Schrödinger Wave Equation

References --
R. M. Eisberg, *Fundamentals of Modern Physics* (Wiley & Sons, New York, 1961).
R. L. Liboff, *Introductory Quantum Mechanics* (Holden Day, New York, 1980).

With this lecture we begin the discussion of quantum mechanical description of nuclei. There are certain properties of a nucleus which can be described properly only by the use of quantum mechanics. The ones which are most familiar to all students are the energy levels of a nucleus and the transitions that can take place from one level to another. Other examples are the various types of nuclear radiation which are sometimes treated as particles and at other times as waves.

It is not our goal in this subject to take up the study of quantum mechanics as a topic by itself. On the other hand, we have no reasons to avoid using quantum mechanics whenever it is the proper way to understand nuclear concepts and radiation interactions. Indeed a serious student in 22.101 has little choice in deciding whether or not to learn quantum mechanics. This is because the concepts and terminologies in quantum mechanics are such integral parts of nuclear concepts and the interaction of radiation with matter that some knowledge of quantum mechanics is *essential* to having full command of the language of nuclear physics. One can go further to say that it is inconceivable that any self-respecting nuclear engineering student will choose not to be exposed to this language, because in all likelihood this experience will come in handy someday. The position we adopt throughout the term is to learn enough quantum mechanics to appreciate the fundamental concepts of nuclear physics, and let each student go beyond this level if he/she is interested. What this means is that we will not always derive the basic equations and expressions that we will use; the student is expected to work with them as postulates when this happens (as always, with the privilege of reading up on the background material on your own).

Waves and Particles

We review some basic properties of waves and the concept of wave-particle duality. In classical mechanics the equation for a one-dimensional periodic disturbance $\xi(x,t)$ is

$$\frac{\partial^2 \xi}{\partial t^2} = c^2 \frac{\partial^2 \xi}{\partial x^2} \tag{2.1}$$

which has as a general solution,

$$\xi(x,t) = \xi_o e^{i(kx - \omega t)} \tag{2.2}$$

where $\omega = 2\pi\nu$ is the circular frequency, ν the linear frequency, and k is the wavenumber related to the wavelength λ by $k = 2\pi/\lambda$. If (2.2) is to be a solution of (2.1), then k and ω must satisfy the relation

$$\omega = ck \tag{2.3}$$

So our solution has the form of a traveling wave with phase velocity equal to c, which we denote by v_{ph}. In general the relation between frequency and wavenumber is called the *dispersion relation*. We will see that different kinds of particles can be represented as waves which are characterized by different dispersion relations.

The solution (2.2) is called a plane wave. In three dimensions a plane wave is of the form $\exp(i\underline{k} \cdot \underline{r})$. It is a wave in space which we can visualize as a series of planes perpendicular to the wavevector $\underline{k}$; at any spatial point on a given plane the phase of the wave is the same. That is to say, the perpendicular planes are *planes of constant phase*. When we include the time variation $\exp(-i\omega t)$, then $\exp[i(\underline{k} \cdot \underline{r} - \omega t)]$ becomes a traveling plane wave, meaning that the planes of constant phase are now moving in the direction along $\underline{k}$ at a speed of ω/k, which is the phase velocity of the wave.

The wave equation (2.1) also admits solutions of the form

$$\xi(x,t) = a_o \sin kx \cos \omega t \tag{2.4}$$

These are standing wave solutions. One can tell a standing wave from a traveling wave by the behavior of the nodes, the spatial positions where the wave function is zero. For a standing wave the nodes do not move, or change with time, whereas for a traveling wave, (2.2), the nodes are $x_n = (n\pi + \omega t)/k$. Clearly the nodes are positions moving in the +x direction with the velocity $dx/dt = \omega/k$. We will see below that the choice between traveling and standing wave solutions depends on the physical solution of interest (which kind of problem one is solving). For the calculation of energy levels of a nucleus, the bound state problem, we will be concerned with standing wave solutions. In contrast, for the discussion of scattering problem (see the later lecture on neutron-proton scattering) it will be more appropriate to consider traveling wave solutions.

