

Thurs: HW by 5pmWeds: Read. 5.2, 5.3, 5.4.HW Note: Integration

In general one can check integrals using tables or software such as Wolfram Alpha, MAPLE, Mathematica. You can do this for HW for integrals that are not simple polynomials or trig functions.

Certain integrals cannot be evaluated in their indefinite form. For example

$$\int e^{-x^2/a^2} dx = ?? \quad \text{OR} \quad \int \frac{\sin^2 x}{x^2} dx = ??$$

However for extreme ranges of integration limits, these can be evaluated.

So

$$\underbrace{\int_0^{\infty} e^{-x^2/a^2} dx = \frac{a}{2} \sqrt{\pi}} \quad \underbrace{\int_0^{\infty} \frac{\sin^2 x}{x^2} dx = \frac{\pi}{2}}$$

look up / can be proved.

Schrödinger equation for a free particle in one dimension

Consider a free particle in one dimension.

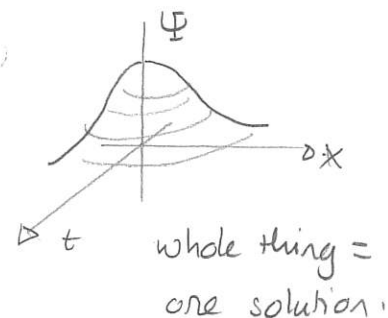
The wave function for the free particle satisfies

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

where m is the mass of the particle.

This is an example of a differential equation. The solution to such a differential equation is:

1) an entire function of two variables (x, t)



2) the function must be such that when substituted into the original differential equation, the resulting expressions are true at all positions and also all times.

Quiz 1 50% - 90%

In this case consider substitution:

Left

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}$$

$$= -\frac{\hbar^2}{2m} \frac{\partial}{\partial x} 2A(x-Bt)$$

$$= -\frac{\hbar^2}{2m} 2A$$

Right

$$i\hbar \frac{\partial \Psi}{\partial t}$$

$$= i\hbar 2A(-B)(x-Bt)$$

$$= -i\hbar 2AB(x-Bt)$$

↙ imaginary part.

These are not the same function. If one sets the two sides equal then

$$-\frac{\hbar^2}{2m} 2A = -i\hbar 2AB(x-Bt) \Rightarrow 1 = i\hbar m B(x-Bt) \text{ may work for}$$

$$x = Bt + \frac{1}{2i\hbar m B} \text{ not all } t, x !!$$

Thus this function does not solve the Schrödinger equation.

Consider another possibility:

$$\Psi(x,t) = A e^{i(kx - \omega t)}$$

Quiz 2 60%

Left	$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}$	Right	$i\hbar \frac{\partial \Psi}{\partial t}$
	$-\frac{\hbar^2}{2m} \frac{\partial}{\partial x} \left[\frac{\partial}{\partial x} A e^{i(kx - \omega t)} \right]$		$i\hbar \frac{\partial}{\partial t} A e^{i(kx - \omega t)}$
	$= -\frac{\hbar^2}{2m} \frac{\partial}{\partial x} i k A e^{i(kx - \omega t)}$		$= i\hbar A (-i\omega) A e^{i(kx - \omega t)}$
	$= -\frac{\hbar^2}{2m} (ik)^2 A e^{i(kx - \omega t)}$		$= \hbar\omega A e^{i(kx - \omega t)}$
	$= \frac{k^2 \hbar^2}{2m} A e^{i(kx - \omega t)}$		

Then setting these equal (to check) gives:

$$\frac{k^2 \hbar^2}{2m} A e^{i(kx - \omega t)} = \hbar\omega A e^{i(kx - \omega t)}$$
$$\Rightarrow \omega = \frac{k^2 \hbar}{2m}$$

We have eliminated x, t from both sides and the proposed solution is a solution if

$$\omega = \frac{k^2 \hbar}{2m}$$

Using $k = p/\hbar$ (de Broglie) gives: $\omega \hbar = \frac{p^2}{2m} = E \quad !!$

Note that we have solutions of the form

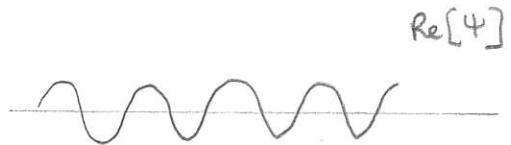
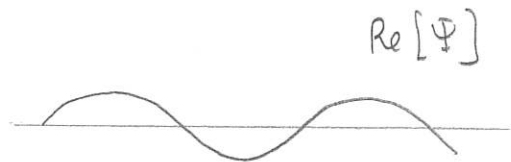
$$\Psi(x,t) = A e^{i(px - Et)/\hbar}$$

where $E = \frac{p^2}{2m}$. There are many possible solutions and these differ by

