Chapter 1

The Schroedinger Equation

Classical Mechanics

- Classical Mechanics uses Newton laws to describe the state of motion of a mechanical system.
- Knowledge of initial conditions are necessary to completely predict the future motion.
- Force is the cause of the motion.
- Potential is conveniently used instead of force
- “Give me the potential” and I will tell you how the system evolve in time

Wave function, not particle

- In QM, the physical entity (e.g. particle) is represented by the wavefunction Ψ
- Ψ is governed by the Schroedinger equation (SE).
- Solving the SE for special cases of various potential U(*x*), and abstract physical information from the solution is the major objectives of ZCT 205.

The time-dependent Schroeding Equation

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

Ψ, *ψ* are pronounced as /ˈsaɪ/, /ˈpsaɪ/

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

- Time evolution of the WF, i.e., the LHS, is determined by the action of kinetic energy and potential energy operators on the WF (the RHS).

$$LHS{:}-i\hbar\frac{\partial}{\partial t}\Psi$$

$$RHS{:}\left(-\frac{\hbar}{2\mathrm{m}}\frac{\partial^2}{\partial x^2}+U\right)\Psi$$

$$H=\left(K+U\right)\Psi$$

- *H* is known as the hamiltonian
- Given (1) initial condition $\Psi(x,0)$ and (2) the potential *V*, the SE completely determines the time evolution of Ψ.

"Anatomy of the SE"

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

- $i\hbar\frac{\partial \Psi}{\partial t}$ Time-evolution of the wavefunction
- : $-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2}$ Kinetic energy
- $V\Psi$ Potential energy

Statistical Interpretation

$|\Psi(x,t)|^2$ = the probability density to find a particle at location *x*

- To be more precise:

- $\int_a^b |\Psi(x,t)|^2 \, dx$ probability of finding
- the particle between *a* and *b* at time *t*.
-

$$\int_a^b |\Psi(x,t)|^2 \, dx$$

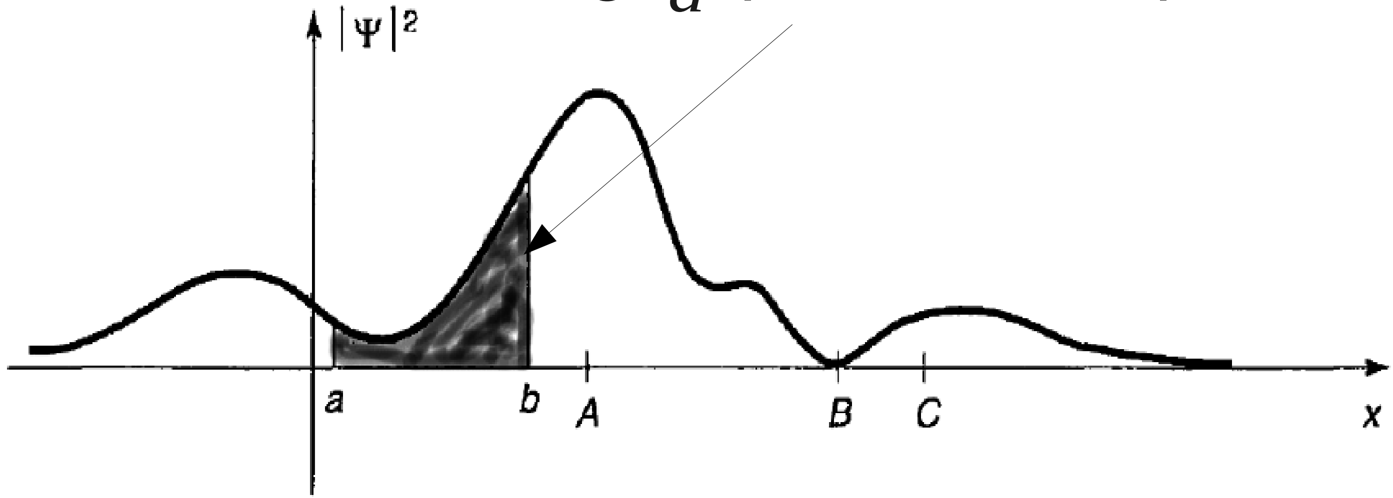


FIGURE 1.2: A typical wave function. The shaded area represents the probability of finding the particle between *a* and *b*. The particle would be relatively likely to be found near *A*, and unlikely to be found near *B*.

Inherent indeterminancy

- Even we know everything about the wave function and the equation governing it, we still can not predict with certainty the outcome of a simple experiment to measure the position. QM only offers statistical information about the possible results.

WF collapse

- Wave function collapse due to a measurement act.
- Two distinct kinds of physical entity: that before and after a measurement.

Quantum Zeno effect

- Particle before measurement is governed by SE, and the wavefunction is evolving in time. This state has inherent indeterminancy.
- Once it is measured, the system is forced into a definite state and stop evolving in time, and will stay in the measured state, at least right immediately the WF collapses.
- The system is completely determined and loss the indeterminancy, at least temporarily after the measurement.
- If the measurement process is persistently carried out on the system, it will stay at that last measured state – QZE.