Our interest in the properties of waves lies in the fact that the quantum mechanical description of a nucleus is based on the wave representation of the nucleus. It was first postulated by deBroglie (1924) that one can associate a particle of momentum p and total energy E with a group of waves (wave packet) which are characterized by a wavelength λ and a frequency ν, with the relation

$$\lambda = h/p \tag{2.5}$$

$$\nu = E/h \tag{2.6}$$

Moreover, the motion of the particle is governed by the propagation of the wave packet. This statement is the essence of particle-wave duality, a concept which we adopt throughout our study of nuclear physics [see, for example, Eisberg, chap 6].

It is important to distinguish between a single wave and a group of waves. This distinction is seen most simply by considering a group of two waves of slightly different wavelengths and frequencies. Suppose we take as the wave packet

$$\Psi(x,t) = \Psi_1(x,t) + \Psi_2(x,t) \tag{2.7}$$

with

$$\Psi_1(x,t) = \sin(kx - \omega t) \tag{2.8}$$

$$\Psi_2(x,t) = \sin[k(k+dk)x - (\omega + d\omega)t] \tag{2.9}$$

Using the identity

$$\sin A + \sin B = 2\cos[(A-B)/2]\sin[(A+B)/2] \tag{2.10}$$

we rewrite $\Psi(x,t)$ as

$$\Psi(x,t) = 2\cos[(dks - d\omega t)/2]\sin\{[(2k+dk)x - (2\omega + d\omega)]t/2\}$$

$$\approx 2\cos[(dkx - d\omega t)/2]\sin(kx - \omega t) \tag{2.11}$$

In this approximation, terms of higher order in dk/k or $d\omega/\omega$ are dropped. Eq. (2.11) shows two oscillations, one is the wave packet oscillating in space with a period of $2\pi/k$, while its amplitude oscillates with a period of $2\pi/dk$ (see Fig. 1). Notice that the latter oscillation has its
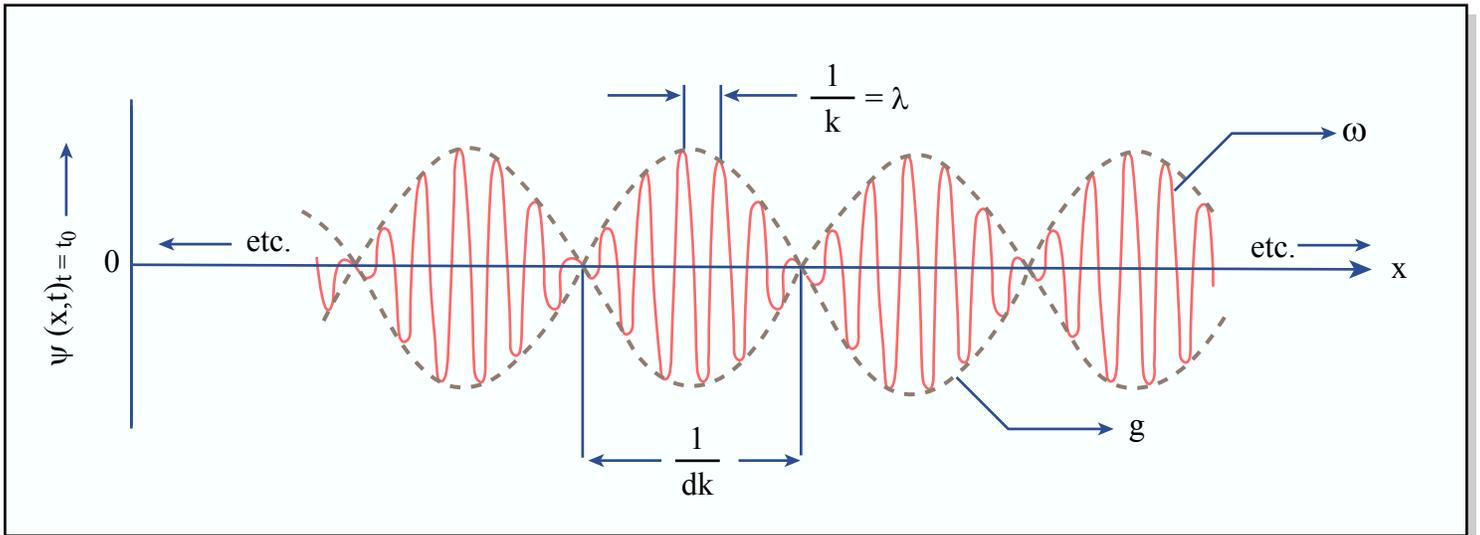
Figure by MIT OCW.

