

22.101 Applied Nuclear Physics (Fall 2006)
Lecture 3 (9/13/06)

Bound States in One Dimensional Systems – Particle in a Square Well

References --

R. L. Liboff, *Introductory Quantum Mechanics* (Holden Day, New York, 1980).

We will solve the Schrödinger wave equation by considering the simplest problem in quantum mechanics, a particle in a potential well. The student will see from this calculation how the problem is treated by dividing the system into two regions, the *interior* where the particle feels the potential, and the *exterior* where the particle is a free particle (zero potential). The solutions to the wave equation have to be different in these two regions to reflect the binding of the particle - the wave function is oscillatory in the interior region and exponentially decaying (non-oscillatory) in the exterior region. Matching these two solutions at the boundary where the potential goes from a finite value (interior) to zero (exterior) gives a condition on the wavenumber (or wavelength), which turns out to be the condition of *quantization*. The meaning of quantization is that solutions exist only if the wavenumbers take on certain discrete values, which then translate into discrete energy levels for the particle. For a given potential well of certain depth and width, only a discrete set of wave functions can exist in the potential well. These wave functions are the eigenfunctions of the Hamiltonian (energy) operator, with corresponding energy levels as the eigenvalues. Finding the wavefunctions and the spectrum of eigenvalues is what we mean by solving the Schrödinger wave equation for the particle in a potential well. Changing the shape of the potential means a different set of eigenfunctions and the eigenvalues. The procedure to find them, however, is the same.

For a one-dimensional system the time-independent wave equation is

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \quad (3.1)$$

We will use this equation to investigate the bound-states of a particle in a square well potential of depth V_0 and width L . The physical meaning of (3.1) is essentially the

statement of energy conservation, the total energy E , a negative and constant quantity in the present problem of bound-state calculations, is the sum of kinetic and potential energies. Since (3.1) holds at every point in space, the fact that the potential energy $V(x)$ varies in space means the kinetic energy of the particle also will vary in space. For a square well potential, $V(x)$ has the form

$$\begin{aligned}
 V(x) &= -V_0 & -L/2 \leq x \leq L/2 \\
 &= 0 & \text{elsewhere}
 \end{aligned}
 \tag{3.2}$$

as shown in Fig. 1. Taking advantage of the piecewise constant behavior of the potential,

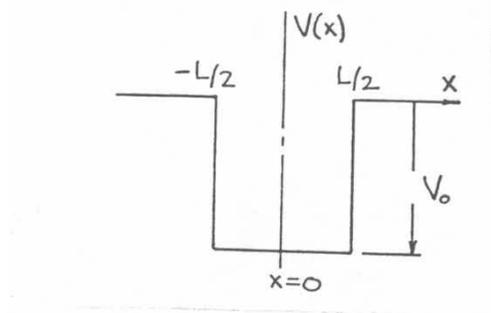


Fig. 1. The square well potential centered at the origin with depth V_0 and width L .

we divide the configuration space (our entire system) into an interior region, where the potential is constant and negative, and an exterior region where the potential is zero. For the interior region the wave equation can be put into the standard form of a second-order differential equation with constant coefficient,

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0 \quad |x| \leq L/2
 \tag{3.3}$$

In (3.3) we purposely introduced the wavenumber k , with $k^2 = 2m(E + V_0)/\hbar^2$ always positive, so that k is real. (As an aside note that we will be doing this consistently in

writing out the wave equation to be solved. In other words, the wavenumber we introduce is always real, whereas the sign of the second term in the wave equation can be plus, as seen in (3.3), or minus, as in (3.4). For k^2 to be positive we understand that the solutions where $-E > V_0$ will be excluded from our considerations.

For the exterior region, the wave equation similarly can be put into the form

$$\frac{d^2\psi(x)}{dx^2} - \kappa^2\psi(x) = 0 \quad |x| \geq L/2 \quad (3.4)$$

where $\kappa^2 = -2mE/\hbar^2$. To obtain the solutions of physical interest to (3.3) and (3.4), we keep in mind that the solutions should have certain symmetry properties, in this case they should have definite parity, or inversion symmetry (see below). This means that when $x \rightarrow -x$, $\psi(x)$ must be either invariant or it must change sign. The reason for this requirement is that the Hamiltonian H is symmetric under inversion (the potential is symmetric given our choice of the coordinate system (see Fig. 1)). Thus we take for our solutions

$$\begin{aligned} \psi(x) &= A \sin kx && |x| \leq L/2 \\ &= B e^{-\kappa x} && x > L/2 \\ &= C e^{\kappa x} && x < -L/2 \end{aligned} \quad (3.5)$$

We have used the condition of definite parity in choosing the interior solution as a sine function, an odd function. The choice of a solution with odd parity is arbitrary because an even-parity solution, $\cos kx$, would be equally acceptable. What about a linear combination of the two solutions, such as the sum, $A \sin kx + B \cos kx$? This particular choice would not be acceptable because the sum of an odd and even parity solutions violates the requirement that all solutions must have definite parity.