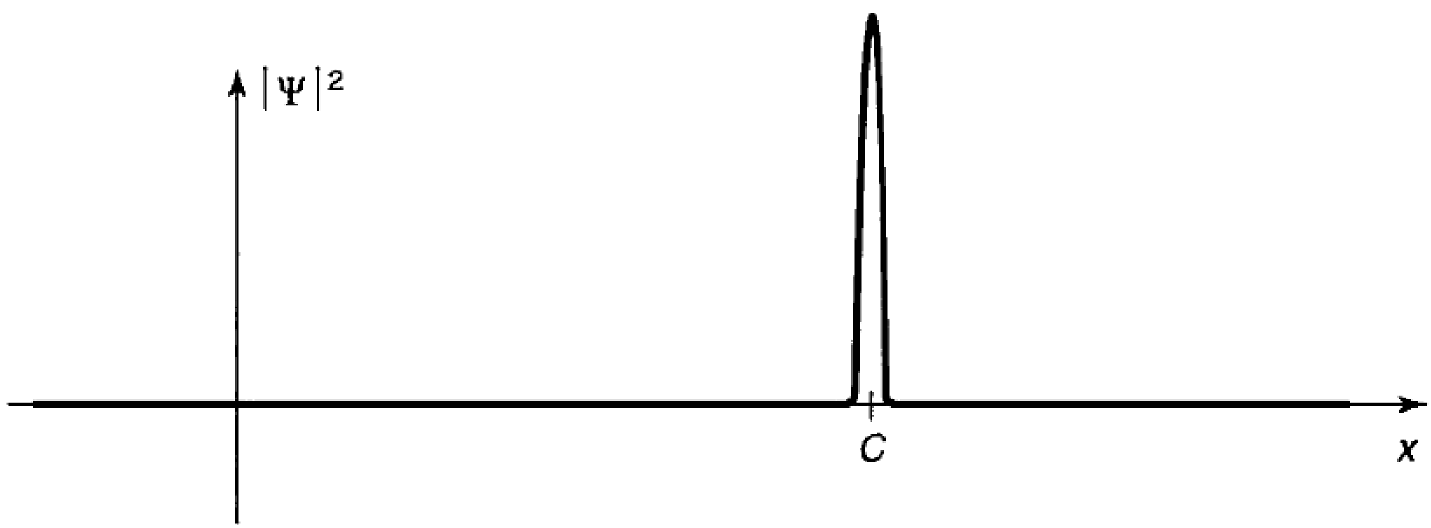


FIGURE 1.3: Collapse of the wave function: graph of $|\Psi|^2$ immediately *after* a measurement has found the particle at point C.

Histogram

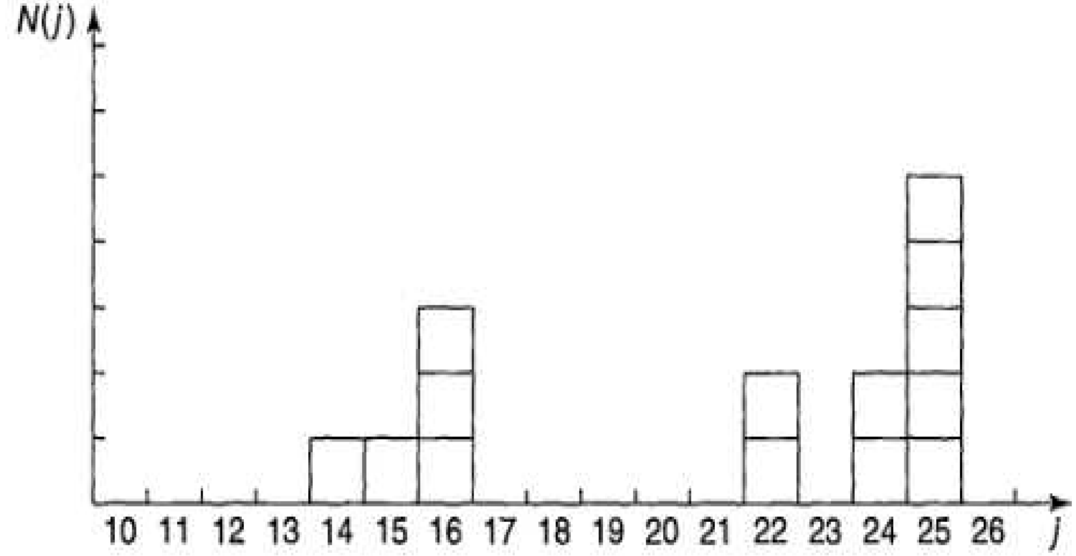


FIGURE 1.4: Histogram showing the number of people, $N(j)$, with age j, for the distribution in Section 1.3.1.

Discrete probability

- *j = age; N*(*j*) number of persons with integer age *j*.

$$N = \sum N(j)$$

$$P(j) = \frac{N(j)}{N}$$

$$\sum P(j) = \sum P(j) = 1$$

$$\langle j \rangle = \sum j P(j) \qquad \langle j^2 \rangle = \sum j^2 P(j)$$

$$\langle f(j) \rangle = \sum f(j) P(j)$$

Discrete probability

- “spread” in the distribution (histrogram)

$$\sigma^2 = \langle (\Delta j)^2 \rangle ;$$
$$\Delta j = j - \langle j \rangle$$

$$\sigma = \sqrt{\sigma^2}$$

“Normalised” version of the histogram

- $N(j)$ vs. j $\longrightarrow$ $\rho(j)$ *vs.* j
- where $\rho(j) = N(j)/N$
- The histogram $\rho(j)$ vs. j is the normalised version of histogram N(j) vs. j
- $\Delta j = 1$, interval between two successive j
- For discrete distribution, normalisation is stated as : $\sum \rho(j)\,\Delta j = 1$
- $\rho(j)$ is PDF

