Quantum Physics Lecture 8

Applications of Steady state Schroedinger Equation

Box of more than one dimension

Harmonic oscillator

Particle meeting a potential step
Waves/particles in a box of >1 dimension

Consider 2-D box
Potential \( U = 0 \) between \( x = 0 \) and \( x = a \)
And between \( y = 0 \) and \( y = b \)
\( U \) infinite elsewhere

Wavefunction \( \Psi \) expressed as \( \Psi(x,y) = f(x)g(y) \) - Separation of variables

Steady state Schrödinger Equation inside box, where \( U = 0 \)

\[
- \frac{\hbar^2}{2m} \left( \frac{\partial^2 \Psi(x,y)}{\partial x^2} + \frac{\partial^2 \Psi(x,y)}{\partial y^2} \right) = E \Psi(x,y)
\]  (Recall \( H\Psi = E\Psi \))

Put in \( \Psi(x,y) = f(x)g(y) \) - noting partial differentials!
Waves/particles in a 2-D box (cont.)

\[-\frac{\hbar^2}{2m} \left( g(y) \frac{\partial^2 f(x)}{\partial x^2} + f(x) \frac{\partial^2 g(y)}{\partial y^2} \right) = Ef(x)g(y)\]

Thus 

\[-\frac{\hbar^2}{2m} \left( \frac{\partial^2 f(x)}{\partial x^2} + \frac{\partial^2 g(y)}{\partial y^2} \right) = E\]

Only one term is \(x\) dependent, and it equals a constant

\[\frac{\partial^2 f(x)}{\partial x^2} = -C\]

So 

\[\frac{\partial^2 f(x)}{\partial x^2} = -Cf(x)\quad \text{Which we have seen before…}\]

Solutions, using boundary conditions, are 

\[f(x) = A \sin \frac{n\pi x}{a} \quad \text{with} \quad C = \frac{n^2 \pi^2}{a^2}\]

Similarly, for \(y\) dependence 

\[g(y) = B \sin \frac{m\pi y}{b}\]

Hence the energy levels in the box are

\[E_{n,m} = \frac{\hbar^2}{2m} \left( \frac{n^2 \pi^2}{a^2} + \frac{m^2 \pi^2}{b^2} \right)\]

With \textbf{TWO} quantum numbers \(n,m\) needed to specify the state
Waves/particles in a 2-D box (cont.)

Ψ is specified by the quantum numbers \( n \) & \( m \)

There are as many states as there are possible \( n,m \) combinations \( (N.B. \ n \ & \ m \ \text{are positive}) \)

Two distinct wave functions are DEGENERATE if they have the same energy.

\( \text{e.g. the states } 1,3 \ \text{and } 3,1 \ \text{are degenerate if } a = b \)

\( \text{If } a/b \ \text{is irrational there are no degeneracies} \)

Readily extended to 3-D….

Useful, especially when filling box with more than one particle.

C.f. black body cavity
Harmonic Oscillator

Examples: mass on spring, diatomic molecule…

Hooke’s Law: “restoring force” $F = -kx$

$$-kx = m \frac{d^2 x}{dt^2}$$

$$\frac{d^2 x}{dt^2} + \frac{k}{m} x = 0$$

$$x = A \cos \omega t$$

Where \( \omega = \sqrt{\frac{k}{m}} \)

Potential energy $U = \frac{1}{2}kx^2$ (potential well, parabolic)

**Expect**

1. quantised energy,
2. $E_{\text{min}} \neq 0$
3. particle outside the classical limits $A$
Apply SSSE to Harmonic Oscillator

\[ \frac{d^2 \psi}{dx^2} + \frac{2m}{\hbar^2} \left( E - \frac{1}{2} kx^2 \right) \psi = 0 \]

or
\[ \frac{d^2 \psi}{dx^2} + \left( \frac{2mE}{\hbar^2} - \frac{km}{\hbar^2} x^2 \right) \psi = 0 \]

write \( y = \left( \frac{\sqrt{km}}{\hbar} \right)^{1/2} x \) and \( dy^2 = \left( \frac{\sqrt{km}}{\hbar} \right) dx^2 \)

\[ \frac{d^2 \psi}{dy^2} + (\alpha - y^2) \psi = 0 \]
\[ \alpha = \frac{2mE}{\hbar^2} \left/ \frac{\sqrt{km}}{\hbar} \right. = \frac{2E}{\hbar} \sqrt{\frac{m}{k}} = \frac{2E}{\hbar \omega} \]
Results for Harmonic Oscillator

