# Physics 4617/5617: Quantum Physics
# Course Lecture Notes

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**Edition 5.1**

**Abstract**

These class notes are designed for use of the instructor and students of the course Physics 4617/5617: Quantum Physics. This edition was last modified for the Fall 2006 semester.

# III. The Time-Independent Schrödinger Equation

## A. Stationary States.

**1.** How does one determine the wave function $\Psi(x,t)$ from first principles?

**a)** It is solved through a knowledge of $V$ (*i.e.*, the potential energy function) in the Schrödinger equation.

**b)** In this class, we will assume that the potential $V$ is *independent of* $t \Longrightarrow$ then the Schrödinger equation can be solved by the method of **separation of variables**:

$$\Psi(x,t) = \psi(x)\, f(t) \ , \tag{III-1}$$

where $\psi$ (lowercase) is a function of $x$ alone and $f$ is a function of $t$ alone.

**c)** For separable solutions we have

$$\frac{\partial \Psi}{\partial t} = \psi\,\frac{df}{dt}, \qquad \frac{\partial^2 \Psi}{\partial x^2} = \frac{d^2\psi}{dx^2}\, f \tag{III-2}$$

(*ordinary* derivatives now) and the Schrödinger equation (Eq. II-1) becomes

$$i\hbar\psi\,\frac{df}{dt} = -\frac{\hbar^2}{2m}\,\frac{d^2\psi}{dx^2}\, f + V\psi f \ . \tag{III-3}$$

**d)** Dividing through by $\psi f$ gives

$$i\hbar\,\frac{1}{f}\,\frac{df}{dt} = -\frac{\hbar^2}{2m}\,\frac{1}{\psi}\,\frac{d^2\psi}{dx^2} + V \ . \tag{III-4}$$

**e)** The left side is a function of $t$ alone, and the right side, a function of $x$ alone $\Longrightarrow$ the only way this can be true is if both sides of the equation are constant (which we will set equal to $E$). Then

$$i\hbar \frac{1}{f}\frac{df}{dt} = E \ , \qquad \text{(III-5)}$$

or

$$\frac{df}{dt} = -\frac{iE}{\hbar} f \ , \qquad \text{(III-6)}$$

and

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V = E \ , \qquad \text{(III-7)}$$

or

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi \ . \qquad \text{(III-8)}$$

**2.** Separation of variables has turned a *partial* differential equation into two *ordinary* differential equations (Eqs. III-6 & III-8).

**a)** Eq. (III-6) is easy to solve by just rearranging terms and integrating:

$$f(t) = Ce^{-iEt/\hbar} \ . \qquad \text{(III-9)}$$

Typically the integration constant $C$ is absorbed into the solution for $\psi$, hence we state the solution to Eq. (III-6) as

$$f(t) = e^{-iEt/\hbar} \ . \qquad \text{(III-10)}$$

**b)** Meanwhile, Eq. (III-8) is referred to as the **time-independent Schrödinger equation** (in one dimension). To solve it, we must specify the potential $V(x)$.

**3.** When is a *separable solution* to the Schrödinger equation valid?

**a)** **Stationary states**:

**i)** These are states which even though the wave function depends upon time:

$$\Psi(x,t) = \psi(x)\, e^{-iEt/\hbar} \ , \qquad \text{(III-11)}$$

the probability density does not:

$$|\Psi(x,t)|^2 = \Psi^*\Psi = \psi^* e^{+iEt/\hbar} \psi e^{-iEt/\hbar} = |\psi(x)|^2 \ . \tag{III-12}$$

**ii)** In a stationary state, $\langle x \rangle$ is constant and $\langle p \rangle = 0$ (from Eq. II-45) $\Longrightarrow$ nothing ever happens in a stationary state.

**b) States of Definite Total Energy**:

**i)** In classical physics, the total energy (kinetic plus potential) is called the **Hamiltonian**:

$$H(x,p) = \frac{p^2}{2m} + V(x) \ . \tag{III-13}$$

**ii)** The corresponding *Hamiltonian operator* is defined by

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \ , \tag{III-14}$$

where the "hat" (*i.e.*, ˆ) means *this is an operator.*

**iii)** Thus the time-independent Schrödinger equation (Eq. III-8) can be written as

$$\hat{H}\psi = E\psi \ . \tag{III-15}$$

**iv)** The expectation value of the total energy is

$$\langle H \rangle = \int_{-\infty}^{+\infty} \psi^* \hat{H} \psi \, dx = E \int_{-\infty}^{+\infty} |\psi|^2 \, dx = E \ . \tag{III-16}$$

**v)** Moreover,

$$\hat{H}^2\psi = \hat{H}(\hat{H}\psi) = \hat{H}(E\psi) = E(\hat{H}\psi) = E^2\psi \ , \tag{III-17}$$

and hence

$$\langle H^2 \rangle = \int_{-\infty}^{+\infty} \psi^* \hat{H}^2 \psi \, dx = E^2 \int_{-\infty}^{+\infty} |\psi|^2 \, dx = E^2 \; . \tag{III-18}$$

**vi)** So the standard deviation in $H$ is given by

$$\sigma_H^2 = \langle H^2 \rangle - \langle H \rangle^2 = E^2 - E^2 = 0 \; . \tag{III-19}$$

**vii)** If $\sigma = 0$, then every member of the sample must share the same value $\Longrightarrow$ the distribution has zero spread.

**viii)** Hence, a separable solution has the property that *every measurement of the total energy is certain to return the value E.*

**c)** The general solution of the time-independent Schrödinger equation is a **linear combination** of separable solutions.

**i)** The time-independent Schrödinger equation yields an infinite collection of solutions ($\psi_1(x), \psi_2(x), \psi_3(x), \ldots$), each with its associated value of the separation constant $(E_1, E_2, E_3, \ldots) \Longrightarrow$ thus there is a different wave function for each **allowed energy**:

$$\Psi_1(x,t) = \psi_1(x) e^{-iE_1 t/\hbar}, \quad \Psi_2(x,t) = \psi_2(x) e^{-iE_2 t/\hbar}, \ldots \tag{III-20}$$

**ii)** Hence the general solution of the wave function for these cases is

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \, \psi_n(x) \, e^{-iE_n t/\hbar} \; . \tag{III-21}$$

**iii)** *Every* solution to the time-independent Schrödinger equation can be written in this form — it is simply a matter of finding the right constants $(c_1, c_2, \ldots)$.

## B. Infinite Square Well.

**1.** Assume we have a potential of the following form:

$$V(x) = \begin{cases} 0, & \text{if } 0 \leq x \leq a, \\ \infty, & \text{otherwise} \end{cases} \tag{III-22}$$

as shown in Figure III-1.

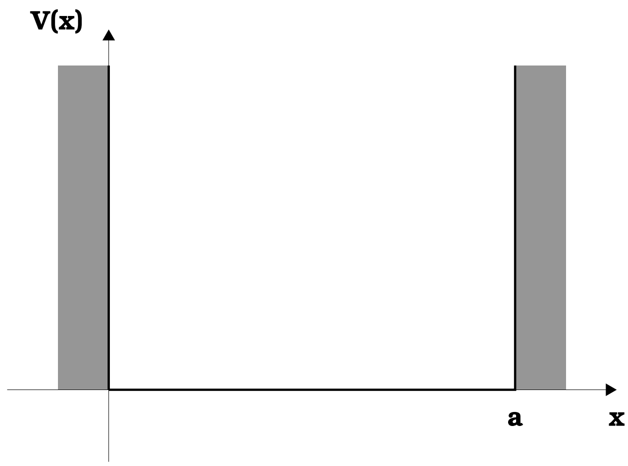


Figure III–1: The infinite square well potential (Eq. III-22).

**a)** A particle in this potential is completely free, except at the two ends ($x = 0$ and $x = a$), where an infinite force prevents it from escaping.

**b)** Outside the well, $\psi(x) = 0 \Longrightarrow$ the probability of finding the particle there is zero.

**c)** Inside the well, $V = 0$, and the time-independent Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \ , \tag{III-23}$$

or

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \quad \text{where } k \equiv \frac{\sqrt{2mE}}{\hbar} \ . \tag{III-24}$$

**d)** Eq. (III-24) is just the (classical) **simple harmonic oscillator** equation with the general solution of

$$\psi(x) = A \sin kx + B \cos kx \ , \tag{III-25}$$

where $A$ and $B$ are constants that are fixed by the **boundary conditions** of the problem:

**i)** Both $\psi$ and $d\psi/dx$ are continuous.

**ii)** Continuity of $\psi(x)$ requires that

$$\psi(0) = \psi(a) = 0 \ , \tag{III-26}$$

so as to join the solution outside the well, hence,

$$\psi(0) = A \sin 0 + B \cos 0 = B = 0 \ , \tag{III-27}$$

so

$$\psi(x) = A \sin kx \ . \tag{III-28}$$

**iii)** At the other boundary, $\psi(a) = A \sin ka = 0$. Since $\psi$ must be normalizable, $A \neq 0$, so

$$ka = 0, \pm\pi, \pm 2\pi, \pm 3\pi, \ldots \tag{III-29}$$

**iv)** But $k = 0$ is no good since that would give $\psi(x) = 0$, and the negative solutions give nothing new, since $\sin(-\theta) = -\sin(\theta)$ and we can absorb the minus sign into $A$. So the *distinct* solutions are

$$k_n = \frac{n\pi}{a}, \qquad \text{with } n = 1, 2, 3, \ldots \tag{III-30}$$

**v)** Note that the boundary condition at $x = a$ does not determine $A$, but rather the constant $k$, and hence the possible values of $E$:

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \ . \tag{III-31}$$

**Exercise:** Prove Eq. (III-25) is the solution to Eq. (III-24).
**Exercise:** Prove Eq. (III-31).

**e)** Unlike the classical case, a quantum particle in the infinite square well cannot have just *any* old energy — it can only have the *allowed* values of Eq. (III-31) $\Longrightarrow$ **allowed states**.

**f)** As usual, we find the amplitude $A$ from the normalization criterion:

$$\begin{aligned}
1 &= \int_0^a \psi^* \psi \, dx \\
&= \int_0^a |A|^2 \sin^2(kx)\, dx \\
&= |A|^2 \int_0^a \frac{1}{2}[1 - \cos(2kx)]\, dx \\
&= \frac{|A|^2}{2} \left[ \int_0^a dx - \int_0^a \cos(2kx)\, dx \right] \\
&= \frac{|A|^2}{2} \left[ x|_0^a - \frac{1}{2k} \sin(2kx)|_0^a \right] \\
&= \frac{|A|^2}{2} \left\{ a - \frac{1}{2k} \left[ \sin 2\left(\frac{n\pi}{a}\right) a - \sin 0 \right] \right\} \\
&= \frac{|A|^2}{2} \left( a - \frac{1}{2k} \sin 2n\pi \right) \\
&= |A|^2 \frac{a}{2} \\
A &= \sqrt{\frac{2}{a}} \qquad \text{(III-32)}
\end{aligned}$$

(we are only worried about the magnitude of $A$ here), so our final wave function becomes

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) \ . \qquad \text{(III-33)}$$

**2.** As can be seen, for an infinite square well, there are an infinite amount of solutions to the time-independent Schrödinger equation. Figure III-2 shows the first 3 of these *stationary states* — as can be seen, these are just standing waves.

