PHY2005
Atomic Physics

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(3) QM and the Schrödinger Equation

Learning goals

1. To revise the principles of quantum mechanics, including the wavefunction and the time-independent Schrödinger equation.
2. To revise and elaborate the concepts of operators, eigenfunctions and eigenvalues in quantum mechanics.
3. To appreciate the concepts of *compatible* and *incompatible* quantities in quantum mechanics.
4. To revise the description of angular momentum in quantum mechanics, including operators for components and magnitude (in Cartesian and spherical polar representations).
5. To establish the compatibility of angular momentum operators.
6. To introduce the vector model for angular momentum.

The wavefunction (reminder)

The wavefunction:

$$\Psi(\mathbf{r}, t)$$

describes a system in quantum mechanics. Measureable quantities can be calculated from the wavefunction. E.g.

$$|\Psi|^2 = \Psi^* \Psi$$

gives a probability density.

The wavefunction (reminder)

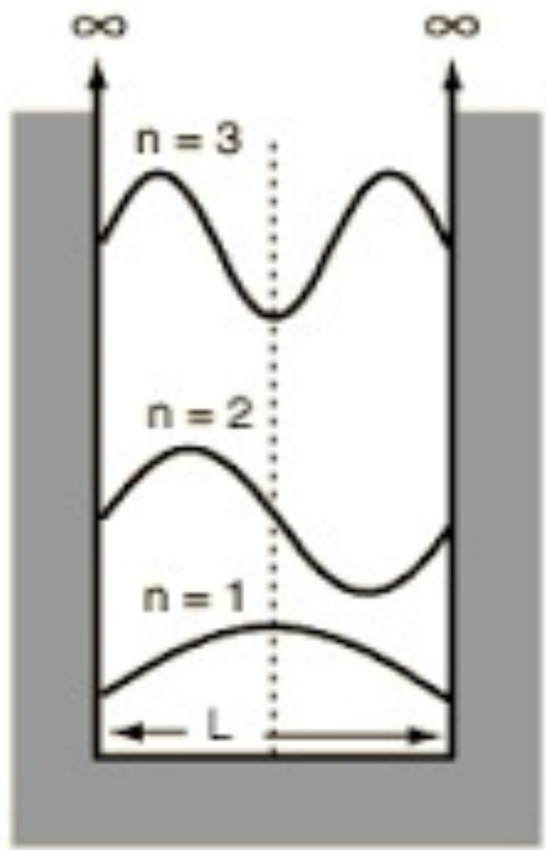
Since the probability density represents a physical quantity $\Psi(\mathbf{r}, t)$ must:

1. everywhere be finite;
2. everywhere be single valued;
3. everywhere be continuous; and
4. vanish at ∞.

These requirements put constraints on finding wavefunctions, which lead to quantisation.

Quantization from boundary conditions

E.g. in PHY2001 you have seen that allowed energy levels come about by requiring that the wavefunction goes to zero at the edges of an infinite square well.



x = 0 at left wall of box.

Schrödinger Equation

The wavefunction obeys the **time-dependent Schrödinger Equation**:

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

For time-independent *V*, can find separable solutions

$\Psi(\mathbf{r},t) = \psi(\mathbf{r})T(t)$ where $T(t) = \exp\left(-iEt/\hbar\right)$

Schrödinger Equation

Then $\psi(\mathbf{r})$ obeys the **time-independent Schrödinger Equation (TISE)**

$$\frac{-\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

$\psi(\mathbf{r})$ describes a stationary state of the system: a state with fixed total energy *E* in which e.g. the probability density is time-independent.

Such states are what we mean by "energy levels".

TISE as eigenvalue equation

Introduce the Hamiltonian operator:

$$\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + V$$

TISE is energy eigenvalue equation

$$\hat{H}\psi = E\psi$$

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Eigenfunction (or **Eigenstate**)

TISE as eigenvalue equation

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TISE is energy eigenvalue equation

Eigenvalue (what we'd actually measure)

Operator representing physics variable (total energy, in this case)

$$\hat{H}\psi = E\psi$$

Eigenfunction (or **Eigenstate**)

Eigenstates and measurements in QM

If the wavefunction of a QM system is an eigenfunction of the operator associated with a physical quantity, then that system will have a definite value of that quantity. The measured value will be the eigenvalue.

If the wavefunction is not an eigenfunction of the appropriate operator, the result of a measurement of the associated quantity is uncertain.

