\cancel{\hbar}}}\left[\frac{1}{2}\cancel{\left(\frac{\hbar}{2am}\right)^{1/2}} - \frac{1}{4}\cancel{\left(\frac{\hbar}{2am}\right)^{1/2}}\right]$

$= \hbar^{\cancel{2}}\,\frac{\cancel{4}am}{\cancel{\hbar}}\cdot\frac{1}{\cancel{4}} = \hbar am$

(d) $\sigma_x = \sqrt{\langle x^2\rangle - \cancel{\langle x\rangle^2}^{\,0}} = \sqrt{\frac{\hbar}{4am}}$

$\sigma_p = \sqrt{\langle p^2\rangle - \cancel{\langle p\rangle^2}^{\,0}} = \sqrt{\hbar am}$

$\sigma_x\sigma_p = \sqrt{\frac{\hbar^2 a\cancel{m}}{4a\cancel{m}}} = \frac{\hbar}{2} \overset{\checkmark}{\geq} \frac{\hbar}{2} \Rightarrow$ consistent with Heisenberg uncertainty principle!

P1.14 Let $P_{ab}(t)$ be the probability of finding the particle in the range $(a<x<b)$, at time t.

switch?

(a) Show that $\frac{dP_{ab}}{dt} = J(a,t) - J(b,t)$,

where $J(x,t) \equiv \frac{i\hbar}{2m}\left(\Psi \frac{\partial \Psi^*}{\partial x} - \Psi^* \frac{\partial \Psi}{\partial x}\right)$. ("probability current")

+ What are the units of $J(x,t)$?

(b) Find the probability current for the wave function in P1.9.

(a) $$P_{ab}(t) = \int_a^b |\Psi(x,t)|^2 dx = \int_a^b \Psi^*(x,t)\Psi(x,t)\,dx$$

$$\frac{dP_{ab}}{dt} = \frac{d}{dt}\int_a^b \Psi^*(x,t)\Psi(x,t)\,dx = \int_a^b \frac{\partial}{\partial t}\Psi^*(x,t)\Psi(x,t)\,dx$$

$$= \int_a^b \frac{\partial \Psi^*}{\partial t}\Psi + \Psi^*\frac{\partial \Psi}{\partial t}\,dx$$

$$\begin{cases} \frac{\partial \Psi}{\partial t} = \frac{i}{\cancel{\hbar}}\frac{\hbar^{\cancel{2}}}{2m}\frac{\partial^2\Psi}{\partial x^2} + \frac{i}{\hbar}V\Psi \\ \frac{\partial \Psi^*}{\partial t} = -\frac{i}{\cancel{\hbar}}\frac{\hbar^{\cancel{2}}}{2m}\frac{\partial^2\Psi^*}{\partial x^2} - \frac{i}{\hbar}V\Psi^* \end{cases}$$

(Schrödinger Equation)

$$= \frac{i\hbar}{2m}\int_a^b \left(-\frac{\partial^2\Psi^*}{\partial x^2}\Psi - \cancel{\frac{2m}{\hbar^2}V\Psi^*\Psi} + \Psi^*\frac{\partial^2\Psi}{\partial x^2} + \cancel{\frac{2m}{\hbar^2}\Psi^*V\Psi}\right)dx$$

$$= \frac{i\hbar}{2m}\int_a^b \Psi^*\frac{\partial^2\Psi}{\partial x^2} - \Psi\frac{\partial^2\Psi^*}{\partial x^2}\,dx$$

$$= \frac{i\hbar}{2m}\int_a^b \left(\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \Psi\frac{\partial^2\Psi^*}{\partial x^2} + \frac{\partial\Psi^*}{\partial x}\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\frac{\partial\Psi}{\partial x}\right)dx$$

$$-\frac{\partial}{\partial x}\left(\Psi\frac{\partial\Psi^*}{\partial x}\right)$$

$$\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x}\right)$$

$$= \frac{i\hbar}{2m}\int_a^b \frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right)dx$$

Fundamental Theorem of Calculus

$$= \frac{i\hbar}{2m}\left(\Psi^*(b,t)\frac{\partial\Psi(b,t)}{\partial x} - \Psi(b,t)\frac{\partial\Psi^*(b,t)}{\partial x}\right) - \frac{i\hbar}{2m}\left(\Psi^*(a,t)\frac{\partial\Psi(a,t)}{\partial x} - \Psi(a,t)\frac{\partial\Psi^*(a,t)}{\partial x}\right)$$

$$= J(b,t) - J(a,t)$$

$[s^{-1}]$ from $\frac{dP_{ab}}{dt}$ ← unitless, ← [s]