Genetic expectation value in discrete distribution

-
- In terms of discrete PDF,

$$\langle Q \rangle = \sum \rho(j) Q(j) \Delta j$$

Continuous variable

- If *j* is a continuous variable *x*,

$$1 = \int_{-\infty}^{\infty} \rho(x)\,dx,$$

$$\langle x \rangle = \int_{-\infty}^{\infty} x\rho(x)\,dx,$$

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} f(x)\rho(x)\,dx,$$

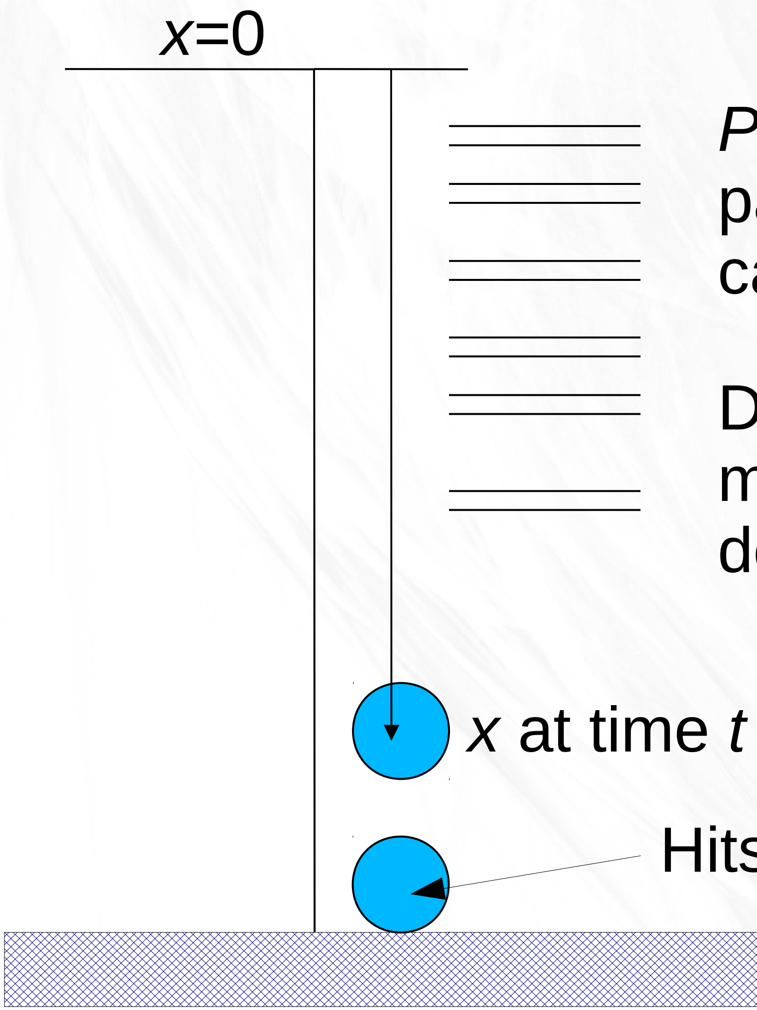
$$\sigma^2 \equiv \langle (\Delta x)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$$

$$\int_{-\infty}^{\infty} \rho(x)\,dx = 1 \qquad \rho(x) = \frac{N(x)}{\int_{-\infty}^{\infty} N(x)\,dx} = \frac{N(x)}{N}$$

Example

- This example illustrates the application of PDF.
- Suppose I drop a rock off a cliff of height *h*. As it falls. I snap a million photographs, at random intervals. On each picture I measure the distance the rock has fallen. Question: What is the average of all these distances? That is to say, what is the time average of the distance traveled?

Calculate $\rho(x)$



$P = \Delta t/T$; Δx width of the snapshot; A particle falling through Δx will be captured at a probability P.

Derive $\rho(x)$ using classical mechanics, and from there you can determine $\langle x \rangle$

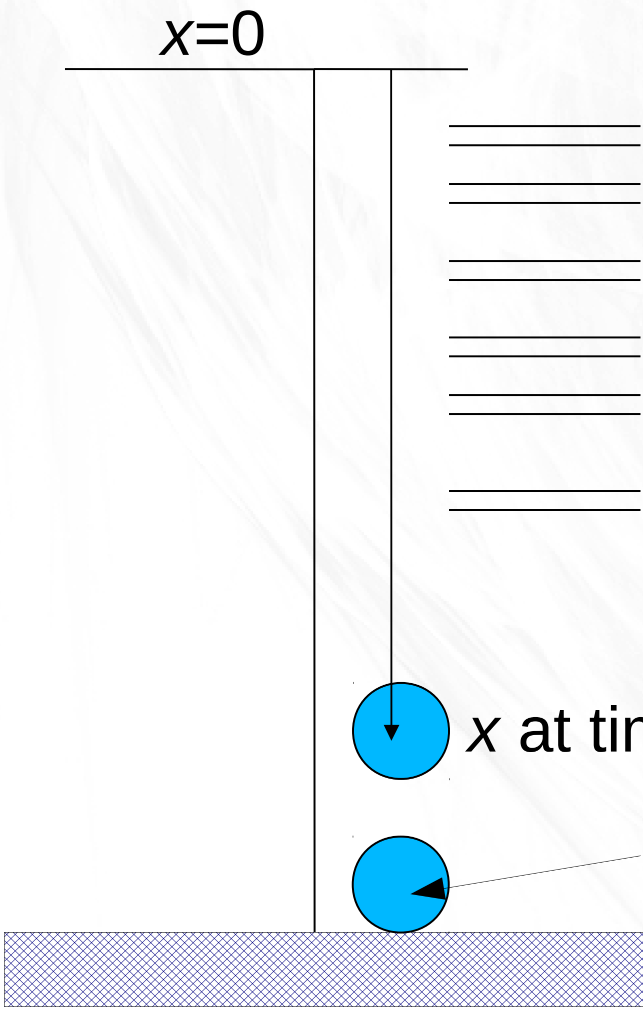
Hits ground $x=h$ when $t=T=\sqrt{(2h/g)}$