For the exterior region we have applied condition (i) in Lec2 to discard the exponentially growing solution. This is justified on physical grounds; for a bound state

the particle should be mostly localized inside the potential well, which is another way of saying that away from the well the wave function should be decaying rather than growing.

In the solutions we have chosen there are three constants of integration, A, B, and C. These are to be determined by applying boundary conditions at the interface between the interior and exterior regions, plus a normalization condition (2.23). Notice there is another constant in the problem which has not been specified, the energy eigenvalue E. All we have said thus far is that E should be negative. We have already utilized the boundary condition at infinity and the inversion symmetry condition of definite parity. The conditions which we have not yet applied are the continuity conditions (ii) and (iii) in Lec2. At the interface, $x_o = \pm L/2$, the boundary conditions are

$$\psi_{\text{int}}(x_o) = \psi_{\text{ext}}(x_o) \quad (3.6)$$

$$\left. \frac{d\psi_{\text{int}}(x)}{dx} \right|_{x_o} = \left. \frac{d\psi_{\text{ext}}(x)}{dx} \right|_{x_o} \quad (3.7)$$

with subscripts int and ext denoting the interior and exterior solutions respectively.

The four conditions at the interface do not allow us to determine the four constants because our system of equations is homogeneous. As in situations of this kind, the proportionality constant is fixed by the normalization condition (2.23). We therefore obtain $C = -B$, $B = A \sin(kL/2) \exp(\kappa L/2)$, and

$$\cot(kL/2) = -\kappa/k \quad (3.8)$$

with the constant A determined by (2.23). Eq.(3.8) is the most important result of this calculation; it is sometimes called a dispersion relation. It is a relation which determines the allowed values of E, a quantity that appears in both k and κ . These are then the discrete (quantized) energy levels which the particle can have in the particular potential well given, a square well of width L and depth V_o . Eq.(3.8) is the consequence of

choosing odd-parity solutions for the interior wave. For the even-parity solutions, $\psi_{\text{int}}(x) = A' \cos kx$, the corresponding dispersion relation is

$$\tan(kL/2) = \kappa/k \quad (3.9)$$

Since both solutions are equally acceptable, one has two distinct sets of energy levels, given implicitly by (3.8) and (3.9). To see what are these levels more explicitly, further analysis is necessary.

We consider a graphical analysis of (3.8) and (3.9). We first put the two equations into dimensionless form,

$$\xi \cot \xi = -\eta \quad (\text{odd-parity}) \quad (3.10)$$

$$\xi \tan \xi = \eta \quad (\text{even-parity}) \quad (3.11)$$

where $\xi = kL/2$, $\eta = \kappa L/2$. Then we notice that

$$\xi^2 + \eta^2 = 2mL^2|V_o|/4\hbar^2 \equiv \Lambda \quad (3.12)$$

is a constant for fixed values of V_o and L . In Fig. 4 we plot the left- and right-hand sides of (3.10) and (3.11), and obtain from their intersections the allowed energy levels. The graphical method thus reveals the following features. There exists a minimum value of

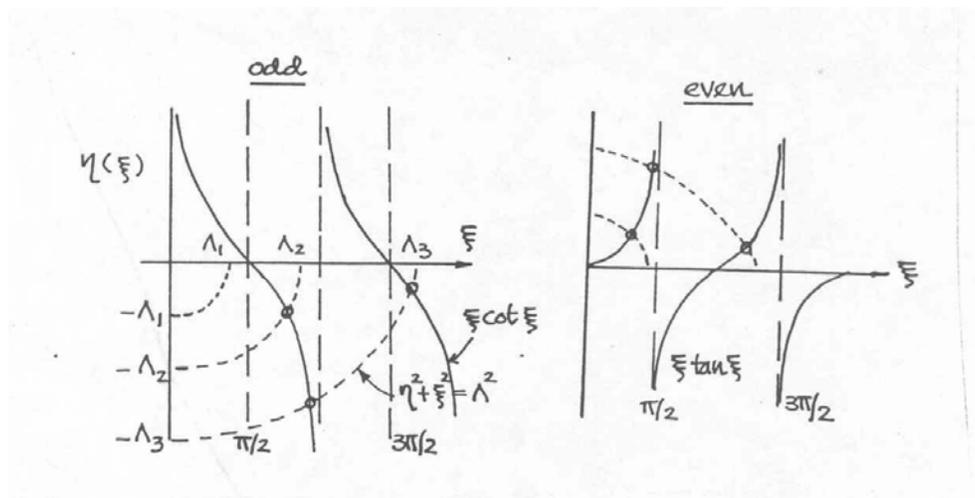


Fig. 4. Graphical solutions of (3.10) and (3.11) showing that there could be no odd-parity solutions if Λ is not large enough (the potential is not deep enough or not wide enough), while there is at least one even-parity solution no matter what values are the well depth and width.

Λ below which no odd-parity solutions are allowed. On the other hand, there is always at least one even-parity solution. The first even-parity energy level occurs at $\xi < \pi/2$, whereas the first odd-parity level occurs at $\pi/2 < \xi < \pi$. Thus, the even- and odd-parity levels alternate in magnitudes, with the lowest level being even in parity. We should also note that the solutions depend on the potential function parameters only through the variable Λ , or the combination of $V_0 L^2$, so that the effect of any change in well depth can be compensated by a change in the square of the well width.