Solution requires:

\[ \frac{d^2 \psi}{dy^2} + (\alpha - y^2) \psi = 0 \]

\[ \alpha = 2n + 1 \quad \text{for } n = 0, 1, 2, 3... \]

\[ E_n = \frac{\hbar \omega}{2} \alpha = \frac{\hbar \omega}{2} (2n + 1) = \left(n + \frac{1}{2}\right) \hbar \omega \]

\[ E_0 = \frac{1}{2} \hbar \omega \quad \text{a.k.a. “zero point energy} \]

Recall Planck’s assumption & blackbody formula (Lecture 6):
Oscillator energies assumed \[ E_n = n\hbar \omega \]

Later, found additional detail & statistics, \( C_v \) etc. but…
Right ideas on quantisation: “fortunate guesswork!”
Wavefunctions of Harmonic Oscillator

Comparing with infinite square well case, $\psi$ has approximately same shape except:

1. width of well is changing
2. $\psi$ extends beyond classical limit
3. amplitude increases at well edge

Look at (2) and (3) via the probability density…..
Probability Density of Harmonic Oscillator

(1) Finite probability of particle outside the classical limits

(2) the quantum picture only approaches the classical picture at large n values
(classical - probability maximum at extremities of oscillation - slower)
- Correspondence Principle

Footnote: compare square well \([E_n \propto n^2]\) and harmonic oscillator \([E_n \propto (n + 1/2)]\) and Bohr H atom \([E_n \propto -1/n^2]\) for energies.
  Differing shapes of the potential wells.
Particle meeting step potential

2 types: “step-up” \[ \rightarrow \] \[ U=U_0 \] \[ U=0 \] “step-down” \[ \rightarrow \] \[ U=U_0 \] \[ U=0 \]

Particle direction “left-to-right”; potential flat apart from step region;

Particle energy \( E \) and step size \( U_o \); 3 distinct situations:

“up” \( E < U_o \) \[ E \] \[ U=U_0 \] \[ U=0 \]
“up” \( E > U_o \) \[ E \] \[ U=U_0 \] \[ U=0 \]
“down” \( E > U_o \) \[ E \] \[ U=U_0 \] \[ U=0 \]

Find elements of “propagating” and “decaying” wavefunctions;
Solutions may not be standing waves (as previously)
cannot draw (\( \cdot \cdot complex \ \psi \)) but can always draw \( |\psi|^2 \) (real).
Apply SSSE to step-up potential \((E < U_o)\)

Classically, particle is reflected!

\[
\frac{d^2 \psi}{dx^2} + \frac{2m}{\hbar^2} (E - U) \psi = 0
\]

For region I, solution is complex exponentials:

\[
\psi_I = A \exp(ik_1x) + B \exp(-ik_1x)
\]

For region II, solutions are real exponentials:

\[
\psi_{II} = C \exp(k_2x) + D \exp(-k_2x)
\]

Also, require \(C = 0\), to keep \(\psi\) finite at large +ve \(x\):

\[
\psi_{II} = D \exp(-k_2x)
\]
Apply boundary matching

\[ \psi_{II} = \psi_I \text{ at } x = 0 \]
\[ D \exp(0) = A \exp(0) + B \exp(0) \]
\[ D = A + B \]
\[ d\psi_{II}/dx = d\psi_I/dx \text{ at } x = 0 \]
\[ -k_2 D \exp(0) = i k_1 A \exp(0) - i k_1 B \exp(0) \]
\[ (i k_2/k_1) D = A - B \]

Convenient to write A and B in terms of D:

\[ \psi_I = D/2 \left( 1 + \frac{i k_2}{k_1} \right) \exp(i k_1 x) + D/2 \left( 1 - \frac{i k_2}{k_1} \right) \exp(-i k_1 x) \]

meaning?

incident particle(s) \hspace{1cm} reflected particle(s)

\[ \psi_{II} = D \exp(-k_2 x) \]

particle(s) probability decays into wall!
Particle reflection

Reflection Coefficient $R = B^*B/A^*A$

\[
R = \frac{(1 - i \frac{k_2}{k_1})^* (1 - i \frac{k_2}{k_1})}{(1 + i \frac{k_2}{k_1})^* (1 + i \frac{k_2}{k_1})} = \frac{(1 + i \frac{k_2}{k_1})(1 - i \frac{k_2}{k_1})}{(1 - i \frac{k_2}{k_1})(1 + i \frac{k_2}{k_1})} = 1
\]

As expected, in agreement with classical picture!