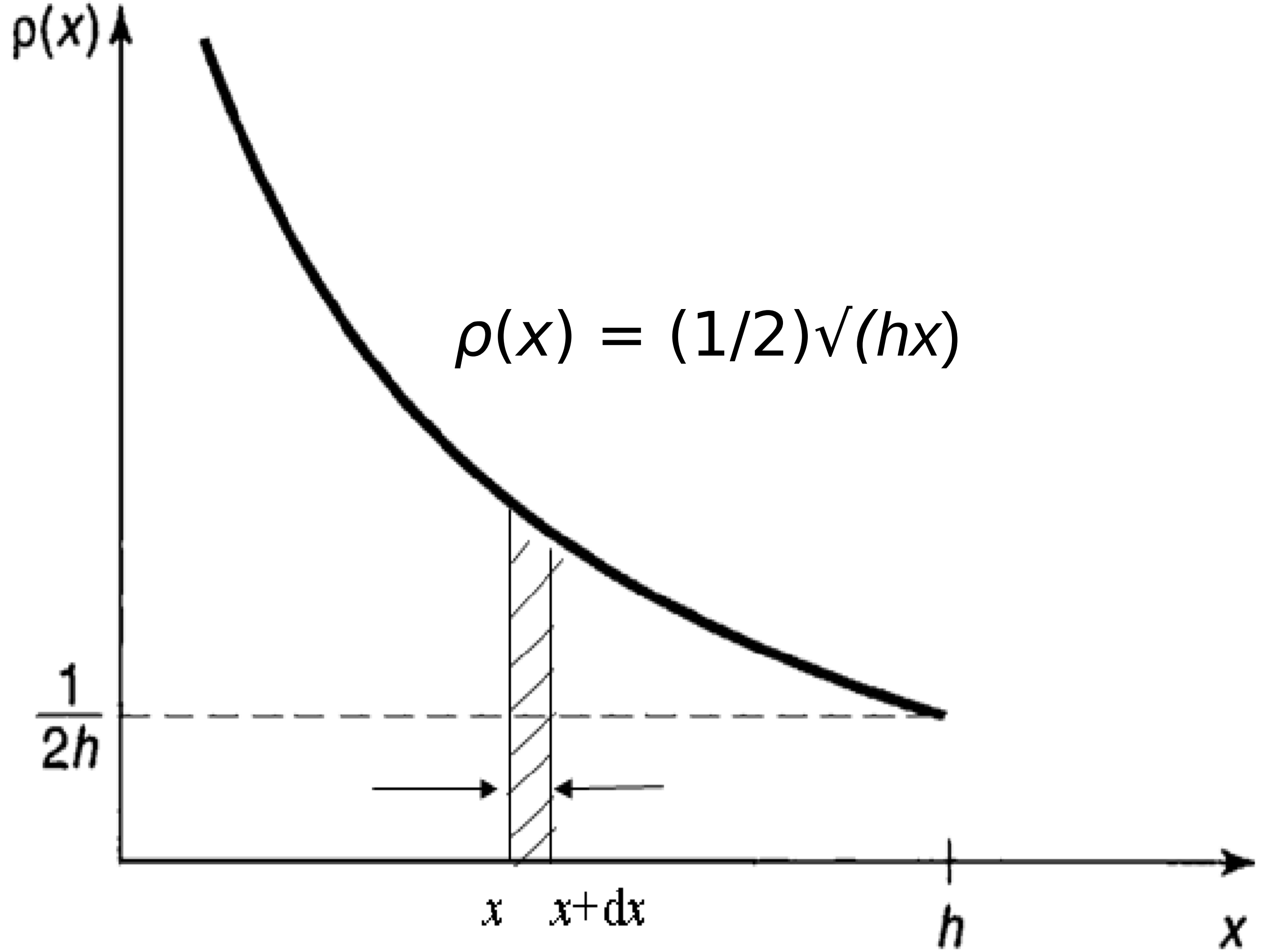
Calculate $\rho(x)$

By definition, $P = \rho(x)\Delta x$
Equate $P = \Delta t/T = \rho(x)\Delta x$

From Newton's law,
$x = (1/2)gt^2$; $t = \sqrt{(2x/g)}$; $dx = gt\, dt$

In the limit $\Delta t \to 0$,
$P = dt/T = (dx/gt)/\sqrt{(2h/g)} = \rho(x)dx$
$\rho(x) = (1/2)\sqrt{(hx)}$





$$\langle x \rangle = \int_0^h x \frac{1}{2\sqrt{hx}} dx = \frac{1}{2\sqrt{h}} \left(\frac{2}{3} x^{3/2} \right) \Big|_0^h = \frac{h}{3} < \frac{h}{2}$$

What's the point of the example?

- Knowing the PDF of a system allows you to abstract averaged dynamical information from it.

Square-integrable

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx < \infty$$

$\Psi(x,t)$ must go to zero faster than $1/\sqrt{|x|}$ as $|x| \to \infty$.

$$\Psi(x,t) \to 0 \text{ as } |x| \to \infty$$

Normalisation

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

$$\frac{d}{dt}\left(\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx\right) = 0$$

Normalisation condition is preserved in all time *t.*
If the WF is normalised at *t*=0, it is normalised for the rest of the time.