Fig. 1. Spatial variation of a sum of two waves of slightly different frequencies and wavenumbers showing the wave packet moves with velocity w which is distinct from the propagation (group) velocity g of the amplitude [from Eisberg, p. 144].

own propagation velocity, $d\omega/dk$. This velocity is in fact the speed with which the associated particle is moving. Thus we identify

$$g = d\omega/dk \qquad (2.12)$$

as the group velocity. The group velocity should not be confused with the propagation velocity of the wave packet, called the phase velocity, given by

$$w = \nu\lambda = E/p = c\sqrt{1+(m_o c/p)^2} \qquad (2.13)$$

Here m_o is the rest mass of the particle and c the speed of light. We see the wave packet moves with a velocity greater than c, whereas the associated particle speed is necessarily less than c. This means the phase velocity is greater than or equal to the group velocity.

In this class we will be dealing with three kinds of particles whose wave representations are of interest. These are (i) nucleons or nuclides which can be treated as non-relativistic particles for our purposes, (ii) electrons and positrons which usually should be treated as relativistic particles since their energies tend to be comparable or greater than the rest-mass energy, and (iii) photons which are fully relativistic since they have zero rest-mass energy. For a non-relativistic particle of mass m moving with momentum p, the associated wavevector $\underline{k}$ is $\underline{p} = \hbar\underline{k}$. Its kinetic energy is T =

$p^2/2m = \hbar^2 k^2/2m$. This is the "particle view". The corresponding "wave view" would have the momentum magnitude p = h/λ, with $\lambda = 2\pi/k$, and energy (usually denoted as E rather than T) as $h\nu = \hbar\omega$. The wavevector, or its magnitude, the wavenumber k, is a useful variable for the discussion of particle scattering since in a beam of such particles the only energies are kinetic, and both momentum and energy can be specified by giving $\underline{k}$. For electromagnetic waves, the associated particle, the photon, has momentum $\underline{p}$, which is also given by $\hbar\underline{k}$, but its energy is $E = \hbar ck = \hbar p$. Comparing these two cases we see that the dispersion relation is $\omega = \hbar k^2/2m$ for a non-relativistic particle, and $\omega = ck$ for a photon. The group velocity, according to9 (2.12), is $v_g = \hbar k/m = p/m$ and

$v_g = c$, respectively, which is consistent with our intuitive notion about particle speed and the universal speed of a photon.

The Schrödinger Wave Equation

The Schrödinger equation is the fundamental equation governing the deBroglie wave with which we associate a particle. The wave or wave function is to be treated as a space- and time-dependent quantity, $\Psi(\underline{r},t)$. One does not derive the Schrödinger equation in the same sense that Newton's equation of motion, $\underline{F} = m\underline{a}$, is postulated, and not derived. The wave equation is therefore a postulate which one accepts when studying physical phenomena using quantum mechanics. Of course one can give systematic motivations to suggest why such an equation is valid [see Eisberg, chap 7 for a development]. Such discussions would be beyond the scope of this class. We now write down the Schrödinger equation in its time-dependent form for a particle in a potential field V(r),

$$i\hbar \frac{\partial \Psi(\underline{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) \right]\Psi(\underline{r},t) \tag{2.14}$$

