

Lecture 8 - Schrödinger equation with interactions

What's important:

- energy operator
- SE with potential energy
- Schrödinger equation in three dimensions

Text: Gasiorowicz, Chaps. 3

Energy operator

Recall again the form of the Schrödinger equation for a free particle in one dimension:

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} \quad (1)$$

In the previous lecture, we established that the momentum operator p_{op} could be represented by

$$p = -i\hbar \frac{\partial}{\partial x} \quad (2)$$

when operating on wavefunctions in position-space, $\psi(x,t)$. From now on, we drop the "op" subscript unless we need it for clarity. Squaring this (not complex square!),

$$p^2 = -\hbar^2 \frac{\partial^2}{\partial x^2} \quad (3)$$

which bears a resemblance to the right-hand side of Eq. (1). Substituting, (1) becomes

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \frac{p^2}{2m} \psi(x,t)$$

Now, $p^2 / 2m$ is just the non-relativistic kinetic energy, so the action of the right hand side is to operate on $\psi(x,t)$ with the kinetic energy operator. Note that we say "operate on", not "multiply by", as there are derivatives in the position-space representation of p . The total energy of a system is just the sum of the kinetic and potential energies,

$$E = p^2/2m + V(x) \quad (4)$$

where we have made the restrictive assumption that V does not explicitly depend on time (other than the changing positions of the particles) nor does it depend on momentum or velocity (like drag).

Corresponding to the physical observable E is the energy operator H_{op} , called the **Hamiltonian**, analogous to the Hamiltonian of classical mechanics (see supplementary lectures to PHYS 211 for a short introduction to Lagrange's and Hamilton's approach to classical mechanics):

$$H_{\text{op}} = p^2/2m + V(x) \quad (5)$$

Schrödinger equation with interactions

Armed with the concept of the energy operator, Schrödinger proposed the basic equation of quantum mechanics with interactions is

$$\hbar \frac{\partial \psi(x,t)}{\partial t} = H_{\text{op}} \psi(x,t). \quad (6)$$

Because p_{op} is Hermitian, then so is H_{op} as long as V is real. The effect of the Hermitian H_{op} is to yield the "real" energy E . It's easy to see how to generalize this one-dimensional equation to three dimensions, from the form of the Hamiltonian:

$$H_{3\text{D}} = (p_x^2 + p_y^2 + p_z^2)/2m + V(x,y,z) \quad (7)$$

which has the operator form

$$H_{\text{op}} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(x,y,z). \quad (8)$$

A common shorthand for Eq. (8) is to introduce the gradient operator ,

$$\nabla = \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \quad (\text{vector!}) \quad (9)$$

such that

$$H_{\text{op}} = (\hbar^2/2m) \nabla^2 + V(x,y,z). \quad (10)$$

The ∇^2 operator is commonly referred to as the *Laplacian*.

Summary

In most courses in quantum mechanics, it is common at this point to lay out a set of postulates which summarize or motivate the formalism of quantum mechanics. There are a variety of starting points; most are based on Heisenberg's uncertainty principle, which may be implemented in various ways: commutation relations, density operators... Let's summarize the approach we've taken here, originally motivated by the idea of wavepackets to represent the probability distribution of position and momentum of a single, non-interacting particle. We follow Gasiorowicz:

1. The mechanics is described by a wavefunction $\psi(x,t)$ which obeys

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = H_{\text{op}} \psi(x,t)$$

where the energy operator is

$$H_{\text{op}} = (\hbar^2/2m) \nabla^2 + V(x,y,z).$$

This equation tells us how $\psi(x,t)$ evolves in time.

2. The probability density for finding the particle at position x is $|\psi(x,t)|^2$, which requires $\psi(x,t)$ to be square integrable.

3. The momentum p and position x are operators which do not commute:

$$[p,x] = -i\hbar.$$

In the position representation, the momentum operator has the form

$$p = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

4. For every physical observable A of the system there corresponds a linear Hermitian operator A_{op} . If a measurement of A gives the same value a every time it is made, then A obeys the equation

$$A_{\text{op}} \psi(x,t) = a \psi(x,t),$$

where a is the eigenvalue of A_{op} and ψ is the eigenfunction. If the measurement does not yield a every time, then the ensemble average of measurements obeys

$$\langle a \rangle = \int \psi^*(x,t) A_{\text{op}} \psi(x,t) dx$$

in one dimension, where $\psi(x,t)$ is normalized to unity:

$$\int \psi^*(x,t) \psi(x,t) dx = 1.$$