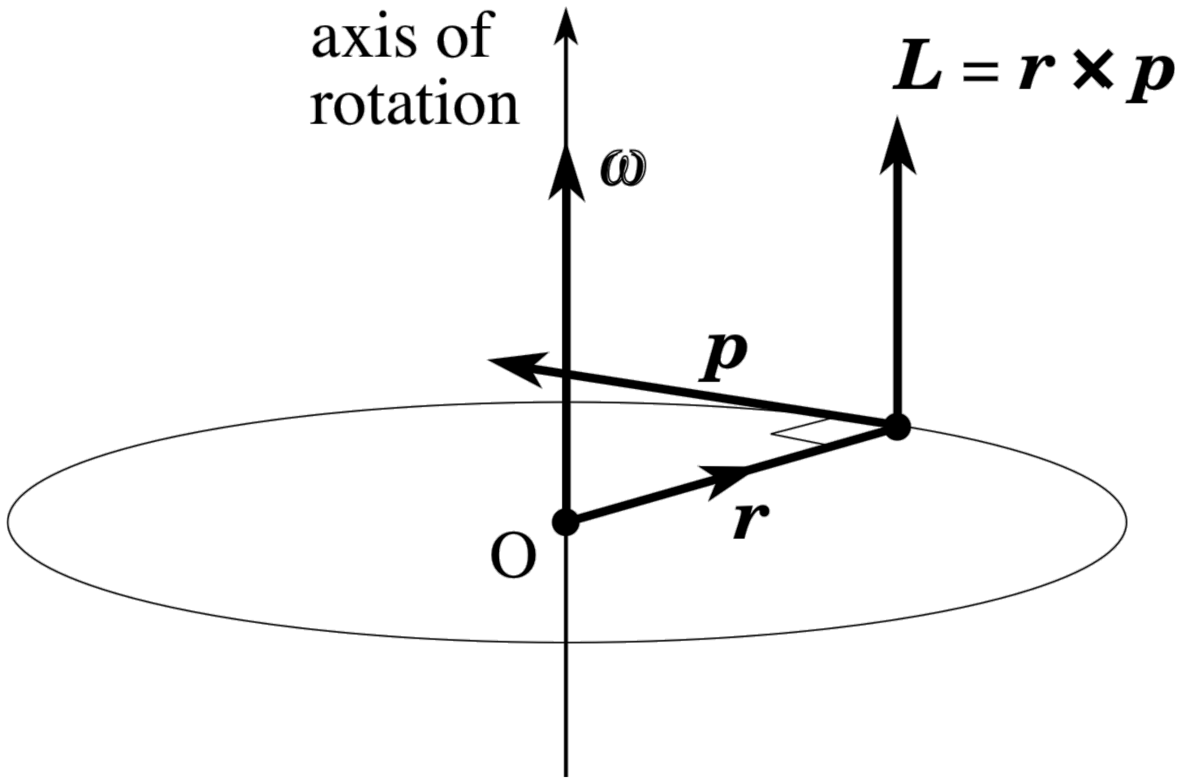
Compatible observables

Measureable quantities are compatible if they can be known simultaneously with no uncertainty.

They are incompatible if they can not.

In the language of eigenfunctions, quantities are compatible if their operators have a common set of eigenfunctions, and incompatible if they do not.

Angular momentum



Angular momentum

Angular momentum operator:

$$\hat{\mathbf{L}} = \mathbf{r} \times \hat{\mathbf{p}} = -i\hbar \mathbf{r} \times \nabla$$

Cartesian components:

$$\hat{L}_z = -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$$

$$\hat{L}_y = -i\hbar \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right)$$

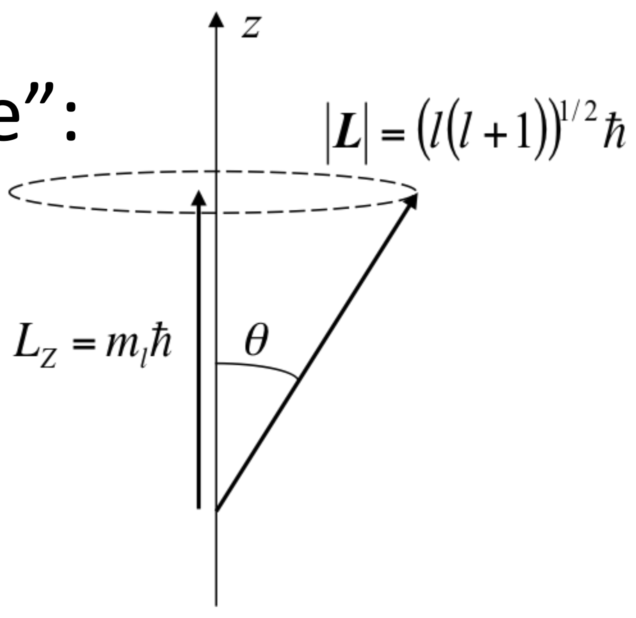
$$\hat{L}_x = -i\hbar \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$$

Angular momentum

We can know the magnitude of the orbital angular momentum and one component only.

The other two components are incompatible.

Can use a vector model to "visualize":



Summary/Revision

- All information about a quantum state is contained in the *wave-function*.
- Physical quantities (observables) are associated with operators that can be applied to the wavefunction.
- The eigenfunctions of an operator are states with a definite value for the associated physical quantity. The value for the quantity is the eigenvalue.
- The Hamiltonian is associated with the total energy. The time-independent Schrödinger equation is an energy eigenvalue equation: wavefunctions satisfying this equation have definite energy and are *stationary states*.
- Physical quantities are *compatible* if they posses a simultaneous set of eigenstates and *incompatible* if they do not. If two quantities are incompatible they cannot both be specified without uncertainty.
- L_x, L_y and L_z are incompatible with each other, but compatible with $\mathbf{L}^2$.
- The vector model is one means to visualise what we can know about angular momentum in quantum mechanics.
- Operators for the z-component of the angular momentum and for the square of the magnitude of the angular momentum are given by Eqns 25 and 26.