Normalisation is time-independent. Proove it.

$$\frac{d}{dt}\left(\int_{-\infty}^{\infty}|\Psi(x,t)|^2 dx\right) = 0$$

.

Example

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

(a) Normalize Ψ (that is, find A in terms of a and b).

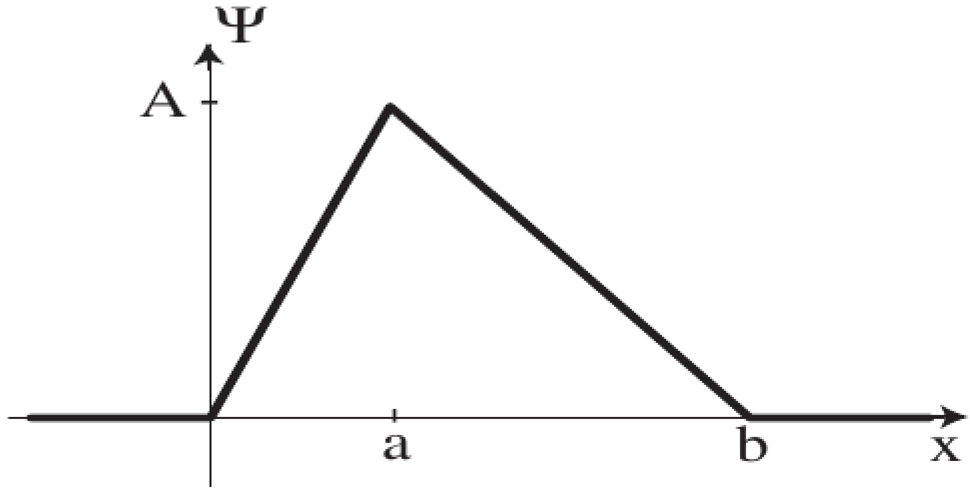
(b) Sketch $\Psi(x,0)$ as a function of x

(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* = 2*a*.

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

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



$$P = \int_0^a |\Psi|^2 dx = \frac{|A|^2}{a^2}\int_0^a x^2 dx = |A|^2 \frac{a}{3} = \boxed{\frac{a}{b}}.$$

$$P = 1 \quad \text{if } \; b = a, \; \checkmark$$

$$P = 1/2 \text{ if } \; b = 2a. \; \checkmark$$

Measuring the expectation value

- The expectation value is the average of repeated measurements on an ensemble of identically prepared systems, not the average of repeated measurements on one and the same system.

Measuring momentum

- Calculate the expectation value of the momentum of a particle described by Ψ

$$\langle p \rangle = m \frac{d\langle x \rangle}{dt}$$

$$\langle x \rangle = \int_{-\infty}^{\infty} x|\Psi(x,t)|^2 dx.$$

Observables are represented as operators in QM

$$\frac{d}{dt}\langle x\rangle = \int x\frac{\partial}{\partial t}|\Psi|^2 dx = \cdots = \frac{-i\hbar}{2m}\int\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)dx = \cdots$$

$$= \frac{1}{m}\int\Psi^*\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi\right)dx \equiv \frac{\langle p\rangle}{m}.$$

$$\langle x\rangle = \int\Psi^* x\Psi dx,$$

$$\langle p\rangle = \int\Psi^*\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi dx.$$

Axiom: For any generic dynamical observable

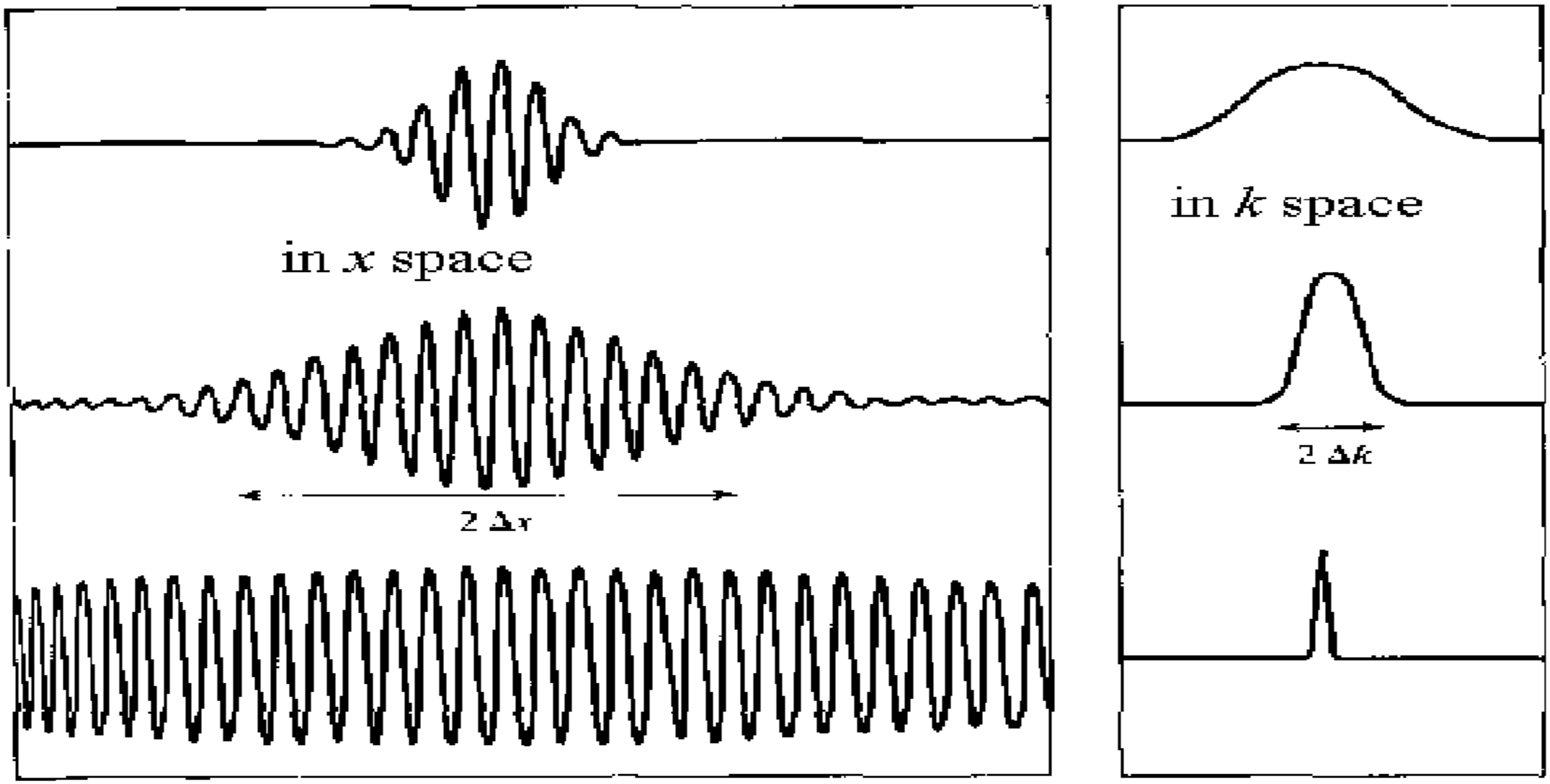
$$\langle Q(x,p)\rangle = \int \Psi^* Q\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi\, dx$$

