PHY202 – Quantum Mechanics
Summary of Topic 0: Mathematics for Quantum Mechanics

1 Differential Equations

Consider the linear 2nd order differential equation:

$$\frac{\partial^2 \psi}{\partial x^2} + \omega^2 \psi = 0. \tag{1}$$

Solutions exist of the form

$$\psi(x) = A\cos(kx) + B\sin(kx), \tag{2}$$

where A, B and k are constants (to be determined). We find that:

$$\frac{\partial \psi}{\partial x} = -Ak\sin(kx) + Bk\cos(kx), \tag{3}$$

and

$$\frac{\partial^2 \psi}{\partial x^2} = -Ak^2\cos(kx) - Bk^2\sin(kx), \tag{4}$$

and subsituting we finally obtain $k = \pm\omega$.

Alternatively we can use as trial solution

$$\psi(x) = A\exp(ikx) + B\exp(-ikx), \tag{5}$$

in which case

$$\frac{\partial \psi}{\partial x} = Aik\exp(ikx) - Bik\exp(-ikx), \tag{6}$$

and

$$\frac{\partial^2 \psi}{\partial x^2} = -Ak^2\exp(ikx) - Bk^2\exp(-ikx), \tag{7}$$

and subsituting we finally obtain $k = \pm\omega$.

Thirdly we may observe that if

$$\frac{\partial^2 \psi}{\partial x^2} + \omega^2 \psi = 0, \tag{8}$$

then

$$\left(\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}\right) + \omega^2\right)\psi = 0, \tag{9}$$

where $\frac{\partial}{\partial x}$ is the differential *operator*. From the properties of operators (see next section) we may then write:

$$\left(\frac{\partial}{\partial x} + i\omega\right)\left(\frac{\partial}{\partial x} - i\omega\right)\psi = 0. \tag{10}$$

This may be satisfied if

$$\left(\frac{\partial}{\partial x}+i\omega\right)\psi=0 \quad \text{or} \quad \left(\frac{\partial}{\partial x}-i\omega\right)\psi=0 \tag{11}$$

These linear first order equations can in turn be solved with

$$\psi(x)=A\exp(\pm ikx), \tag{12}$$

and hence the general solution can be constructed from the linear combination:

$$\psi(x)=A\exp(ikx)+B\exp(-ikx). \tag{13}$$

2 Operators and Commutators

An operator is a mathematical object which acts on everything to its right in a product and for which the order in which it is applied in general can affect the result. Operators are denoted with 'hats' (e.g. $\hat{A}$). Special examples include the differential operator $\partial/\partial x$. To work with operators it is often easiest to include a function for them to operate upon in order to keep track of terms.

The commutator of two operators describes the effect of exchanging their order in an expression:

$$[\hat{A},\hat{B}]\equiv\hat{A}\hat{B}-\hat{B}\hat{A}. \tag{14}$$

This is non-zero only for 'non-commuting' operators. The differential operator by contrast is an example of a commuting operator for which $[\hat{A},\hat{B}]=0$. Some useful identities are:

$$[\hat{A},\hat{A}]=0 \quad \text{and} \quad [\hat{A},\hat{B}]=-[\hat{B},\hat{A}], \tag{15}$$

and also:

$$[\hat{A},\hat{B}\hat{C}]=[\hat{A},\hat{B}]\hat{C}+\hat{B}[\hat{A},\hat{C}], \tag{16}$$

and

$$[\hat{A}\hat{B},\hat{C}]=\hat{A}[\hat{B},\hat{C}]+[\hat{A},\hat{C}]\hat{B}. \tag{17}$$

As an example consider the following commutator between the Quantum Mechanical position ($\hat{x}=x$) and momentum ($\hat{p}=-i\hbar\partial/\partial x$) operators (I have included a function ψ for the operators to act upon to keep track of terms):

$$\begin{aligned}
[\hat{x},\hat{p}]\psi &\equiv (\hat{x}\hat{p}-\hat{p},\hat{x})\,\psi,\\
&= \hat{x}\hat{p}\psi-\hat{p}\hat{x}\psi,\\
&= x\left(-i\hbar\frac{\partial}{\partial x}\right)\psi-\left(-i\hbar\frac{\partial}{\partial x}\right)x\psi\\
&= -i\hbar x\frac{\partial\psi}{\partial x}+i\hbar\left(\frac{\partial x}{\partial x}\psi+x\frac{\partial\psi}{\partial x}\right)\\
&= i\hbar\psi.
\end{aligned} \tag{18}$$

hence $[\hat{x},\hat{p}]=i\hbar$.