Notice that the quantity in the bracket is the Hamiltonian H of the system. H is a mathematical operator whose physical meaning is the total energy. Thus it consists of the kinetic part $p^2/2m$ and the potential part V(r). The appearance of the Laplacian operator ∇^2 is to be expected, since the particle momentum $\underline{p}$ is an operator in configuration space, with $\underline{p} = -i\hbar\underline{\nabla}$. The momentum operator is therefore a first-order differential operator in configuration space. By defining the Hamiltonian H as the operator

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(r) \tag{2.15}$$

we can express the time-dependent Schrödinger equation in operator notation,

$$ i\hbar \frac{\partial \Psi(\underline{r},t)}{\partial t} = H\Psi(\underline{r},t) \qquad (2.16) $$

As a side remark (2.14) is valid only for a non-relativistic particle, whereas (2.16) is more general if H is left unspecified. This means that one can use a relativistic expression for H, then (2.16) would lead to an equation first derived by Dirac. The Dirac equation is what one should consider if the particle were an electron. Compared to the classical wave equation, (2.1), which relates the second spatial derivative of the wave function to the second-order time derivative, the time-dependent Schrödinger wave equation, (2.14) or (2.16), is seen to relate the spatial derivative of the wave function to the *first-order* time derivative. This is a significant distinction, although we have no need to go into it further in this class. Among the implications is the fact that the classical wave is real and measurable (for example, an elastic string or an electromagnetic wave), whereas the Schrödinger wave function is *complex, and therefore not measurable*. To ascribe physical meaning to the wave function one needs to consider the probability density defined as $\Psi^*(\underline{r},t)\Psi(\underline{r},t)$, where $\Psi^*(\underline{r},t)$ is the complex conjugate of the wave function.

Almost all our discussions are concerned with the time-independent form of the Schrödinger equation. This is obtained by considering a periodic solution to (2.16) of the form

$$ \Psi(\underline{r},t) = \psi(\underline{r})e^{iEt/\hbar} \qquad (2.17) $$

where E is a constant (soon to be identified as the total energy). Inserting this solution into (2.16) gives the time-independent Schrödinger equation,

$$ H\psi(\underline{r}) = E\psi(\underline{r}) \qquad (2.18) $$

We see that (2.18) has the form of an eigenvalue problem with H being a linear operator, E the eigenvalue, and $\psi(\underline{r})$ the eigenfunction.

It is instructive to point out a certain similarity between the Schrödinger equation and the classical wave equation when the latter incorporates the concept of deBroglie waves. To show this we first write the three-dimensional generalization (2.1) as

$$\frac{\partial^2 \xi(\underline{r},t)}{\partial t^2} = v_{ph}^2 \nabla^2 \xi(\underline{r},t) \tag{2.19}$$

and use (2.13),

$$v_{ph} = \frac{E}{p} = \frac{E}{\sqrt{2m(E-V)}} \tag{2.20}$$

For periodic solutions, $\xi(\underline{r},t) = \varsigma(\underline{r})e^{iEt/\hbar}$, we see that one is led immediately to (2.19). Notice that the connection between the classical wave equation and the Schrödinger equation is possible only in terms of the time-independent form of the equations. As mentioned above, the two equations, in their time-dependent forms, differ in important ways, consequently different properties have to be ascribed to the classical wave function and the Schrödinger wave function.