Example:

$$\langle T\rangle = -\frac{\hbar^2}{2m}\int \Psi^* \frac{\partial^2 \Psi}{\partial x^2} dx$$

1-D Wave

- A wave well defined in wavelength ($\sigma_\lambda \ll 1$) is ill-defined in location ($\sigma_x \gg 1$), and vice versa.



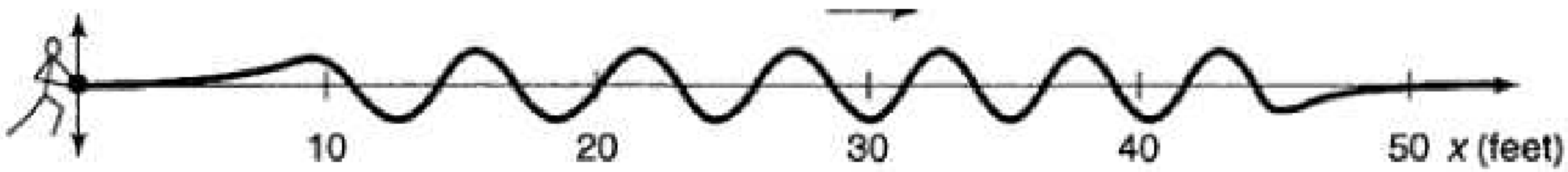


FIGURE 1.7: A wave with a (fairly) well-defined *wavelength*, but an ill-defined *position*.

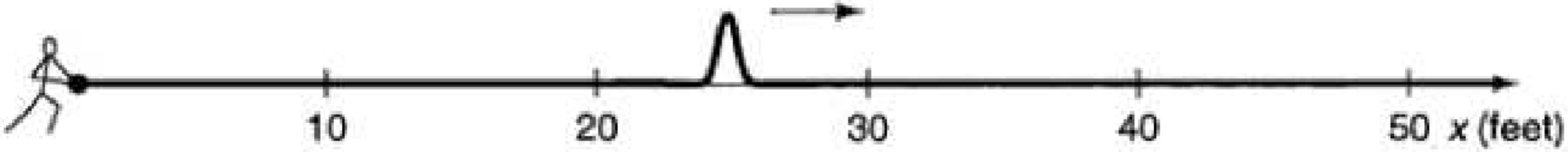


FIGURE 1.8: A wave with a (fairly) well-defined *position*, but an ill-defined *wavelength*.

de Broglie postulate

- The wavelength of Ψ is related to the momentum of the particle by the de Broglie formula

$$p = \frac{h}{\lambda} = \frac{2\pi\hbar}{\lambda}$$

Heisenberg's uncertainty principle

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

Simulation of wave packet using Mathematica

http://www2.fizik.usm.my/tlyoon/teaching/ZCT205_1112/wave.nb

(i) adding many waves of different wavelength results in a wave packet,
(ii) the wave packet's "spread" in x (the "width" of the wave packet) is inversely proportional to the "spread" in wave number ($\Delta k = N_k \Delta$) of the waves that are used to form the wave packet.

Example

- A particle of mass m is in the state

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

- where *A* and a are positive real constants.
- (a) Find *A*.
- (b) For what potential energy function *V* (x) does *Ψ* satisfy the Schroedinger 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?