(b) $\Psi(x,t) = Ae^{-a\left[\frac{mx^2}{\hbar} + it\right]}$

$$\Psi^*(x,t) = Ae^{-a\left[\frac{mx^2}{\hbar} - it\right]}$$

$$\frac{\partial \Psi}{\partial x} = -\frac{2amx}{\hbar} Ae^{-a\left[\frac{mx^2}{\hbar} + it\right]}$$

$$\frac{\partial \Psi^*}{\partial x} = -\frac{2amx}{\hbar} Ae^{-a\left[\frac{mx^2}{\hbar} - it\right]}$$

$$J(x,t) = \frac{i\hbar}{2m}\left(Ae^{-a\left[\frac{mx^2}{\hbar} - it\right]} \cdot -\frac{2amx}{\hbar} Ae^{-a\left[\frac{mx^2}{\hbar} + it\right]} + Ae^{-a\left[\frac{mx^2}{\hbar} + it\right]} \cdot \frac{2amx}{\hbar} Ae^{-a\left[\frac{mx^2}{\hbar} - it\right]}\right)$$

$$= 0$$

P1.18 Very roughly speaking, quantum mechanics is relevant when the de Broglie wavelength of the particle in question $\left(\frac{h}{p}\right)$ is greater than the characteristic size of the system (d). In thermal equilibrium at (Kelvin) temperature T, the average kinetic energy of a particle is

$$\frac{p^2}{2m} = \frac{3}{2}k_B T$$ (where k_B is Boltzmann's constant), so the typical

de Broglie wavelength is $\lambda = \dfrac{h}{\sqrt{3mk_BT}}$

The purpose of this problem is to determine which systems will have to be treated quantum mechanically, and which can safely be described classically.

(a) Solids. The lattice spacing in a typical solid is around $d = 0.3\,\text{nm}$. Find the temperature below which the unbound electrons in a solid are quantum mechanical. ✓

\+ Below what temperature are the nuclei in a solid quantum mechanical? ✓ (Use silicon as an example.)

Moral: The free electrons in a solid are always quantum mechanical; the nuclei are generally not quantum mechanical.

(b) Gases. For what temperatures are the atoms in an ideal gas at pressure P quantum mechanical? Hint: Use the ideal gas law ($PV = Nk_BT$) ✓ to deduce all the interatomic spacing.

Answer: $T < \dfrac{1}{k_B}\left(\dfrac{h^2}{3m}\right)^{3/5} P^{2/5}$. Obviously (for the gas to show quantum behaviour) we want m to be as small as possible, and P as large as possible. Put in the numbers for helium at atmospheric pressure. ✓ Is hydrogen in outer space (where the interatomic spacing is about 1 cm and the temperature is at least 3K) quantum mechanical? ✓ (assume it's monatomic hydrogen, not H_2)

(a) $\frac{h}{p} > d \rightarrow \lambda > d \rightarrow \frac{h}{\sqrt{3mk_BT}} > d$

$$\Rightarrow T < \frac{h^2}{3mk_Bd^2}$$

① electrons: $m_e = 9.109 \times 10^{-31}$ kg $h = 6.626 \times 10^{-34}$ J·s

$k_B = 1.381 \times 10^{-23}$ JK^{-1} $d = 0.3 \times 10^{-9}$ m

$T < 1.293 \times 10^5$ K

mass of Si nucleus

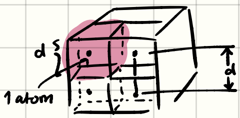
② Si nuclei: $m = 28.085 \cancel{amu} \times \frac{1.661 \times 10^{-27} kg}{1 \cancel{amu}} = 4.665 \times 10^{-26}$ kg $Si^{14}_{28.085\ amu}$

$1\ amu = 1.661 \times 10^{-27}$ kg

with same constants as before and same assumed lattice spacing $d = 0.3$nm:

$T < 2.525$K

(b) $PV = Nk_BT \Rightarrow Pd^3 = \cancel{N}^{1} k_BT \rightarrow d = \left(\frac{k_BT}{P}\right)^{1/3}$



$\frac{h}{\sqrt{3mk_BT}} > \left(\frac{k_BT}{P}\right)^{1/3} \rightarrow \frac{h^3P}{(3m)^{3/2}k_B^{5/2}} > T^{5/2}$

$\Rightarrow T < \frac{P^{2/5}h^{6/5}}{(3m)^{3/5}k_B}$

$2/5$ $3/2$

For helium: $He^2_{4.003\ amu}$

$m = 4.003 \cancel{amu} \times \frac{1.661 \times 10^{-27} kg}{1 \cancel{amu}} = 6.649 \times 10^{-27}$ kg

$1\ atm = 1.013 \times 10^5$ Pa

$P = 1.013 \times 10^5$ Pa

$T < 2.936$ K

For monatomic hydrogen:

$H^{1}_{1.008\,amu}$

$$m = 1.008\,\cancel{amu} \times \frac{1.661\times10^{-27}\,kg}{1\,\cancel{amu}} = 1.674\times10^{-27}\,kg$$

$$d = 0.01\,m$$

$$T < \frac{\hbar^2}{3mk_Bd^2} \implies T < 6.332\times10^{-14}\,K \implies \text{MUCH smaller than } 3K$$

$\Rightarrow$ No, H in outer space is NOT quantum mechanical