**a)** The lowest energy state, $\psi_1$ is called the **ground state**.

**b)** The higher energy states scale as $n^2$ and are called **excited states**.

**c)** These states alternate from **even** to **odd**, with respect to the center of the well. ($\psi_1$ is even, $\psi_2$ is odd, $\psi_3$ is even, and so on.)

**d)** As you go up in energy, each successive state has one more **node** (zero crossing). $\psi_1$ has none (the end points don't count), $\psi_2$ has 1, $\psi_3$ has 2, etc.

**e)** They are mutually **orthogonal** (*i.e.*, the wave functions are said to be **orthonormal**), in the sense that

$$\int \psi_m^*(x)\,\psi_n(x)\,dx = \delta_{mn} \;, \tag{III-34}$$

where $\delta_{mn}$ is the **Kronecker delta**:

$$\delta_{mn} = \begin{cases} 0, & \text{if } m \neq n; \\ 1, & \text{if } m = n. \end{cases} \tag{III-35}$$

**f)** They are **complete**, in the sense that any *other* function, $f(x)$, can be expressed as a linear combination of them:

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{a}x\right) \;. \tag{III-36}$$

Proof of this *completion* criterion requires knowledge of **Fourier series** (see below).

**Exercise:** Prove Eq. (III-34) with the wave function in Eq. (III-33).

**3.** The time-dependent form of the solution to this Schrödinger

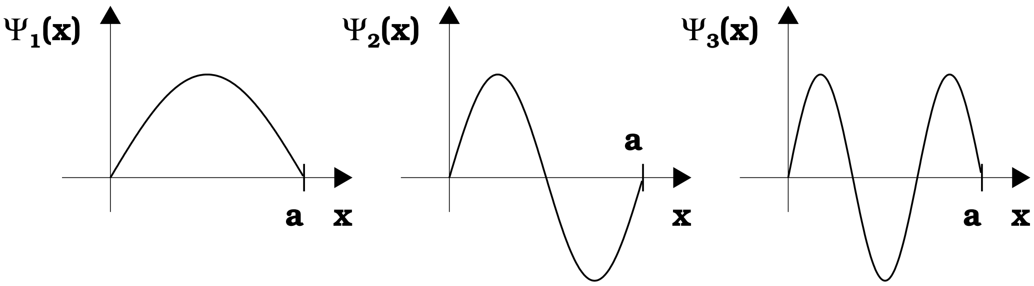


Figure III–2: The first 3 stationary states of the infinite square well.

equation is thus

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-i(n^2\pi^2\hbar/2ma^2)t} \ . \qquad \text{(III-37)}$$

**a)** Then our *initial condition* equation becomes

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x) \ . \qquad \text{(III-38)}$$

**b)** By making use of the orthonormality of the solutions, the initial condition equations then give us the mechanism for finding the coefficients of the series:

$$c_n = \sqrt{\frac{2}{a}} \int_0^a \sin\left(\frac{n\pi}{a}x\right) \Psi(x,0)\, dx \ . \qquad \text{(III-39)}$$

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**Example III–1.** A particle in an infinite square well has the initial wave function

$$\Psi(x,0) = Ax(a-x) \ .$$

**(a)** Normalize $\Psi(x,0)$. Graph it. Which stationary state does it most closely resemble? On that basis, estimate the expectation value of the energy.

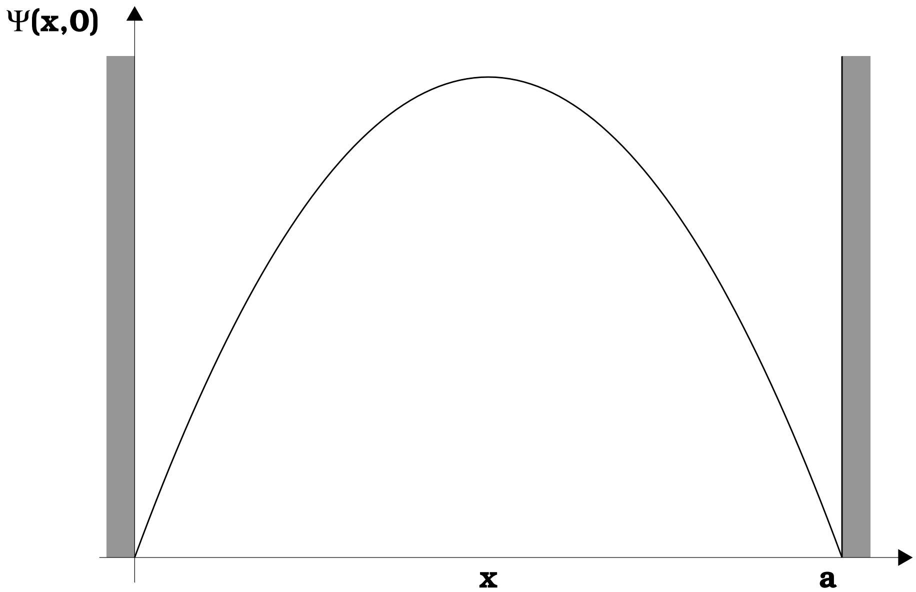
**(b)** Compute $\langle x \rangle$, $\langle p \rangle$ and $\langle H \rangle$, at $t = 0$. (*Note*: This time you cannot get $\langle p \rangle$ by differentiating $\langle x \rangle$, because you only know $\langle x \rangle$ at one instant in time.) How does $\langle H \rangle$ compare with your estimate in (a)?

**Solution (a):**

$$\begin{aligned}
\Psi(x,0) &= Ax(a-x) \\
\Psi^*(x,0) &= Ax(a-x) \\
1 &= \int_0^a \Psi^*\Psi\,dx = A^2\int_0^a x(a-x)x(a-x)\,dx \\
&= A^2\int_0^a x^2\left(a^2-2ax+x^2\right)\,dx \\
&= A^2\int_0^a \left(a^2x^2-2ax^3+x^4\right)\,dx \\
&= A^2\left[\frac{1}{3}a^2x^3-\frac{1}{2}ax^4+\frac{1}{5}x^5\right]_0^a \\
&= A^2\left[\frac{1}{3}a^5-\frac{1}{2}a^5+\frac{1}{5}a^5\right] \\
&= \frac{A^2}{30}\left[10a^5-15a^5+6a^5\right] = \frac{A^2}{30}a^5 \\
A &= \sqrt{\frac{30}{a^5}}\ .
\end{aligned}$$

To graph this function, note that at the endpoints (*i.e.*, $x=0$ and $x=a$), $\Psi(x,0)=0$. Also, expanding out the integrand gives $ax-x^2$, which clearly indicates that this wave function has a parabolic shape. We can find the extrema of this parabola by taking the derivative and setting it equal to 0: $a-2x=0$, or $x=a/2$. The second derivative tells us the orientation of the parabola: $-2$, so the curve is concave downward as shown on the graph on the next page. As one can see from an inspection of this curve (see figure on next page), this wave function resembles the harmonic oscillator solution in the ground state ($n=1$) since it resembles a sine function (note that we will be investigating simple harmonic oscillators in section III.E). As such, we can guess the expectation value of the energy will follow Eq. (III-31):

$$E = \frac{\pi^2\hbar^2}{2ma^2} = 4.93\frac{\hbar^2}{ma^2}\ .$$




The wave function $\Psi(x,0) = x(a-x)$.

**Solution (b):**

$$\begin{aligned}
\langle x \rangle &= \int_0^a \Psi^* x \Psi \, dx = A^2 \int_0^a \left[ x(a-x)x^2(a-x) \right] dx \\
&= A^2 \int_0^a \left[ x^3(a-x)^2 \right] dx \\
&= A^2 \int_0^a \left[ x^3(a^2 - 2ax + x^2) \right] dx \\
&= A^2 \int_0^a \left( a^2x^3 - 2ax^4 + x^5 \right) dx \\
&= A^2 \left[ \frac{1}{4}a^2x^4 - \frac{2}{5}ax^5 + \frac{1}{6}x^6 \right]_0^a \\
&= A^2 \left[ \frac{1}{4}a^6 - \frac{2}{5}a^6 + \frac{1}{6}a^6 \right] \\
&= \frac{30}{60a^5} \left( 15a^6 - 24a^6 + 10a^6 \right) \\
&= \frac{1}{2a^5}a^6 = \frac{a}{2} \, .
\end{aligned}$$

Which is just what you would expect from the appearance of the graph.

$$\langle p \rangle = \int_0^a \Psi^* \frac{\hbar}{i} \frac{\partial}{\partial x} \Psi \, dx = A^2 \frac{\hbar}{i} \int_0^a \left\{ x(a-x) \frac{\partial}{\partial x} \left[ x(a-x) \right] \right\} dx$$

$$
\begin{aligned}
&= A^2\frac{\hbar}{i}\int_0^a [x(a-x)(a-2x)]\,dx \\
&= A^2\frac{\hbar}{i}\int_0^a \left[x(a^2-3ax+2x^2)\right]\,dx \\
&= A^2\frac{\hbar}{i}\int_0^a \left[a^2x-3ax^2+2x^3\right]\,dx \\
&= A^2\frac{\hbar}{i}\left[\frac{1}{2}a^2x^2-ax^3+\frac{2}{4}x^4\right]_0^a \\
&= A^2\frac{\hbar}{2i}\left(a^4-2a^4+a^4\right)=0\ .
\end{aligned}
$$

The particle initially has an expectation of being at rest.

$$
\langle H\rangle = \int_0^a \Psi^*\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V\right)\Psi\,dx\ .
$$

Now,

$$
\frac{\partial^2}{\partial x^2}\Psi = \frac{\partial^2}{\partial x^2}[x(a-x)] = \frac{\partial}{\partial x}(a-2x) = -2\ ,
$$

so

$$
\begin{aligned}
\langle H\rangle &= -\frac{\hbar^2}{2m}\int_0^a \Psi^*\frac{\partial^2\Psi}{\partial x^2}\,dx + V\int_0^a \Psi^*\Psi\,dx \\
&= \frac{\hbar^2}{m}A^2\int_0^a x(a-x)\,dx + V \\
&= \frac{\hbar^2}{m}A^2\left[\frac{1}{2}ax^2-\frac{1}{3}x^3\right]_0^a + V \\
&= \frac{\hbar^2}{m}A^2\left(\frac{1}{2}a^3-\frac{1}{3}a^3\right) + V \\
&= \frac{\hbar^2}{6m}A^2\left(3a^3-2a^3\right) + V \\
&= \frac{\hbar^2}{6m}\frac{30}{a^5}a^3 + V \\
&= \frac{5\hbar^2}{ma^2} + V\ .
\end{aligned}
$$

From this, it is clear that

$$
E = 5\frac{\hbar^2}{ma^2}\ ,
$$

which is close to the solution found for the harmonic oscillator.