3 Eigenvalue equations

Eigenvalue equations have the typical form

$$\hat{A}\psi = a\psi, \tag{19}$$

where a is a number determined by solving the equation and there is one function ψ for each possible value of a. We call the a the eigenvalues of the operator $\hat{A}$ and ψ the eigenfunctions. There is a one-to-one mapping between the properties of the operators, eigenvalues and eigenfunctions with matrices, eigenvalues and eigenvectors. Indeed matrices can be used to represent operators.

Differential equations can sometimes be written as eigenvalue equations. For example Eqn. 1 can be written as an eigenvalue equation where the operator is $\partial^2/\partial x^2$, ψ is the eigenfunction and $-\omega^2$ is the eigenvalue.

4 Boundary conditions and normalisation

Returning to Eqn. 1, let's assume

$$\begin{aligned} \psi = 0 \quad &\text{when} \quad x = 0, \\ \psi = 0 \quad &\text{when} \quad x = L. \end{aligned} \tag{20}$$

From Eqn. 2

$$\psi(x) = A\cos(kx) + B\sin(kx), \tag{21}$$

we find that $A = 0$ (from the first condition) and that

$$B\sin(kL) = 0, \tag{22}$$

and so $k = n\pi/L$ where n is an integer. So $\psi = B\sin\left(\frac{n\pi x}{L}\right)$.

If we interpret $|\psi|^2$ as a probability then we can determine B by normalising the probability to unity (i.e. to 1). If we assume that ψ is zero everywhere except in the range $0 < x < L$ then we should require:

$$\int_0^L |\psi|^2 dx = 1. \tag{23}$$

Thus

$$\int_0^L B^2 \sin^2\left(\frac{n\pi x}{L}\right) dx = 1, \tag{24}$$

which we can solve for B by using the trigonometric identity $\sin^2 y \equiv \frac{1}{2}(1 - \cos 2y)$. The result is that $B = \sqrt{2/L}$ and so $\psi = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$.

5 Expectation values

An important question in quantum mechanics is the average value of a quantity x which is distributed according to a probability distribution function $f(x)$. This is obtained from the weighted mean value of x, where the weighting is provided by $f(x)$. For a continuous variable this weighted mean or 'expectation value' $\langle x \rangle$ is calculated by integrating $xf(x)$ over all x. For the example above this gives:

$$\begin{aligned}
\langle x \rangle &= \frac{2}{L}\int_0^L x\sin^2\left(\frac{n\pi x}{L}\right)dx, \\
&= \frac{2}{L}\int_0^L \left(\frac{x}{2} - \frac{x}{2}\cos\left(\frac{2n\pi x}{L}\right)dx\right), \\
&= \frac{2}{L}\left(\frac{L^2}{4} - \frac{1}{2}\int_0^L x\cos\left(\frac{2n\pi x}{L}\right)dx\right), \\
&= \frac{2}{L}\left(\frac{L^2}{4} - \frac{1}{2}\left(\frac{L^2}{4n\pi^2}\left(\cos\left(\frac{2n\pi L}{L} - 1\right)\right)\right)\right), \\
&= \frac{L}{2}, \qquad (25)
\end{aligned}$$

as we might have expected given that $\sin(x)$ is a symmetric function about $x = L/2$.

6 Time dependence

Consider a modified version of Eqn. 1:

$$\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = i\alpha\frac{\partial\psi}{\partial t}. \qquad (26)$$

This equation possesses plane-wave solutions of the following form (try substituting to show this!):

$$\begin{aligned}
\psi(x,t) &= A\exp(i(kx - \omega t) \\
&\equiv \psi(x)\exp(-i\omega t). \qquad (27)
\end{aligned}$$