Hint

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2} du.$$

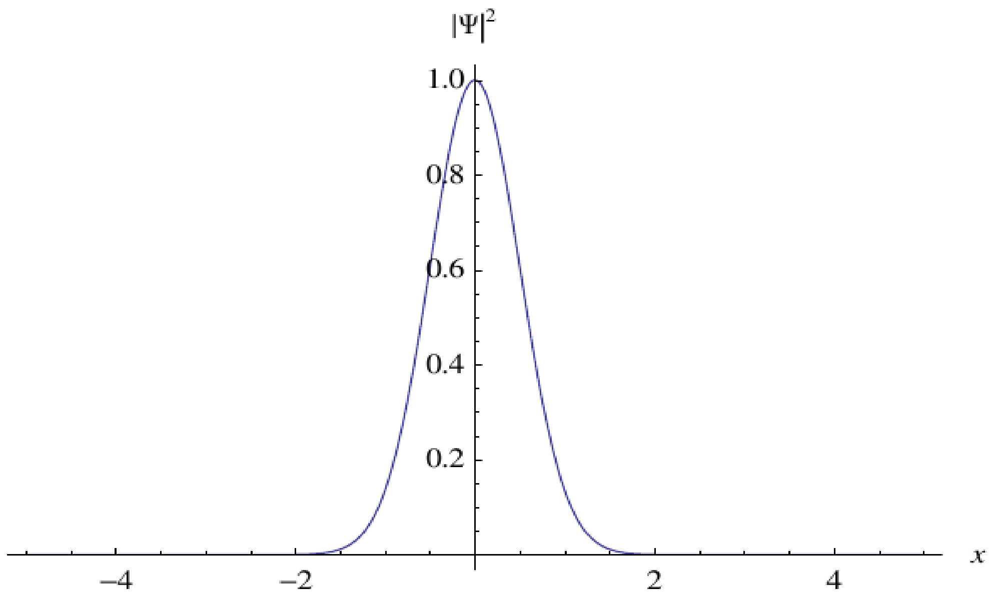
$$\mathrm{erf}(x \to \pm\infty) = \pm 1$$

(a) Find *A*

- Use normalisation condition. Cast the integral into the form of erf(x)

$$|\Psi|^2 = \Psi^* \Psi = \left(A \exp\left[-a\left(\frac{mx^2}{\hbar}\right) + iht \right] \right)^* \cdot \left(A \exp\left[-a\left(\frac{mx^2}{\hbar}\right) + iht \right] \right)$$

$$= A^2 \exp\left[-2\mathrm{a}\left(\frac{mx^2}{\hbar}\right) \right]$$



$$\int_{-\infty}^{\infty} A^2 \exp\left[-\left(\frac{2am}{\hbar}\right)x^2\right]dx = 1$$

$$\int_{-\infty}^{\infty} A^2 \exp\left[-\left(\frac{2am}{\hbar}\right)x^2\right]dx = 2A^2\int_0^{\infty} \exp\left(-y^2\right)dx$$

$$y^2 = \frac{2ma}{\hbar}x^2, y = \sqrt{\frac{2ma}{\hbar}}x, dy = \sqrt{\frac{2ma}{\hbar}}dx$$

$$\frac{2A^2}{\sqrt{\frac{2ma}{\hbar}}} \cdot \sqrt{\frac{\pi}{2}} \cdot \sqrt{\frac{2}{\pi}} \int_0^{\infty} \exp\left(-y^2\right)dy = \frac{2A^2}{\sqrt{\frac{2ma}{\hbar}}} \cdot \sqrt{\frac{\pi}{2}} = 1$$

$$A = \left(\frac{ma}{\pi\hbar}\right)^{\frac{1}{4}}$$

•(b) For what potential energy function *V* (x) does *Ψ* satisfy the Schroedinger equation?

$$\frac{\partial \Psi}{\partial t} = -ia\Psi; \quad \frac{\partial \Psi}{\partial x} = -\frac{2amx}{\hbar}\Psi;$$

$$\frac{\partial^2 \Psi}{\partial x^2} = -\frac{2am}{\hbar}\left(\Psi + x\frac{\partial \Psi}{\partial x}\right) = -\frac{2am}{\hbar}\left(1 - \frac{2amx^2}{\hbar}\right)\Psi.$$

Plug these into the Schrödinger equation,

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

$$V\Psi = i\hbar(-ia)\Psi + \frac{\hbar^2}{2m}\left(-\frac{2am}{\hbar}\right)\left(1 - \frac{2amx^2}{\hbar}\right)\Psi$$

$$\boxed{V(x) = 2ma^2x^2.}$$

$$\langle x \rangle = \int_{-\infty}^{\infty} x|\Psi|^2 dx = \boxed{0.} \qquad \text{[Odd integrand.]}$$

$$\langle x^2 \rangle = 2|A|^2 \int_0^{\infty} x^2 e^{-2amx^2/\hbar} dx =$$

$$2|A|^2 \frac{1}{2^2(2am/\hbar)} \sqrt{\frac{\pi\hbar}{2am}} = \boxed{\frac{\hbar}{4am}.}$$

$$\langle p \rangle = m\frac{d\langle x \rangle}{dt} = \boxed{0.}$$

$$\langle p^2 \rangle = \int \Psi^* \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 \Psi dx = -\hbar^2 \int \Psi^* \frac{\partial^2 \Psi}{\partial x^2} dx$$

$$= -\hbar^2 \int \Psi^* \left[-\frac{2am}{\hbar}\left(1 - \frac{2amx^2}{\hbar}\right)\Psi\right] dx$$

$$= 2am\hbar \left\{ \int |\Psi|^2 dx - \frac{2am}{\hbar} \int x^2 |\Psi|^2 dx \right\}$$