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## C. Fourier Analysis.

**1.** As we continue on with our work with the Schrödinger equation, we will often encounter wave functions that take the form

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k)\, e^{i(kx-\omega t)}\, dk \ . \tag{III-40}$$

**a)** In the wave function, $x$ and $t$ represent their usual meanings of the *position* and *time* independent variables, respectively. The new variables introduced here in the integral are:

**i)** The **wave number**, $k$, which is inversely related to the wavelength, $\lambda$, of a wave through

$$k \equiv \frac{2\pi}{\lambda} \ .$$

Using Eq. (I-77) we can show that the wave number is related to the particle/wave's linear momentum via

$$p = \hbar k \ .$$

**ii)** The **angular frequency**, $\omega$, which is directly related to the frequency, $\nu$, of a wave through

$$\omega \equiv 2\pi\nu \ .$$

Using Eq. (I-77) we can show that the angular frequency is related to the particle/wave's energy via

$$E = \hbar\omega \ .$$

**iii)** Finally note that one can write a dispersion relation for a wave with these new variables. Using

Eq. (I-75) for a non-relativistic free particle (*i.e.*, $V = 0$), the total energy of the wave is

$$E = \frac{p^2}{2m} \ .$$

Making use of our relations above, this energy-momentum equation becomes the following dispersion relation:

$$\omega(k) = \frac{\hbar k^2}{2m} \ .$$

**b)** At $t = 0$, this equation takes on a form that may be familiar:

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k)\, e^{ikx}\, dk \ . \qquad \text{(III-41)}$$

**c)** Eq. (III-41) reveals that the *amplitude function* $A(k)$ *is the Fourier transform of the wave function* $\Psi(x,t)$ *at* $t$ *= 0* $\Longrightarrow$ the amplitude function is related to the wave function at $t = 0$ by a Fourier integral.

**2. Fourier analysis** — the generation and deconstruction of Fourier series and integrals are the mathematical methods that underlies the construction of wave packets by superposition.

**a)** Mathematicians commonly use Fourier analysis to rip functions apart, representing them as sums or integrals of simple component functions, each which is characterized by a single frequency.

**b)** This method can be applied to any function $f(x)$ that is *piecewise continuous* — *i.e.*, that has at most a finite number of finite discontinuities. As we have already noted, wave functions must be continuous, so as such, satisfies this condition and so are prime candidates for Fourier analysis.

**c)** Whether we represent $f(x)$ via a Fourier series or Fourier integral depends on whether or not this function is *periodic* $\Longrightarrow$ any function that repeats itself is said to be periodic.

**d)** More precisely, if there exists a finite number $L$ such that $f(x+L) = f(x)$, then $f(x)$ is **periodic** with **period** $L$.

**e)** We can write any function that is periodic (or that is defined on a *finite* interval) as a *Fourier series.*

**f)** However if $f(x)$ is non-periodic or is defined on the *infinite* interval from $-\infty$ to $+\infty$, we must use a *Fourier integral.*

**3. Fourier Series**. Fourier series are not mere mathematical devices; they can be generated in the laboratory (or telescope) $\Longrightarrow$ a *spectrometer* decomposes an electromagnetic wave into spectral lines, each with a different frequency and amplitude (intensity). Thus, a spectrometer decomposes a periodic function in a fashion analogous to the Fourier series.

**a)** Suppose we want to write a periodic, piecewise continuous function $f(x)$ as a series of simple functions. Let $L$ denote the period of $f(x)$, and choose as the origin of coordinates the midpoint of the interval defined by this period $-L/2 \leq x \leq L/2$.

**b)** If we let $a_n$ and $b_n$ denote (real) expansion coefficients, we can write the Fourier series of this function as

$$f(x) = a_0 + \sum_{n=1}^{\infty} \left[ a_n \cos\left(2\pi n \frac{x}{L}\right) + b_n \sin\left(2\pi n \frac{x}{L}\right) \right] . \tag{III-42}$$

**c)** We calculate the coefficients in Eq. (III-42) from the function $f(x)$ as

$$a_0 = \frac{1}{L} \int_{-L/2}^{L/2} f(x)\, dx \ , \qquad \text{(III-43)}$$

$$a_n = \frac{2}{L} \int_{-L/2}^{L/2} f(x) \cos\left(2\pi n \frac{x}{L}\right) dx \quad (n = 1, 2, \ldots) \qquad \text{(III-44)}$$

$$b_n = \frac{2}{L} \int_{-L/2}^{L/2} f(x) \sin\left(2\pi n \frac{x}{L}\right) dx \quad (n = 1, 2, \ldots) \ . \qquad \text{(III-45)}$$

**d)** Notice that the summation in Eq. (III-42) contains an *infinite number of terms.* In practice we retain only a finite number of terms $\Longrightarrow$ this approximation is called **truncation**.

**i)** Truncation is viable only if the sum converges to whatever accuracy we want *before* we chop it off.

**ii)** Truncation is not as extreme an act as it may seem. If $f(x)$ is normalizable, then the expansion coefficients in Eq. (III-42) decrease in magnitude with increasing $n$, *i.e.*,

$$|a_n| \rightarrow 0 \text{ and } |b_n| \rightarrow 0 \text{ as } n \rightarrow \infty \ .$$

**iii)** Under these conditions, which are satisfied by physically admissible wave functions, the sum in Eq. (III-42) can be truncated at some finite maximum value $n_{\text{max}}$ of the index $n$. (Trial and error is typically needed to determine the value of $n_{\text{max}}$ that is required for the desired accuracy.)

**iv)** If $f(x)$ is particularly simple, all but a small, finite number of coefficients may be zero. One should always check for zero coefficients first before evaluating the integrals in Eqs. (III-43, 44, 45).

4. **The Power of Parity.** One should pay attention as to whether one is integrating an **odd** or an **even** function. Trigonometric functions have the well-known parity properties:

$$\begin{aligned} \sin(-x) &= -\sin x \quad \text{(odd)} \qquad \text{(III-46)} \\ \cos(-x) &= +\cos x \quad \text{(even)}\ . \qquad \text{(III-47)} \end{aligned}$$

As such, if $f(x)$ is even or odd, then half of the expansion coefficients in its Fourier series are zero.

**a)** If $f(x)$ is **odd** $[f(-x) = -f(x)]$, then

$$\begin{cases} a_n = 0 \quad (n = 0, 1, 2, 3, \ldots) \\ \\ f(x) = \sum\limits_{n=1}^{\infty} b_n \sin\left(2\pi n \dfrac{x}{L}\right)\ . \end{cases} \qquad \text{(III-48)}$$

**b)** If $f(x)$ is **even** $[f(-x) = +f(x)]$, then

$$\begin{cases} b_n = 0 \quad (n = 1, 2, 3, \ldots) \\ \\ f(x) = \sum\limits_{n=0}^{\infty} a_n \cos\left(2\pi n \dfrac{x}{L}\right)\ . \end{cases} \qquad \text{(III-49)}$$

**c)** If $f(x)$ is either an *even* or and *odd* function, it is then said to have *definite* parity.

5. **The Complex Fourier Series**: If $f(x)$ does not have a definite parity, we can expand it in a complex Fourier series.

**a)** To derive this variant on the Fourier series in Eq. (III-42), we just combine the coefficients $a_n$ and $b_n$ so as to introduce the complex exponential function $e^{i2\pi nx/L}$:

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{i2\pi nx/L}\ . \qquad \text{(III-50)}$$

**b)** Note carefully that in the complex Fourier series in Eq. (III-50) the summation runs from $-\infty$ to $\infty$. The expansion coefficients $c_n$ for the complex Fourier series are

$$c_n = \frac{1}{L} \int_{-L/2}^{L/2} f(x)\, e^{-i2\pi nx/L}\, dx \ . \tag{III-51}$$

**Exercise:** Derive Eqs. (III-50) and (III-51) and thereby determine the relationship of the coefficients $c_n$ of the complex Fourier series of a function to the coefficients $a_n$ and $b_n$ of the corresponding real series.

**6. Fourier Integrals**: Any normalizable function can be expanded in an infinite number of sine and cosine functions that have infinitesimally differing arguments. Such an expansion is called a **Fourier integral**.

**a)** A function $f(x)$ can be represented by a Fourier integral provided the integral $\int_{-\infty}^{\infty} |f(x)|^2\, dx$ exists $\Longrightarrow$ all wave functions satisfy this condition for they are normalizable.

**b)** The Fourier integral has the form

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{ikx}\, dk \ , \tag{III-52}$$

which is the *inverse Fourier transform.*

**c)** The function $g(k)$ plays the role analogous to that of the expansion coefficients $c_n$ in the complex series (Eq. III-50). The relationship of $g(k)$ to $f(x)$ is more clearly exposed by the inverse of Eq. (III-52),

$$g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx}\, dx \ , \tag{III-53}$$

which is the famed *Fourier transform* equation. In mathematical parlance, $f(x)$ and $g(k)$ are said to be Fourier transforms of one another.

**d)** More precisely, $g(k)$ is the **Fourier transform** of $f(x)$, and $f(x)$ is the **inverse Fourier transform** of $g(k)$.

**e)** When convenient, we will use the shorthand notation

$$\boxed{A(k) = \mathcal{F}\left[\Psi(x,0)\right] \qquad \text{and} \qquad \Psi(x,0) = \mathcal{F}^{-1}\left[A(k)\right]} \tag{III-54}$$

to represent Eqs. (III-53) and (III-52), respectively.

**f)** Many useful relationships follow from the intimate relationship between $f(x)$ and $g(k)$. For our purposes, the most important is the **Bessel-Parseval relationship**:

$$\int_{-\infty}^{\infty} |f(x)|^2 \, dx = \int_{-\infty}^{\infty} |g(k)|^2 \, dk \ . \tag{III-55}$$

## D. The Gaussian Wave Packet.

**1.** In Eqs. (III-40) and (III-41), we stated that there will often be time when the wave function will be expressed in terms of an integral of an *amplitude function* $\Longrightarrow$ calculating the wave function is the inverse Fourier transform of the amplitude function.

**2.** Hence, to calculate the **amplitude function**, one merely takes the Fourier transform of the wave function:

$$A(k) = \mathcal{F}[\Psi(x,0)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} \, dx \ . \tag{III-56}$$

**3.** The Bessel-Parseval relationship (Eq. III-55) guarantees that the Fourier transform of a normalized function is normalized:

$$\int_{-\infty}^{\infty} |A(k)|^2 \, dk = \int_{-\infty}^{\infty} |\Psi(x,0)|^2 \, dx = 1 \ . \tag{III-57}$$

---

**Example III–2. The Amplitude Function for a Gaussian**. The Gaussian function is a wave packet with a well-defined center and a single peak. Its amplitude function has the same properties. Initially (*i.e.*, $t = 0$), the Gaussian function contains one parameter, a real number $L$ that governs its width. Show how the amplitude function of a Gaussian scales with $L$ and prove that both the Gaussian wave function and its amplitude function obey normalization rules.