At this point it can be noted that we anticipate that for a particle in a potential well in three dimensions (next chapter), the cosine solution to the wave function has to be discarded because of the condition of regularity (wave function must be finite) at the origin. This means that there will be a minimum value of Λ or $V_0 L^2$ below which no bound states can exist. This is a feature of problems in three dimensions which does not apply to problems in one dimension.

We now summarize our results for the allowed energy levels of a particle in a square well potential and the corresponding wave functions.

$$\psi_{\text{int}}(x) = A \sin kx \quad \text{or} \quad A' \cos kx \quad |x| \leq L/2 \quad (3.13)$$

$$\begin{aligned} \psi_{\text{ext}}(x) &= B e^{-\kappa x} & x > L/2 \\ &= C e^{\kappa x} & x < -L/2 \end{aligned} \quad (3.14)$$

where the energy levels are

$$E = -|V_0| + \frac{\hbar^2 k^2}{2m} = -\frac{\hbar^2 \kappa^2}{2m} \quad (3.15)$$

The constants B and C are determined from the continuity conditions at the interface, while A and A' are to be fixed by the normalization condition. The discrete values of the bound-state energies, k or κ , are obtained from (3.8) and (3.9). In Fig. 5 we show a

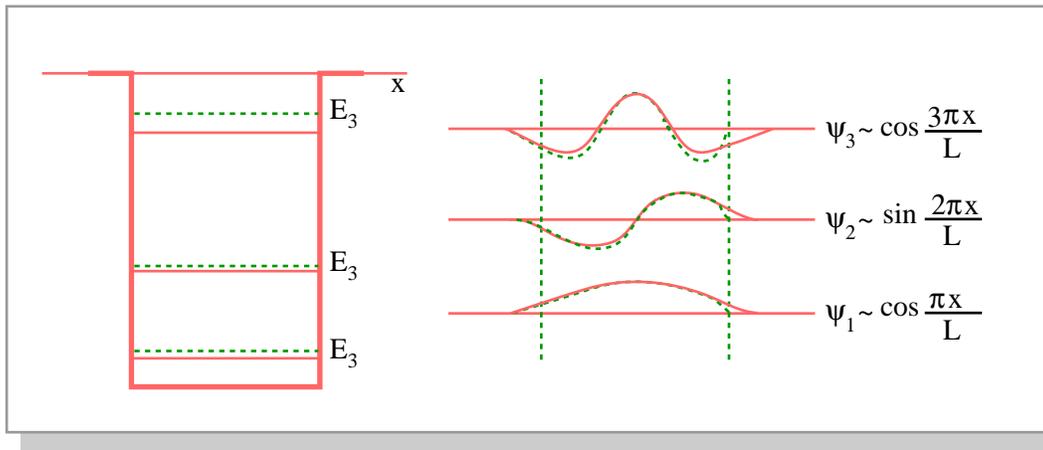


Figure by MIT OCW.

Fig. 5. Ground-state and first two excited-state solutions [from Cohen, p. 16].

Approximate solutions given by the condition of vanishing wavefunction at the potential boundary are indicated by the dashed lines.

sketch of the three lowest-level solutions, the ground state with even parity, the first excited state with odd parity, and the second excited state with even parity. Notice that the number of excited states that one can have depends on the value of V_0 because our solution is valid only for negative E. This means that for a potential of a given depth, the particle can be bound only in a finite number of states.

To obtain more explicit results it is worthwhile to consider an approximation to the boundary condition at the interface. Instead of the continuity of ψ and its derivative at the interface, one might assume that the penetration of the wave function into the external region can be neglected, and therefore require that ψ vanishes at $x = \pm L/2$. Applying this condition to (3.13) gives $kL = n\pi$, where n is any integer, or equivalently,

$$E_n = -|V_o| + \frac{n^2 \pi^2 \hbar^2}{2mL^2}, \quad n = 1, 2, \dots \quad (3.16)$$

This shows explicitly how the energy eigenvalue E_n varies with the level index n , which is the quantum number for the one-dimensional problem under consideration. The corresponding wave functions under this approximation are

$$\begin{aligned} \psi_n(x) &= A_n \cos(n\pi x/L), \quad n = 1, 3, \dots \\ &= A_n' \sin(n\pi x/L) \quad n = 2, 4, \dots \end{aligned} \quad (3.17)$$

The first solutions in this approximate calculation are also shown in Fig. 5. We see that requiring the wave function to vanish at the interface has the effect of confining the particle in a potential well of width L with infinitely steep walls (the infinite well potential or limit of $V_o \rightarrow \infty$). It is therefore to be expected that the problem becomes independent of V_o and there is no limit on the number of excited states. Clearly, the approximate solutions become the more useful the greater is the well depth, and the error is always an overestimate of the energy levels as a result of squeezing of the wave function (physically, this makes the wave have a shorter period or a larger wavenumber).