Bound (E < 0) and Scatterig (E > 0) State Solutions

Following our previous statement about the different types of wave solutions, we can ask what types of solutions to the Schrödinger equation are of interest. To answer this question we consider (2.18) in one dimension for the sake of illustration. Writing out the equation explicitly, we have

$$\frac{d^2 \psi(x)}{dx^2} = -k^2 \psi(x) \tag{2.21}$$

where $k^2 = 2m[E - V(x)]/\hbar^2$. In general k^2 is a function of x because of the potential energy V(x), but for piecewise constant potential functions such as a rectangular well or barrier, we can write a separate equation for each region where V(x) is constant, and thereby treat k^2 as a constant in (2.21). A general solution to (2.21) is then

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \tag{2.22}$$

where A and B are constants to be determined by appropriate boundary conditions. Now suppose we are dealing with finite-range potentials so that $V(x) \to 0$ as $x \to \infty$, then k becomes $(2mE/\hbar^2)^{1/2}$. For $E > 0$, k is real and Ψ, as given by (2.17), is seen to have the form of traveling plane waves. On the other hand, if $E < 0$, $k = i\kappa$ is imaginary, then $\Psi \approx e^{-\kappa x}e^{-i\omega t}$, and the solution has the form of a standing wave. What this means is that for the description of scattering problems one should use *positive-energy* solutions (these are called scattering states), while for bound-state calculations one should work with *negative-energy* solutions. Fig. 2 illustrates the behavior of the two types of solutions. The condition at infinity, $x \to \pm\infty$, is that ψ is a plane wave in the scattering problem, and an exponentially decaying function in the bound-state problem. In other words, outside the potential (the exterior region) the scattering state should be a plane wave representing the presence of an incoming or outgoing particle, while the bound state should be represented by an exponentially damped wave signifying the localization of the particle inside the potential well. Inside the potential (the interior region) both solutions are seen to be oscillatory, with the shorter period corresponding to higher kinetic energy $T = E - V$.
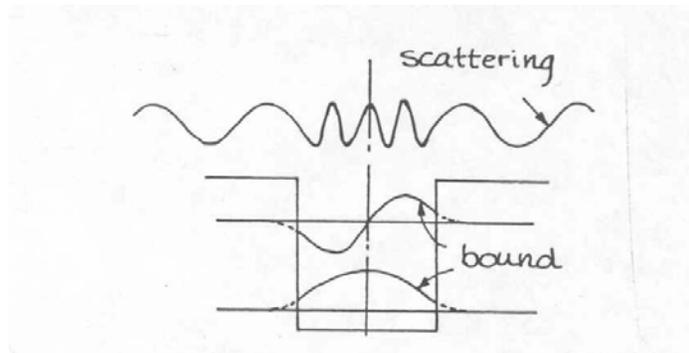
Fig. 2. Traveling and standing wave functions as solutions to scattering and bound-state problems respectively.

There are general properties of Ψ which we require for either problem. These arise from the fact that we are seeking physical solutions to the wave equation, and that $|\psi(\underline{r})|^2 d^3r$ has the interpretation of being the probability of finding the particle in an element of volume d3r about $\underline{r}$. In view of (2.17) we see $|\Psi(\underline{r},t)|^2 = |\psi(\underline{r})|^2$, which means that we are dealing with stationary solutions. Since a time-independent potential cannot create or destroy particles, the normalization condition

$$\int d^3r |\psi(\underline{r})|^2 = 1 \qquad (2.23)$$

can be applied to the bound-state solutions with integration limits extending to infinity. For scattering solutions one needs to specify an arbitrary but finite volume Ω for the normalization of a plane wave. This turns out not to be a difficulty; in any calculation all physical results will be found to be independent of Ω. Other properties of Ψ or ψ which can be invoked as conditions for the solutions to be physically meaningful are:

(i)   finite everywhere

(ii)   single-valued and continuous everywhere

(iii)   first derivative continuous

(iv) $\Psi \rightarrow 0$ when $V \rightarrow \infty$

Condition (iii) is equivalent to the statement that the particle current must be continuous everywhere. The current is related to the wave function by the expression

$$\underline{j}(\underline{r}) = \frac{\hbar}{2mi}[\psi^+(\underline{r})\underline{\nabla}\psi(\underline{r}) - \psi(\underline{r})\underline{\nabla}\psi^+(\underline{r})] \qquad (2.24)$$

This is a generally useful relation which can be derived directly from (2.18).