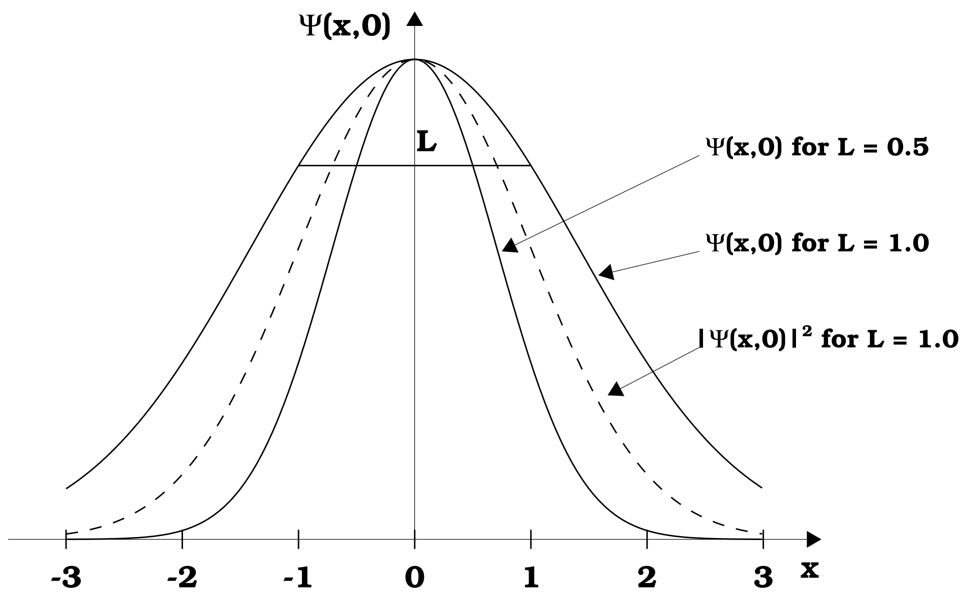
**Solution:**

The most general form of such a function has a center at $x_\circ \neq 0$ and corresponds to an amplitude function that is centered at $k_\circ \neq 0$:

$$\Psi(x,0) = \left(\frac{1}{2\pi L^2}\right)^{1/4} e^{ik_\circ x} e^{-[(x-x_\circ)/(2L)]^2} \ .$$

For simplicity though, assume the Gaussian is centered at $x_\circ = 0$ with an amplitude function centered at $k_\circ = 0$, *i.e.*,

$$\Psi(x,0) = \left(\frac{1}{2\pi L^2}\right)^{1/4} e^{-x^2/(4L^2)} \ .$$




Two Gaussian wave packets of the form in Example III-2; parameter $L$ for these functions takes on the values $L = 0.5$ and $L = 1.0$ (solid curves). The corresponding probability density for $L = 1.0$ is shown as a dashed curve.

In the figure above, you'll find two such wave packets (with different values of $L$). Each exhibits the characteristic shape of a Gaussian function

($i.e.$, a *Bell-shaped* curve): Each has a single peak and decreases rather sharply as $|x|$ increases from zero. But because the Gaussian function decays *exponentially*, it never actually equals zero for finite $|x|$. (It is, nonetheless, normalizable.) You'll also find in this figure above that the probability density $|\Psi(x,0)|^2$ for a Gaussian. This figure illustrates one of the special properties of a Gaussian wave function $\Longrightarrow$ its probability is also a Gaussian function, one that has the same center but is narrower than the state function from which it is calculated.

To find the amplitude function for this Gaussian, make sure that both the state function and the amplitude function are normalized as requested in the problem. We begin by substituting the state function listed above into Eq. (III-56) for the amplitude function:

$$A(k) = \frac{1}{\sqrt{2\pi}} \left(\frac{1}{2\pi L^2}\right)^{1/4} \int_{-\infty}^{\infty} \exp\left[-\frac{1}{4L^2}x^2 - ikx\right] dx \ .$$

We note that a Table of Integrals give

$$\int_{-\infty}^{\infty} e^{-\alpha x^2 - \beta x}\, dx = \sqrt{\frac{\pi}{\alpha}}\, e^{\beta^2/(4\alpha)} \quad (\alpha > 0) \ .$$

Let $\alpha = 1/(4L^2)$ and $\beta = ik$, then we see that

$$A(k) = \left(\frac{2}{\pi}L^2\right)^{1/4} e^{-k^2L^2} \ .$$

Comparing the *mathematical form* of the amplitude function and the initial wave function, we see that the Fourier transform of a Gaussian function of variable $x$ is a Gaussian of variable $k$.

Now, check for normalization

$$\begin{aligned}
\int_{-\infty}^{\infty} \Psi^*\Psi\, dx &= \left(\frac{1}{2\pi L^2}\right)^{1/2} \int_{-\infty}^{\infty} e^{-x^2/(2L^2)}\, dx \\
&= \left(\frac{1}{2\pi L^2}\right)^{1/2} 2\int_{0}^{\infty} e^{-x^2/(2L^2)}\, dx \\
&= \left(\frac{1}{2\pi L^2}\right)^{1/2} 2\frac{1}{2/\sqrt{2}L}\sqrt{\pi}
\end{aligned}$$

$$
\begin{aligned}
&= \left(\frac{1}{2\pi L^2}\right)^{1/2} \sqrt{2\pi} L \\
&= \left(\frac{2\pi L^2}{2\pi L^2}\right)^{1/2} \\
&= \sqrt{1} = 1\ . \quad \text{QED}
\end{aligned}
$$

$$
\begin{aligned}
\int_{-\infty}^{\infty} A(k)^* A(k)\, dk &= \left(\frac{2}{\pi}L^2\right)^{1/2} \int_{-\infty}^{\infty} e^{-2k^2L^2}\, dk \\
&= \left(\frac{2}{\pi}L^2\right)^{1/2} 2\int_{0}^{\infty} e^{-2k^2L^2}\, dk \\
&= \left(\frac{2}{\pi}L^2\right)^{1/2} 2\frac{1}{2\sqrt{2}L}\sqrt{\pi} \\
&= \left(\frac{2}{\pi}L^2\right)^{1/2} \sqrt{\frac{\pi}{2L^2}} \\
&= \left(\frac{2\pi L^2}{2\pi L^2}\right)^{1/2} \\
&= \sqrt{1} = 1\ . \quad \text{QED}
\end{aligned}
$$

---

## E. The Quantum Simple Harmonic Oscillator.

**1.** From classical mechanics, the equation of motion of a mass connected to a spring is govern by **Hooke's Law**:

$$F = -kx = m\frac{d^2x}{dt^2}\ ,$$

where $k$ is the **spring constant**.

**2.** The solution to Hooke's Law gives a *simple harmonic oscillation* in position:

$$x(t) = A\sin(\omega t) + B\cos(\omega t)\ ,$$

where $A$ and $B$ are constants determined from either initial conditions or boundary conditions, and

$$\omega = \sqrt{\frac{k}{m}} \tag{III-58}$$

is the (angular) frequency of oscillation. The potential energy is

$$V(x) = \frac{1}{2}kx^2 \ . \tag{III-59}$$

**3.** As can be seen by the above equation, the potential for Hooke's law is parabolic. Practically any potential can be *approximated* by a parabola, if one takes the limits small enough in the neighborhood of a local minimum.

**a)** One can expand any function about a local minimum in a **Taylor series**. In the case of the potential:

$$V(x) = V(x_\circ) + \frac{1}{1!}V'(x_\circ)(x - x_\circ) + \frac{1}{2!}V''(x_\circ)(x - x_\circ)^2 + \cdots \tag{III-60}$$

where $x_\circ$ is the location of the local minimum.

**b)** We can set $V(x_\circ) = 0$ since the value of this constant is irrelevant to the force. Also $V'(x_\circ) = 0$ since $x_\circ$ is a minimum. If we drop terms higher than the second derivative, we get

$$V(x) \cong \frac{1}{2}V''(x_\circ)(x - x_\circ)^2 \ , \tag{III-61}$$

which describes simple harmonic oscillation about the point $x_\circ$, with an effective spring constant $k = V''(x_\circ)$.

**c)** It should be noted from this Taylor series approximation that *any* oscillatory motion is approximately simple harmonic, as long as the amplitude is small.

**4.** The *quantum* problem is to solve the Schrödinger equation for the potential

$$V(x) = \frac{1}{2} m\omega^2 x^2 \ . \tag{III-62}$$

**a)** With this potential, the time-independent Schrödinger's equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2} m\omega^2 x^2 \psi = E\psi \ . \tag{III-63}$$

**b)** There are 2 ways to solve this equation: The **power series expansion** method and the **ladder operator** method. This second method is primarily just clever algebra and we will go through that solution first.

**5.** The **Ladder Operator** (Algebraic) Method.

**a)** Let's rewrite Eq. (III-63) as

$$\frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 + (m\omega x)^2\right]\psi = E\psi \ . \tag{III-64}$$

**b)** We must *factor* the term in the square brackets. We can do this by realizing that if these terms were *numbers*, we could factor them as

$$u^2 + v^2 = (u - iv)(u + iv) \ .$$

However in our case, $u$ and $v$ are operators and operators do not, in general, **commute** (*i.e.*, $uv \neq vu$).