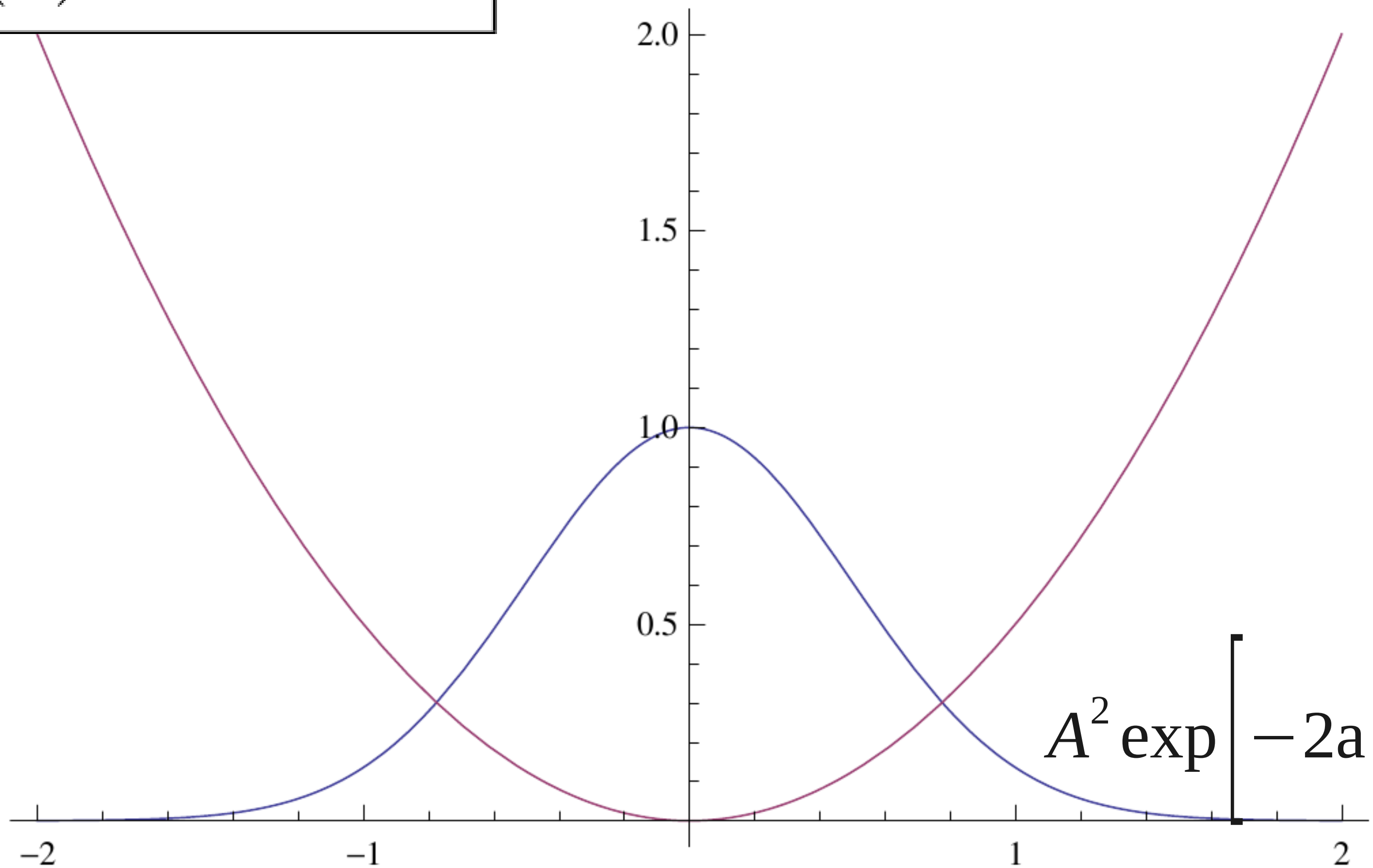
$$= 2am\hbar \left(1 - \frac{2am}{\hbar}\langle x^2 \rangle\right) = 2am\hbar \left(1 - \frac{2am}{\hbar}\frac{\hbar}{4am}\right)$$

$$= 2am\hbar \left(\frac{1}{2}\right) = \boxed{am\hbar.}$$

Check it yourself to verify that, indeed, the solutions you obtain do obey Heisenberg's Uncertainty Principle,

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

$$V(x) = 2ma^2x^2.$$



$$A^2 \exp\left[-2a\left(\frac{mx^2}{\hbar}\right)\right]_x$$

Tutorial to submit online

Please scan your hand-written answer and submit the solution to these tutorial questions online to E-learning

2. Prove that for a wave function that is the solution to the Schroedinger ec
tion, the normalisation of the wave function is time-independent,

$$\frac{d}{dt}\left(\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx\right) = 0.$$

Prove this:

$$\langle p \rangle = \int \Psi^* \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) \Psi dx.$$

Problem 1.17 A particle is represented (at time $t = 0$) by the wave function

$$\Psi(x, 0) = \begin{cases} A(a^2 - x^2), & \text{if } -a \le x \le +a, \\ 0, & \text{otherwise.} \end{cases}$$

(a) Determine the normalization constant A.

(b) What is the expectation value of x (at time $t = 0$)?

(c) What is the expectation value of p (at time $t = 0$)? (Note that you *cannot* get it from $p = md\langle x\rangle/dt$. Why not?)

(d) Find the expectation value of x^2.

(e) Find the expectation value of p^2.

(f) Find the uncertainty in x (σ_x).

Problem 1.16 Show that

$$\frac{d}{dt}\int_{-\infty}^{\infty} \Psi_1^* \Psi_2 \, dx = 0$$

for any two (normalizable) solutions to the Schrödinger equation, Ψ_1 and Ψ_2.