Exercise: use $[\exp(i\theta) = \cos\theta + i\sin\theta]$ to show

\[
\psi_I = D \cos(k_1x) - D \left(\frac{k_2}{k_1}\right) \sin(k_1x)
\]

can be generalised as $\sin(k_1x + \phi)$ i.e. standing wave!
(combination of equal incident and reflected waves)
Plotting $\psi$ and $|\psi|^2$

Because in this case $\psi_i$ is a pure standing wave, it can still be plotted; note how $\psi_i$ matches onto $\psi_{ll}$ (red).

As $U_o$ increases, $k_2$ increases (less penetration of wall) and $\psi_i$ moves closer to simple $\sin(k_1 x)$.

Plot of $|\psi|^2$ always possible
Signature of perfect reflection ($R = 1$):

minimum value of $|\psi|^2 = 0$
Apply SSSE to step-up potential \((E > U_o)\)

Classically: kinetic energy decrease and particle \textit{not} reflected!

\[
\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - U)\psi = 0
\]

For region I, solution is \textit{complex} exponentials as before:

\[
\psi_I = A\exp(ik_1x) + B\exp(-ik_1x) \quad \text{where} \quad k_1 = \frac{\sqrt{2mE}}{\hbar}
\]

For region II, solution is also \textit{complex} exponentials:

\[
\psi_{II} = C\exp(ik_2x) + D\exp(-ik_2x) \quad \text{where} \quad k_2 = \frac{\sqrt{2m(E-U_o)}}{\hbar}
\]

Require \(D = 0\), no \textit{negative-going} wave for \(x > 0\), as all particles are incident in +ve \(x\) direction!

Not so for \(x < 0\), there is \textit{some} reflection!

\[
\psi_{II} = C\exp(ik_2x)
\]
Apply boundary matching

\[ \psi_{II} = \psi_I \text{ at } x = 0 \]

\[ C \exp(0) = A \exp(0) + B \exp(0) \]

\[ C = A + B \]

\[ d\psi_{II}/dx = d\psi_I/dx \text{ at } x = 0 \]

\[ ik_2 C \exp(0) = ik_1 A \exp(0) - ik_1 B \exp(0) \]

\[ (k_2/k_1)C = A - B \]

Convenient to write \( B \) and \( C \) in terms of \( A \):

\[ \psi_I = A \exp(ik_1 x) + A \frac{k_1 - k_2}{k_1 + k_2} \exp(-ik_1 x) \]

meaning?

\[ \psi_{II} = A \frac{2k_1}{k_1 + k_2} \exp(ik_2 x) \text{ particle(s) with reduced energy!} \]
Particle reflection

Recall Reflection Coefficient \( R = \frac{B \cdot B}{A \cdot A} \)

\[
R = \left( \frac{k_1 - k_2}{k_1 + k_2} \right)^2 = \left( \frac{1 - \frac{k_2}{k_1}}{1 + \frac{k_2}{k_1}} \right)^2
\]

Recall the equations for \( k_1 \) and \( k_2 \)

\[
\frac{k_2}{k_1} = \sqrt{2m(E - U_0) \over \sqrt{2mE}} = \sqrt{1 - \frac{U_0}{E}}
\]

\[
R = \left( \frac{1 - \sqrt{1 - \frac{U_0}{E}}}{1 + \sqrt{1 - \frac{U_0}{E}}} \right)^2
\]

for \( E > U_o \) and \( R = 1 \) for \( E < U_o \)
Particle meeting **step-down** potential

compare:  “step-up”  with  “step-down”

Reverse situations, simply exchange $k_1$ and $k_2$:

$$\psi_I = A \exp(ik_2x) + B \exp(-ik_2x)$$
$$\psi_{II} = C \exp(ik_1x)$$

Proceed to determine matching etc.

Significant point is that some **reflection** occurs here too;

**Origin of reflectivity is “change in potential $U$”**

*For quantum ‘lemmings’, some reflect from cliff edge….*
General conclusions

Step-up, where $E < U_o$
- total reflection
- but can exist in wall!

Step-up, where $E > U_o$
- decreased kinetic energy
- and partial reflection!

Step-down, where $E > U_o$
- increased kinetic energy
- also partial reflection!

“solve, match, R and plot”