**c)** Let us introduce the $a$-operators as

$$a_\pm \equiv \frac{1}{\sqrt{2m}}\left(\frac{\hbar}{i}\frac{d}{dx} \pm im\omega x\right) \ . \tag{III-65}$$

Let's check the various products of these operators:

**i)** First,

$$(a_- a_+) f(x) \ = \ \frac{1}{2m}\left(\frac{\hbar}{i}\frac{d}{dx} - im\omega x\right)\left(\frac{\hbar}{i}\frac{d}{dx} + im\omega x\right) f(x)$$

$$
\begin{aligned}
&= \frac{1}{2m}\left(\frac{\hbar}{i}\frac{d}{dx} - im\omega x\right)\left(\frac{\hbar}{i}\frac{df}{dx} + im\omega x f\right) \\
&= \frac{1}{2m}\left[-\hbar^2\frac{d^2 f}{dx^2} + \hbar m\omega\frac{d}{dx}(xf)\right. \\
&\qquad \left. -\hbar m\omega x\frac{df}{dx} + (m\omega x)^2 f\right] \\
&= \frac{1}{2m}\left[-\hbar^2\frac{d^2 f}{dx^2} + \hbar m\omega x\frac{df}{dx} + \hbar m\omega f\right. \\
&\qquad \left. -\hbar m\omega x\frac{df}{dx} + (m\omega x)^2 f\right] \\
&= \frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 + (m\omega x)^2 + \hbar m\omega\right] f(x) \\
a_- a_+ &= \frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 + (m\omega x)^2\right] + \frac{1}{2}\hbar\omega \ . \qquad \text{(III-66)}
\end{aligned}
$$

**ii)** Pulling the $(1/2)\hbar\omega$ term to the other side of the equation, we get the following for Schrödinger's equation:

$$\left(a_- a_+ - \frac{1}{2}\hbar\omega\right)\psi = E\psi \ . \qquad \text{(III-67)}$$

**iii)** From a similar treatment, one can easily show that

$$a_+ a_- = \frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 + (m\omega x)^2\right] - \frac{1}{2}\hbar\omega \ , \quad \text{(III-68)}$$

and the Schrödinger equation becomes

$$\left(a_+ a_- + \frac{1}{2}\hbar\omega\right)\psi = E\psi \ . \qquad \text{(III-69)}$$

**iv)** Also note that

$$a_- a_+ - a_+ a_- = \hbar\omega \ . \qquad \text{(III-70)}$$

**d)** If $\psi$ satisfies the Schrödinger equation with energy $E$, then $a_+\psi$ satisfies the Schrödinger equation with energy $(E +$

$\hbar\omega$):

$$\begin{aligned}\left(a_+a_- + \frac{1}{2}\hbar\omega\right)(a_+\psi) &= \left(a_+a_-a_+ + \frac{1}{2}\hbar\omega a_+\right)\psi \\ = a_+\left(a_-a_+ + \frac{1}{2}\hbar\omega\right)\psi &= a_+\left[\left(a_-a_+ - \frac{1}{2}\hbar\omega\right)\psi + \hbar\omega\psi\right] \\ = a_+(E\psi + \hbar\omega\psi) &= (E+\hbar\omega)(a_+\psi)\ . \quad \text{QED} \end{aligned} \qquad \text{(III-71)}$$

**e)** By the same token, $a_-\psi$ is a solution with energy $(E - \hbar\omega)$:

$$\begin{aligned}\left(a_-a_+ - \frac{1}{2}\hbar\omega\right)(a_-\psi) &= \left(a_-a_+a_- - \frac{1}{2}\hbar\omega a_-\right)\psi \\ = a_-\left(a_+a_- - \frac{1}{2}\hbar\omega\right)\psi &= a_-\left[\left(a_+a_- + \frac{1}{2}\hbar\omega\right)\psi - \hbar\omega\psi\right] \\ = a_-(E\psi - \hbar\omega\psi) &= (E-\hbar\omega)(a_-\psi)\ . \quad \text{QED} \end{aligned} \qquad \text{(III-72)}$$

**f)** We call the $a$-operators the **ladder operators**: $a_+$ is called the **raising operator**, and $a_-$, the **lowering operator** $\Longrightarrow$ if we can find one solution with energy $E$, we can find all other solutions by using these operators.

**g)** There exist a *lowest* energy state for the quantum harmonic oscillator which satisfies

$$a_-\psi_\circ = 0\ , \qquad \text{(III-73)}$$

where $\psi_\circ$ is referred to as the **ground state**.

**i)** As a result, we can write the lowering operator for this ground state as

$$\frac{1}{\sqrt{2m}}\left(\frac{\hbar}{i}\frac{d\psi_\circ}{dx} - im\omega x\psi_\circ\right) = 0\ , \qquad \text{(III-74)}$$

or

$$\frac{d\psi_\circ}{dx} = -\frac{m\omega}{\hbar}x\psi_\circ\ . \qquad \text{(III-75)}$$

**ii)** The solution to this differential equation is trivial:

$$\int \frac{d\psi_\circ}{\psi_\circ} = -\frac{m\omega}{\hbar}\int x\,dx$$

$$\begin{aligned}\ln\psi_\circ &= -\frac{m\omega}{2\hbar}x^2 + \text{ constant}\\ \psi_\circ &= A_\circ e^{-(m\omega/2\hbar)\,x^2}\ . \qquad \text{(III-76)}\end{aligned}$$

**iii)** Plugging this into Schrödinger equation, $(a_+a_- + (1/2)\hbar\omega)\psi_\circ = E_\circ\psi_\circ$ and noting Eq. (III-73), we see that

$$E_\circ = \frac{1}{2}\hbar\omega\ . \qquad \text{(III-77)}$$

Note that

$$\begin{aligned}\omega &= 2\pi\nu\\ \hbar &= \frac{h}{2\pi}\ ,\end{aligned}$$

so

$$\hbar\omega = \frac{h}{2\pi}\cdot 2\pi\nu = h\nu\ .$$

**h)** From this ground state, we can easily calculate the excited states with the raising operator:

$$\boxed{\psi_n(x) = A_n(a_+)^n e^{-(m\omega/2\hbar)\,x^2}, \quad \text{with } E_n = \left(n+\frac{1}{2}\right)\hbar\omega\ .} \qquad \text{(III-78)}$$

**i)** For instance, the first excited state is

$$\begin{aligned}\psi_1 &= A_1 a_+ e^{-(m\omega/2\hbar)\,x^2}\\ &= A_1\frac{1}{\sqrt{2m}}\left(\frac{\hbar}{i}\frac{d}{dx} + im\omega x\right)e^{-(m\omega/2\hbar)\,x^2}\\ &= \frac{A_1}{\sqrt{2m}}\left[\frac{\hbar}{i}\left(-\frac{m\omega}{\hbar}x\right)e^{-(m\omega/2\hbar)\,x^2} + im\omega x e^{-(m\omega/2\hbar)\,x^2}\right]\ .\end{aligned} \qquad \text{(III-79)}$$

**ii)** This simplifies to

$$\psi_1 = (iA_1\omega\sqrt{2m})xe^{-(m\omega/2\hbar)\,x^2}\ . \qquad \text{(III-80)}$$

Note that since $\psi$ must be real, the amplitude $A_1$ must be imaginary (see Example III-3 below).

**Example III–3.** The raising and lowing operators:

**(a)** The raising and lowering operators generate new solutions to the Schrödinger equation, but these new solutions are not correctly normalized. Thus $a_+\psi_n$ is *proportional* to $\psi_{n+1}$, and $a_-\psi_n$ is *proportional* to $\psi_{n-1}$, but we would like to know the precise proportionality constants. Use integration by parts and the Schrödinger equation (Eqs. III-67 and III-69) to show that

$$\begin{aligned} \int_{-\infty}^{\infty} |a_+\psi_n|^2\, dx &= (n+1)\,\hbar\omega && \text{(III-81)} \\ \int_{-\infty}^{\infty} |a_-\psi_n|^2\, dx &= n\hbar\omega\ , && \text{(III-82)} \end{aligned}$$

and hence (with $i$'s to keep the wave function real)

$$\begin{aligned} a_+\psi_n &= i\sqrt{(n+1)\hbar\omega}\ \psi_{n+1} && \text{(III-83)} \\ a_-\psi_n &= -i\sqrt{n\hbar\omega}\ \psi_{n-1}\ . && \text{(III-84)} \end{aligned}$$

**(b)** Use Eq. (III-83) to show that the normalization constant $A_n$ in Eq. (III-78) is

$$A_n = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{(-i)^n}{\sqrt{n!(\hbar\omega)^n}}\ . \qquad \text{(III-85)}$$

**Solution (a):**

$$\begin{aligned} \int_{-\infty}^{\infty} |a_+\psi_n|^2\, dx &= \int_{-\infty}^{\infty} (a_+\psi_n)^*(a_+\psi_n)\, dx \\ &= \frac{1}{2m}\int_{-\infty}^{\infty} \left[\left(\frac{\hbar}{i}\frac{d}{dx} + im\omega x\right)\psi_n\right]^* \\ &\quad \times \left[\left(\frac{\hbar}{i}\frac{d}{dx} + im\omega x\right)\psi_n\right] dx \\ &= \frac{1}{2m}\int_{-\infty}^{\infty} \left(-\frac{\hbar}{i}\frac{d\psi_n^*}{dx} - im\omega x\psi_n^*\right) \\ &\quad \times \left(\frac{\hbar}{i}\frac{d\psi_n}{dx} + im\omega x\psi_n\right) dx \end{aligned}$$

$$\begin{aligned} &= \frac{1}{2m}\int_{-\infty}^{\infty}\left[\hbar^2\frac{d\psi_n^*}{dx}\frac{d\psi_n}{dx} - \hbar m\omega x\frac{d\psi_n^*}{dx}\psi_n\right. \\ &\qquad \left. -\hbar m\omega x\psi_n^*\frac{d\psi_n}{dx} + (m\omega x)^2\psi_n^*\psi_n\right] dx\ . \end{aligned}$$

At this point, note that

$$\frac{d}{dx}(\psi_n^*\psi_n) = \psi_n^*\frac{d\psi_n}{dx} + \frac{d\psi_n^*}{dx}\psi_n\ .$$

As such, we can simplify the integral above as

$$\begin{aligned} \int_{-\infty}^{\infty}|a_+\psi_n|^2\,dx &= \frac{1}{2m}\int_{-\infty}^{\infty}\left[\hbar^2\frac{d\psi_n^*}{dx}\frac{d\psi_n}{dx} + (m\omega x)^2\psi_n^*\psi_n\right. \\ &\qquad \left. -\hbar m\omega x\frac{d}{dx}(\psi_n^*\psi_n)\right] dx \\ &= \frac{1}{2m}\left[\int_{-\infty}^{\infty}\hbar^2\frac{d\psi_n^*}{dx}\frac{d\psi_n}{dx}\,dx + \int_{-\infty}^{\infty}(m\omega x)^2\psi_n^*\psi_n\,dx\right. \\ &\qquad \left. -\int_{-\infty}^{\infty}\hbar m\omega x\frac{d}{dx}(\psi_n^*\psi_n)\,dx\right]\ . \qquad \textbf{(A)} \end{aligned}$$

The first integral in Eq. (A) is found by using integration by parts, let

$$\begin{aligned} u &= \tfrac{d\psi_n}{dx} & dv &= d\psi_n^* \\ du &= \tfrac{d^2\psi_n}{dx^2}\,dx & v &= \psi_n^*, \end{aligned}$$

then

$$\begin{aligned} \int_{-\infty}^{\infty}\hbar^2\frac{d\psi_n^*}{dx}\frac{d\psi_n}{dx}\,dx &= \int_{-\infty}^{\infty}\hbar^2\frac{d\psi_n}{dx}\frac{d\psi_n^*}{dx}\,dx \\ &= \hbar^2\int_{-\infty}^{\infty}\frac{d\psi_n}{dx}d\psi_n^* \\ &= \hbar^2\left[\psi_n^*\,\frac{d\psi_n}{dx}\bigg|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\psi_n^*\frac{d^2\psi_n}{dx^2}\,dx\right] \\ &= -\hbar^2\int_{-\infty}^{\infty}\psi_n^*\frac{d^2\psi_n}{dx^2}\,dx\ , \qquad \textbf{(A1)} \end{aligned}$$

where $\psi_n^*(d\psi_n/dx)|_{-\infty}^{\infty} \to 0$ since the wave function must be normalizable. The second integral in Eq. (A) can be written as

$$\int_{-\infty}^{\infty}(m\omega x)^2\psi_n^*\psi_n\,dx = \int_{-\infty}^{\infty}\psi_n^*(m\omega x)^2\psi_n\,dx\ . \qquad \textbf{(A2)}$$

The third and final integral in Eq. (A) in once again solved with integral by parts, let

$$\begin{array}{rclcrcl} u & = & x & \quad & dv & = & d(\psi_n^* \psi_n) \\ du & = & dx & \quad & v & = & \psi_n^* \psi_n \ , \end{array}$$

then

$$\begin{aligned} \hbar m\omega \int_{-\infty}^{\infty} x \frac{d}{dx}(\psi_n^* \psi_n)\, dx &= \hbar m\omega \int_{-\infty}^{\infty} x d(\psi_n^* \psi_n) \\ &= \hbar m\omega \left[ x\psi_n^* \psi_n |_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \psi_n^* \psi_n \, dx \right] \\ &= -\hbar m\omega \ , \qquad\qquad \textbf{(A3)} \end{aligned}$$

which results once again since $x\psi_n^* \psi_n|_{-\infty}^{\infty} \to 0$ in order for the wave function to be normalizable.