- * amplitude A
- * momentum p

smaller p
→

larger p
→



The multitude of possible solutions is typical of such differential equations. In fact given two solutions we can construct a third by adding

$$\Psi_1(x,t) = A_1 e^{i(p_1x - E_1t)/\hbar}$$

$$E_1 = \frac{p_1^2}{2m}$$

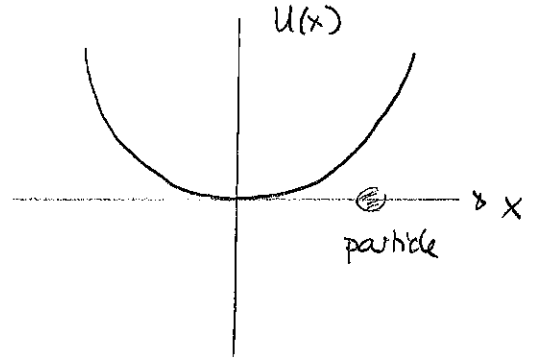
$$\Psi_2(x,t) = A_2 e^{i(p_2x - E_2t)/\hbar}$$

$$E_2 = \frac{p_2^2}{2m}$$

then $\Psi_1(x,t) + \Psi_2(x,t)$ is also a solution. We will still need to select one solution out of the infinitely many possibilities. We usually do so by providing information at some initial time ($t=0$).

Schrödinger equation for any particle in one dimension

Now consider a particle in one dimension that is subject to external interactions. We assume that the external interactions can be described by a potential energy, $U(x)$. For example:



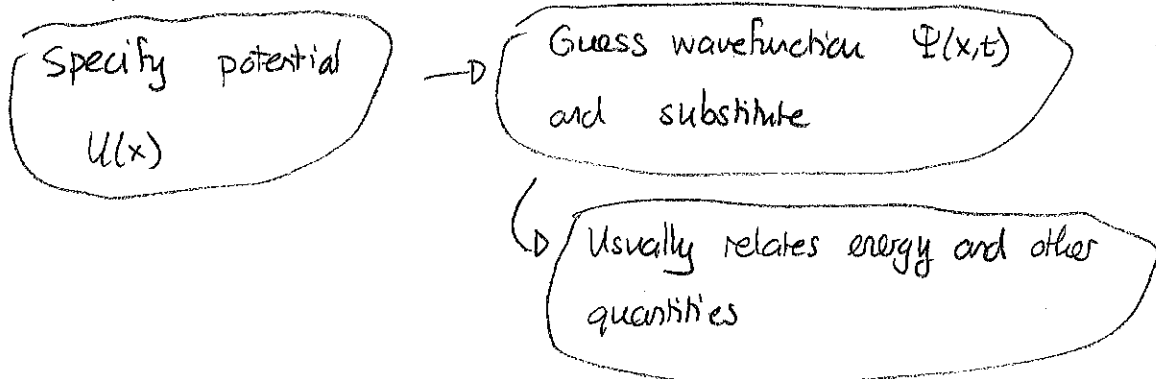
1) particle on a ramp $U(x) = \text{const} \times x$

2) spring/mass oscillator $U(x) = \frac{1}{2} kx^2$

Then we assume that the wavefunction for the particle satisfies the time-dependent Schrödinger equation:

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

Typically the way that we will work with this is:



Stationary States / Energy Eigenstates

For the free particle we saw that one possible solution

$$\Psi(x,t) = A e^{i(px - Et)/\hbar}$$

$$= A e^{i p x / \hbar} e^{-i E t / \hbar}$$

only depends on x only depends on t

can be factorized into a product of a function of time and a different function of energy. We consider this as a broad class of solution. In general

A possible solution to the time-dependent Schrödinger equation has the form:

$$\Psi(x,t) = \underbrace{\Psi(x)}_{\text{only depends on } x} \underbrace{\phi(t)}_{\text{only depends on } t}$$

and then

$$\phi(t) = e^{-iEt/\hbar}$$

where E is the energy of the system and $\Psi(x)$ satisfies the time independent Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2 \Psi}{dx^2} + U(x) \Psi(x) = E \Psi(x)$$

Proof: Substitution gives

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{d^2 \psi}{dx^2} \phi(t)$$

$$\frac{\partial \Psi}{\partial t} = \psi \frac{\partial \phi}{\partial t}$$

Thus:

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} \phi + U \psi \phi = i\hbar \frac{d\phi}{dt} \psi$$

$$\Rightarrow \underbrace{\left[-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + U(x) \psi(x) \right] \frac{1}{\psi}}_{\text{only depends on } x} = \underbrace{i\hbar \frac{1}{\phi} \frac{d\phi}{dt}}_{\text{only depends on } t}$$

This can only be true for all x, t if each side is a constant. Set the constant equal to E .

$$\Rightarrow i\hbar \frac{1}{\phi} \frac{d\phi}{dt} = E \Rightarrow \frac{d\phi}{dt} = \frac{-iE}{\hbar} \phi$$

The solution to this is $\phi = e^{-iEt/\hbar}$.

Separately

$$\left\{ -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + U(x) \psi(x) \right\} \frac{1}{\psi(x)} = E$$

$$\Rightarrow -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + U(x) \psi(x) = E \psi(x)$$