Now plugging Eqs. (A1), (A2), and (A3) back into Eq. (A) gives

$$\begin{aligned} \int_{-\infty}^{\infty} |a_+ \psi_n|^2 \, dx &= \frac{1}{2m} \int_{-\infty}^{\infty} \left[ -\hbar^2 \psi_n^* \frac{d^2 \psi_n}{dx^2} + \psi_n^* (m\omega x)^2 \psi_n \right] dx \\ & \quad - \frac{1}{2m}(-\hbar m\omega) \ , \end{aligned}$$

or with use of the Schrödinger equation (Eq. III-64), we get

$$\begin{aligned} \int_{-\infty}^{\infty} |a_+ \psi_n|^2 \, dx &= \frac{1}{2m} \int_{-\infty}^{\infty} \left[ -\hbar^2 \psi_n^* \frac{d^2 \psi_n}{dx^2} + \psi_n^* (m\omega x)^2 \psi_n \right] dx \\ & \quad + \frac{1}{2}\hbar\omega \\ &= \int_{-\infty}^{\infty} \psi_n^* \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2 \right] \psi_n \, dx + \frac{1}{2}\hbar\omega \\ &= \int_{-\infty}^{\infty} \psi_n^* E_n \psi_n \, dx + \frac{1}{2}\hbar\omega \\ &= E_n \int_{-\infty}^{\infty} \psi_n^* \psi_n \, dx + \frac{1}{2}\hbar\omega \\ &= E_n + \frac{1}{2}\hbar\omega = (n + \frac{1}{2})\, \hbar\omega + \frac{1}{2}\hbar\omega \\ &= (n+1)\, \hbar\omega \ . \qquad\qquad \text{QED} \end{aligned}$$

Note that we could have solved this much more simply by using *operator algebra* and noting that $a_+^* = a_-$ (see next section):

$$\int_{-\infty}^{\infty} (a_+ \psi_n)^* (a_+ \psi_n) \, dx \ = \ \int_{-\infty}^{\infty} (\psi_n^* a_-)(a_+ \psi_n) \, dx$$

$$
\begin{aligned}
= \int_{-\infty}^{\infty} \psi_n^* a_- a_+ \psi_n \, dx &= \int_{-\infty}^{\infty} \psi_n^* (E_n + \frac{1}{2}\hbar\omega)\, \psi_n \, dx \\
= (E_n + \frac{1}{2}\hbar\omega) \int_{-\infty}^{\infty} \psi_n^* \psi_n \, dx &= E_n + \frac{1}{2}\hbar\omega = (n + \frac{1}{2})\,\hbar\omega + \frac{1}{2}\hbar\omega \\
= (n+1)\,\hbar\omega \ . \qquad & \text{QED}
\end{aligned}
$$

Now for the proof of the second integral relation

$$
\begin{aligned}
\int_{-\infty}^{\infty} (a_-\psi_n)^* (a_-\psi_n) \, dx &= \frac{1}{2m} \int_{-\infty}^{\infty} \left[ \left( \frac{\hbar}{i}\frac{d}{dx} - im\omega x \right) \psi_n \right]^* \\
&\quad \times \left[ \left( \frac{\hbar}{i}\frac{d}{dx} - im\omega x \right) \psi_n \right] dx \\
&= \frac{1}{2m} \int_{-\infty}^{\infty} \left( -\frac{\hbar}{i}\frac{d\psi_n^*}{dx} + im\omega x \psi_n^* \right) \\
&\quad \times \left( \frac{\hbar}{i}\frac{d\psi_n}{dx} - im\omega x \psi_n \right) dx \\
&= \frac{1}{2m} \int_{-\infty}^{\infty} \left[ \hbar^2 \frac{d\psi_n^*}{dx}\frac{d\psi_n}{dx} + \hbar m\omega x \frac{d\psi_n^*}{dx}\psi_n \right. \\
&\quad \left. + \hbar m\omega x \psi_n^* \frac{d\psi_n}{dx} + (m\omega x)^2 \psi_n^* \psi_n \right] dx \\
&= \frac{1}{2m} \int_{-\infty}^{\infty} \left[ \hbar^2 \frac{d\psi_n^*}{dx}\frac{d\psi_n}{dx} + (m\omega x)^2 \psi_n^* \psi_n \right. \\
&\quad \left. + \hbar m\omega x \frac{d}{dx}(\psi_n^* \psi_n) \right] dx \ . \quad \textbf{(B)}
\end{aligned}
$$

The first two integrals in Eq. (B) are identical to those in Eq. (A) and the third is just the negative of the third integral in Eq. (A). As such, Eq. (B) reduces to

$$
\begin{aligned}
\int_{-\infty}^{\infty} |a_-\psi_n|^2 \, dx &= \frac{1}{2m} \int_{-\infty}^{\infty} \left[ -\hbar^2 \psi_n^* \frac{d^2\psi_n}{dx^2} + \psi_n^* (m\omega x)^2 \psi_n \right] dx \\
&\quad - \frac{1}{2}\hbar\omega \\
&= \int_{-\infty}^{\infty} \psi_n^* \left[ -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2 \right] \psi_n \, dx - \frac{1}{2}\hbar\omega \\
&= \int_{-\infty}^{\infty} \psi_n^* E_n \psi_n \, dx - \frac{1}{2}\hbar\omega
\end{aligned}
$$

$$
\begin{aligned}
&= E_n \int_{-\infty}^{\infty} \psi_n^* \psi_n \, dx - \frac{1}{2}\hbar\omega \\
&= E_n + \frac{1}{2}\hbar\omega = (n + \frac{1}{2})\hbar\omega - \frac{1}{2}\hbar\omega \\
&= n\hbar\omega \; . \qquad\qquad\qquad \text{QED}
\end{aligned}
$$

We next have to prove the solutions of the raising and lowering operators. Assume that $a_+\psi_n = c\psi_{n+1}$, for some constant $c$. With $\psi_n$ and $\psi_{n+1}$ normalized,

$$\int_{-\infty}^{\infty} |a_+\psi_n|^2 \, dx = |c|^2 \int_{-\infty}^{\infty} |\psi_{n+1}|^2 \, dx = |c|^2 = (n+1)\,\hbar\omega \ ,$$

so $c = \sqrt{(n+1)\hbar\omega}$. Note however, to achieve consistency with the integrals above, $c = i\sqrt{(n+1)\hbar\omega}$, so

$$a_+\psi_n = i\sqrt{(n+1)\hbar\omega} \ \psi_{n+1} \ .$$

Similarly, $a_-\psi_n = b\psi_{n-1}$, for some constant $b$, so

$$\int_{-\infty}^{\infty} |a_-\psi_n|^2 \, dx = |b|^2 \int_{-\infty}^{\infty} |\psi_{n-1}|^2 \, dx = |b|^2 = n\hbar\omega \ ,$$

so $b = \sqrt{n\hbar\omega}$. Once again, to achieve consistency, $b = -i\sqrt{n\hbar\omega}$, so

$$a_-\psi_n = -i\sqrt{n\hbar\omega} \ \psi_{n-1} \ .$$

**Solution (b):** From Eqs. (III-76) and (III-78),

$$
\begin{aligned}
\psi_\circ &= A_\circ e^{-(m\omega/2\hbar)x^2}, \quad e^{-(m\omega/2\hbar)x^2} = \frac{\psi_\circ}{A_\circ} \\
\psi_n &= A_n (a_+)^n e^{-(m\omega/2\hbar)x^2} = \frac{A_n}{A_\circ}(a_+)^n \psi_\circ \\
&= \frac{A_n}{A_\circ}(a_+)^{n-1} \underbrace{(a_+\psi_\circ)}_{i\sqrt{\hbar\omega}\psi_1} = \frac{A_n}{A_\circ}(i\sqrt{\hbar\omega})(a_+)^{n-2} \underbrace{(a_+\psi_1)}_{i\sqrt{2\hbar\omega}\psi_2} = \cdots \\
&= \frac{A_n}{A_\circ}(i\sqrt{\hbar\omega})(i\sqrt{2\hbar\omega})(i\sqrt{3\hbar\omega})\cdots(i\sqrt{n\hbar\omega})\psi_n \\
&= \frac{A_n}{A_\circ} i^n \sqrt{n!(\hbar\omega)^n} \, \psi_n, \\
A_n &= \frac{(-i)^n}{\sqrt{n!(\hbar\omega)^n}} \, A_\circ \ .
\end{aligned}
$$

Normalizing $\psi_\circ$ gives

$$1 = |A_\circ|^2 \int_{-\infty}^{\infty} e^{-m\omega x^2/\hbar}\, dx = |A_\circ|^2 \sqrt{\frac{\pi\hbar}{m\omega}}$$

or

$$A_\circ = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} ,$$

so

$$A_n = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{(-i)^n}{\sqrt{n!(\hbar\omega)^n}} .$$

---

**6.** The **Power Series Expansion** (Analytic) Method.

**a)** Let

$$\xi \equiv \sqrt{\frac{m\omega}{\hbar}}\, x \quad \text{and} \quad \frac{d\xi}{dx} = \sqrt{\frac{m\omega}{\hbar}} \qquad \text{(III-86)}$$

in the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi = E\psi . \qquad \text{(III-87)}$$

Then using the chain rule,

$$\begin{aligned} \frac{d^2\psi}{dx^2} &= \frac{d}{dx}\left(\frac{d\psi}{dx}\right) = \frac{d}{d\xi}\left(\frac{d\psi}{dx}\right)\frac{d\xi}{dx} = \frac{d}{d\xi}\left(\frac{d\psi}{d\xi}\frac{d\xi}{dx}\right)\frac{d\xi}{dx} \\ &= \frac{d}{d\xi}\left(\frac{d\psi}{d\xi}\sqrt{\frac{m\omega}{\hbar}}\right)\sqrt{\frac{m\omega}{\hbar}} = \frac{m\omega}{\hbar}\frac{d^2\psi}{d\xi^2} , \qquad \text{(III-88)} \end{aligned}$$

plugging this back into Eq. (III-87) gives

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{m\omega}{\hbar}\frac{d^2\psi}{d\xi^2} + \frac{1}{2}m\omega^2\left(\frac{\hbar}{m\omega}\right)\xi^2\psi &= E\psi \\ -\frac{\hbar\omega}{2}\frac{d^2\psi}{d\xi^2} + \frac{\hbar\omega}{2}\xi^2\psi &= E\psi \\ \frac{d^2\psi}{d\xi^2} - \xi^2\psi &= -\frac{2E}{\hbar\omega}\psi \end{aligned}$$

$$\frac{d^2\psi}{d\xi^2} = \left(\xi^2 - \frac{2E}{\hbar\omega}\right)\psi$$
$$\frac{d^2\psi}{d\xi^2} = \left(\xi^2 - K\right)\psi\ , \qquad \text{(III-89)}$$

where

$$K \equiv \frac{2E}{\hbar\omega}\ . \qquad \text{(III-90)}$$

Finally, we can rewrite Eq. (III-89) as

$$\boxed{\left(\frac{d^2}{d\xi^2} - \xi^2 + K\right)\ \psi(\xi) = 0\ ,} \qquad \text{(III-91)}$$

which is called **Weber's equation**.

**b)** To solve this DE, let's first look at the asymptotic limit of very large $\xi$ (hence $x$) such that $\xi^2 \gg K$, then

$$\frac{d^2\psi}{d\xi^2} \approx \xi^2\psi\ , \qquad \text{(III-92)}$$

which has the approximate solution

$$\psi(\xi) \approx Ae^{-\xi^2/2} + Be^{+\xi^2/2}\ . \qquad \text{(III-93)}$$

**i)** The $B$ term is clearly not normalizable since $\psi$ blows up as $\xi \rightarrow \infty$.

**ii)** The realistic solution thus has the asymptotic form

$$\psi(\xi) \rightarrow Ae^{-\xi^2/2},\ \ \text{at large } \xi\ . \qquad \text{(III-94)}$$

**c)** Since we know the asymptotic form of the solution, we can re-examine Eq. (III-89 or III-91) and assume the solution to this equation has the functional form

$$\psi(\xi) = A\,h(\xi)\,e^{-\xi^2/2}\ , \qquad \text{(III-95)}$$

where $h$ is some function of $\xi$ that contains the constant energy term $K$ and the coefficient $A$ is determined from the normalization condition. Since we insist that the wave function for a real wave be normalizable, then

$$\lim_{\xi\to\pm\infty}\left(h(\xi)\,e^{-\xi^2/2}\right)\to 0\ . \qquad \text{(III-96)}$$

**i)** Note that $h(\xi)$ must depend upon the energy term $K$ since the asymptotic form $A\,e^{-\xi^2/2}$ does not.

**ii)** Also note that since the asymptotic form is an even function, the $h(\xi)$ portion of the wave function will dictate the **parity** of the complete wave function $\Longrightarrow$ if $h(\xi)$ is an even function, then the wave function will have **even parity**, and if $h(\xi)$ is an odd function, then the wave function will have **odd parity**.

**d)** We now need to come up with the functional form of $h(\xi)$.

**i)** The first derivative of Eq. (III-95) is

$$\frac{d\psi}{d\xi}=A\left(\frac{dh}{d\xi}-\xi h\right)e^{-\xi^2/2}\ . \qquad \text{(III-97)}$$

**ii)** The second derivative is thus

$$\frac{d^2\psi}{d\xi^2}=A\left[\frac{d^2h}{d\xi^2}-2\xi\frac{dh}{d\xi}+(\xi^2-1)h\right]e^{-\xi^2/2}\ . \qquad \text{(III-98)}$$

**iii)** Using these derivatives in the Schrödinger equation (*e.g.*, Eq. III-91) gives

$$\frac{d^2h}{d\xi^2}-2\xi\frac{dh}{d\xi}+(K-1)h=0\ . \qquad \text{(III-99)}$$

**e)** Now, let's assume that $h(\xi)$ can be expressed as a power series

$$h(\xi)=a_0+a_1\xi+a_2\xi^2+\cdots=\sum_{j=0}^{\infty}a_j\xi^j\ . \qquad \text{(III-100)}$$

(Note that the '$a$' parameters here are *series coefficients* and not the raising and lowering operators we were discussing earlier.)

**i)** The first derivative of this series is

$$\frac{dh}{d\xi} = a_1 + 2a_2\xi + 3a_3\xi^2 + \cdots = \sum_{j=0}^{\infty} j a_j \xi^{j-1}. \tag{III-101}$$

**ii)** The second derivative is

$$\begin{aligned} \frac{d^2h}{d\xi^2} &= 2a_2 + 2\cdot 3a_3\xi + 3\cdot 4a_4\xi^2 + \cdots \\ &= \sum_{j=0}^{\infty} (j+1)(j+2)a_{j+2}\xi^j \ . \end{aligned} \tag{III-102}$$

**iii)** Putting these into Eq. (III-99), we find

$$\sum_{j=0}^{\infty} \left[(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j\right]\xi^j = 0 \ . \tag{III-103}$$

**iv)** It follows from the uniqueness of the power series expansion that the coefficient of each power of $\xi$ must vanish,

$$(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j = 0 \ ,$$

and hence that

$$a_{j+2} = \frac{(2j+1-K)}{(j+1)(j+2)} a_j \ . \tag{III-104}$$

**v)** This **recursion formula** is entirely equivalent to the Schrödinger equation itself. Given $a_0$ we can in principle derive $a_2, a_4, a_6, ...$, and given $a_1$ it generates $a_3, a_5, a_7, ....$

**f)** Let us therefore write

$$h(\xi) = h_e(\xi) + h_o(\xi) \ , \qquad \text{(III-105)}$$

where $h_e(\xi)$ are the even terms of the series expansion (*i.e.*, an *even* function):

$$h_e(\xi) \equiv a_0 + a_2\xi^2 + a_4\xi^4 + \cdots \qquad \text{(III-106)}$$

and $h_o(\xi)$ are the odd terms of the series expansion (*i.e.*, an *odd* function):

$$h_o(\xi) \equiv a_1\xi + a_3\xi^3 + a_5\xi^5 + \cdots \qquad \text{(III-107)}$$

**g)** Our next job is to figure out the functional form of the '$a$' coefficients. Essentially, we will guess at a form for $a_j$ and test it to see if it is consistent with Eqs. (III-91) and (III-99). But first, let's note the series expansions of exponential functions.

**i)** For the exponential function, we have

$$e^{\pm\xi} = 1 \pm \xi + \frac{1}{2!}\xi^2 \pm \frac{1}{3!}\xi^3 + \cdots = \sum_{j=0}^{\infty} b_j \xi^j, \quad \text{(III-108)}$$

where

$$b_j = (\pm 1)^j \, \frac{1}{j!} \ . \qquad \text{(III-109)}$$

**ii)** If we now substitute $\xi^2$ for $\xi$ in the above series expansion, we get

$$\begin{aligned} e^{\xi^2} &= 1 + \xi^2 + \frac{1}{2!}(\xi^2)^2 + \frac{1}{3!}(\xi^2)^3 + \frac{1}{4!}(\xi^2)^4 + \cdots \\ &= 1 + \xi^2 + \frac{1}{2}\xi^4 + \frac{1}{6}\xi^6 + \frac{1}{24}\xi^8 + \cdots \\ &= \sum_{\substack{j=0 \\ \text{(even)}}}^{\infty} b_j \xi^j, \end{aligned} \qquad \text{(III-110)}$$

where

$$b_j = \frac{1}{(j/2)!} \ . \qquad \text{(III-111)}$$

**iii)** We next ask if the series expansion above converges. To test this, we use the **d'Alembert ratio test** which takes the limit of the ratio of two successive terms as the counter goes to infinity:

$$\frac{b_{j+2}\xi^{j+2}}{b_j\xi^j} = \frac{\frac{1}{[(j+2)/2]!}\xi^{j+2}}{\frac{1}{(j/2)!}\xi^j} = \frac{1}{(j/2)+1}\xi^2 = \frac{2}{j+2}\xi^2 \ .$$

Now as taking the limit of this ratio as $j \to \infty$, we get

$$\lim_{j\to\infty} \frac{2}{j+2}\xi^2 \approx \lim_{j\to\infty} \frac{2}{j}\xi^2 \to 0 \ , \qquad \text{(III-112)}$$

thus this series converges.

**h)** We are now faced with a wave function solution to the Schrödinger equation of the form

$$\begin{aligned}\psi(\xi) &= A\,h(\xi)\,e^{-\xi^2/2} = A\left(\sum_{j=0}^{\infty} a_j\xi^j\right)e^{-\xi^2/2} \qquad \text{(III-113)}\\ &= \text{(infinite series in } \xi\text{) (decaying Gaussian).}\end{aligned}$$

**i)** For this wave function to be physically admissible, it must go to zero as $\xi \to \infty$. But does the infinite sum produce a finite number? Let's assume that our wave function has even parity. Then we will only look at $h_e(\xi)$ in this case. (We could make a similar argument for the $h_o(\xi)$ odd parity solution.)

**ii)** For very large $j$, we see from Eq. (III-104) that the recursion formula takes on the approximate form of

$$a_{j+2} \approx \frac{2}{j}a_j \ . \qquad \text{(III-114)}$$

**iii)** But what is $a_j$ when $j$ is large? Let us take the ratio of two successive terms and run the d'Alembert ratio test. Using Eq. (III-104), this ratio is

$$\frac{a_{j+2}\xi^{j+2}}{a_j\xi^j} = \frac{2j+1-K}{(j+2)(j+1)}\xi^2 \ .$$

Now as taking the limit of this ratio as $j \to \infty$, we get

$$\lim_{j\to\infty} \frac{2j+1-K}{(j+2)(j+1)}\xi^2 \approx \lim_{j\to\infty} \frac{2j}{j^2}\xi^2 = \lim_{j\to\infty} \frac{2}{j}\xi^2 \ , \qquad \text{(III-115)}$$

which is precisely the same limit for large $j$ as $e^{\xi^2}$! From this coincidence, we can make use of Eq. (III-111) to write that

$$a_j \approx \frac{C}{(j/2)!} \quad \text{(for even } j\text{)} \ , \qquad \text{(III-116)}$$

for some constant $C$ at large $j$.

**iv)** This yields (at large $\xi$, where the higher powers dominate)

$$h(\xi) \approx C \sum \frac{1}{(j/2)!}\xi^j \approx C \sum \frac{1}{k!}\xi^{2k} \approx Ce^{\xi^2}. \qquad \text{(III-117)}$$

**v)** If $h$ goes like $e^{\xi^2}$, then $\psi$ goes like $e^{\xi^2/2}$ (see Eq. III-113), which is precisely the asymptotic behavior we <u>don't</u> want!

**vi)** There is only one way out of this dilemma $\Longrightarrow$ *the power series must terminate*! There must occur some *highest* $j$ (call it $n = j_{\text{max}}$) such that $a_{n+2} = 0$.

**i)** We see from Eq. (III-104) that this will occur when

$$K = 2n + 1 \ , \qquad \text{(III-118)}$$

or using Eq. (II-90), we see that the *requirement that for $h(\xi)$ to be a finite polynomial, the energies of a simple harmonic oscillator are restricted* to the form

$$\begin{aligned} \frac{2E}{\hbar\omega} &= 2n+1 \\ E_n &= \frac{\hbar\omega}{2}(2n+1) \\ &= \left(n+\frac{1}{2}\right)\hbar\omega \quad n=0,1,2,\ldots \qquad \text{(III-119)} \end{aligned}$$

Hence we recover, by a completely different method, the fundamental quantization condition found in Eq. (III-78).

**j)** As a result of this, we see that for any energy not in the form of Eq. (III-119), the wave function of the simple harmonic oscillator blows up at large $\xi$ and the wave function is no longer un-normalizable, hence unphysical. From this we see that the boundary conditions demand **energy quantization**.

**k)** The recursion formula now reads

$$a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)} a_j \quad (j \leq n) \ . \qquad \text{(III-120)}$$

**i)** If $n=0$ (*i.e.*, the ground state), there is only one term in the series (we must pick $a_1 = 0$ to kill $h_o$, and $j=0$ in Eq. (III-120) yields $a_2 = 0$):

$$h_0(\xi) = a_0 \ , \qquad \text{(III-121)}$$

and hence

$$\psi_0(\xi) = A_0 \, a_0 \, e^{-\xi^2/2} \ , \qquad \text{(III-122)}$$

which reproduces Eq. (III-76).

**ii)** For $n=1$ we pick $a_0 = 0$, and Eq. (III-120) with $j=1$ yields $a_3 = 0$, so

$$h_1(\xi) = a_1 \xi \ , \qquad \text{(III-123)}$$

Table III–1: The first few Hermite polynomials, $H_n(x)$.

| | | |
|---|---|---|
| $H_0$ | = | $1$ |
| $H_1$ | = | $2x$ |
| $H_2$ | = | $4x^2 - 2$ |
| $H_3$ | = | $8x^3 - 12x$ |
| $H_4$ | = | $16x^4 - 48x^2 + 12$ |
| $H_5$ | = | $32x^5 - 160x^3 + 120x$ |

and hence

$$\psi_1(\xi) = A_1\, a_1\, \xi\, e^{-\xi^2/2} \qquad \text{(III-124)}$$

confirming Eq. (III-80).

**iii)** For $n = 2$, $j = 0$ yields $a_2 = -2a_0$, and $j = 2$ gives $a_4 = 0$, so

$$h_2(\xi) = a_0(1 - 2\xi^2) \qquad \text{(III-125)}$$

and

$$\psi_2(\xi) = A_2\, a_0\, (1 - 2\xi^2)\, e^{-\xi^2/2}\ , \qquad \text{(III-126)}$$

and so on.

**l)** $h_n(\xi)$ is thus a polynomial of degree $n$ in $\xi$, involving even powers only, if $n$ is an even integer, and odd powers only, if $n$ is an odd integer $\Longrightarrow$ **Hermite polynomials** (designated by $H_n(\xi)$) share these same characteristics (see Table III-1). **Note that in Hermite polynomials, the coefficient of the term with the maximum power is arbitrarily set to $2^n$.**

**m)** **Normalization**.

**i)** Finally, we need to figure out the functional form of the normalization constant $A_n$. We need to convert back to the $x$ label (from $\xi$, see Eq. III-86). To simplify matters, let

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}} \quad \text{so} \quad \xi = \beta\, x \qquad \text{(III-127)}$$

for the ground state.

**ii)** For the $n = 0$ ground state, normalization gives

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} \psi^* \psi \, dx \\ &= \int_{-\infty}^{\infty} A_0^2 e^{-\beta^2 x^2} \, dx \\ &= A_0^2 \sqrt{\frac{\pi}{\beta^2}} \\ A_0 &= \left(\frac{\beta^2}{\pi}\right)^{1/4} . \end{aligned} \qquad \text{(III-128)}$$

**iii)** We can continue this for some of the higher-order wave functions (I leave it to the students to do this on their own). We can compare these results to derive the following recursion relationship for the normalization constant:

$$A_n = \frac{1}{\sqrt{2^n n!}} A_0 = \frac{1}{\sqrt{2^n n!}} \left(\frac{\beta^2}{\pi}\right)^{1/4} . \qquad \text{(III-129)}$$

**iv)** With this, the normalized stationary states for the simple harmonic oscillator are

$$\psi_n(\xi) = \left(\frac{\beta^2}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2} , \qquad \text{(III-130)}$$

which is identical to Eq. (III-78).

**v)** Finally, we can write the complete wave equation by including the time dependence (*i.e.*, Eqs. III-10, III-119, III-129, and III-130) as

$$\boxed{\Psi_n(x,t) = \left[\left(\frac{\beta^2}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}}\right] H_n(\beta x)\, e^{-\beta^2 x^2/2} e^{-i(2n+1)\omega_0 t/2}\ ,} \tag{III-131}$$

where $\beta = \sqrt{m\omega_0/\hbar}$ (see Eq. III-127).

---

**Example III–4.** In the ground state of the harmonic oscillator, what is the probability (correct to 3 significant digits) of finding the particle outside the *classically* allowed region? *Hint:* Look in a math table under "Normal Distribution" or "Error Function."

**Solution:**

For the ground state, the wave function is

$$\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\xi^2/2}\ ,$$

so the probability is

$$P = 2\sqrt{\frac{m\omega}{\pi\hbar}} \int_{x_0}^{\infty} e^{-\xi^2}\, dx = 2\sqrt{\frac{m\omega}{\pi\hbar}}\sqrt{\frac{\hbar}{m\omega}} \int_{\xi_0}^{\infty} e^{-\xi^2}\, d\xi\ .$$

The classically allowed region extends out to: $\frac{1}{2}m\omega^2 x_0^2 = E_0 = \frac{1}{2}\hbar\omega$, or $x_0 = \sqrt{\hbar/m\omega}$, so $\xi_0 = 1$. Therefore,

$$P = \frac{2}{\sqrt{\pi}} \int_1^{\infty} e^{-\xi^2}\, d\xi = 2[1 - F(\sqrt{2})] = 0.157\ ,$$

where $F(z)$ is the notation used in the CRC Tables.

---

**Example III–5.** In this problem we explore some of the more useful theorems (stated without proof) involving Hermite polynomials.

(a) The **Rodrigues formula** states that

$$H_n(\xi) = (-1)^n e^{\xi^2} \left(\frac{d}{d\xi}\right)^n e^{-\xi^2}.$$

Use it to derive $H_3$ and $H_4$.

**(b)** The following recursion relation gives you $H_{n+1}$ in terms of the 2 preceding Hermite polynomials:

$$H_{n+1}(\xi) = 2\xi H_n(\xi) - 2nH_{n-1}(\xi) \ .$$

Use it, together with your answer to (a), to obtain $H_5$ and $H_6$.

**(c)** If you differentiate an $n$-th order polynomial, you get a polynomial of order $(n-1)$. For the Hermite polynomials, in fact:

$$\frac{dH_n}{d\xi} = 2nH_{n-1}(\xi) \ .$$

Check this by differentiating $H_5$ and $H_6$.

**(d)** $H_n(\xi)$ is the $n$-th $z$-derivative, at $z=0$, of the **generating function** $\exp(-z^2+2z\xi)$; or, to put it another way, it is the coefficient of $z^n/n!$ in the Taylor series expansion for the function:

$$e^{-z^2+2z\xi} = \sum_{n=0}^{\infty} \frac{z^n}{n!} H_n(\xi) \ .$$

Use this to rederive $H_0$, $H_1$, and $H_2$.

**Solution (a):**

$$\begin{aligned}
\frac{d}{d\xi}(e^{-\xi^2}) &= -2\xi e^{-\xi^2} \\
\left(\frac{d}{d\xi}\right)^2 e^{-\xi^2} &= \frac{d}{d\xi}(-2\xi e^{-\xi^2}) = (-2+4\xi^2)e^{-\xi^2} \\
\left(\frac{d}{d\xi}\right)^3 e^{-\xi^2} &= \frac{d}{d\xi}[(-2+4\xi^2)e^{-\xi^2}] = [8\xi + (-2+4\xi^2)(-2\xi)]e^{-\xi^2} \\
&= (12\xi - 8\xi^3)e^{-\xi^2} \\
\left(\frac{d}{d\xi}\right)^4 e^{-\xi^2} &= \frac{d}{d\xi}[(12\xi - 8\xi^3)e^{-\xi^2}] \\
&= [12 - 24\xi^2 + (12\xi - 8\xi^3)(-2\xi)]e^{-\xi^2} \\
&= (12 - 48\,\xi^2 + 16\,\xi^4)e^{-\xi^2} \\
H_3(\xi) &= -e^{\xi^2}\left(\frac{d}{d\xi}\right)^3 e^{-\xi^2} = \boxed{-12\xi + 8\xi^3}
\end{aligned}$$

$$H_4(\xi) \;=\; -e^{\xi^2}\left(\frac{d}{d\xi}\right)^4 e^{-\xi^2} = \boxed{12 - 48\,\xi^2 + 16\,\xi^4\ .}$$

**Solution (b):**

$$\begin{aligned}
H_5(\xi) &= 2\xi H_4 - 8H_3 = 2\xi(12 - 48\,\xi^2 + 16\,\xi^4) - 8(-12\xi + 8\xi^3) \\
&= \boxed{120\xi - 160\xi^3 + 32\xi^5} \\
H_6(\xi) &= 2\xi H_5 - 10H_4 \\
&= 2\xi(120\xi - 160\xi^3 + 32\xi^5) - 10(12 - 48\,\xi^2 + 16\,\xi^4) \\
&= \boxed{-120 + 720\xi^2 - 480\xi^4 + 64\xi^6\ .}
\end{aligned}$$

**Solution (c):**

$$\begin{aligned}
\frac{dH_5}{d\xi} &= 120 - 480\xi^2 + 160\xi^4 = 10(12 - 48\xi^2 + 16\xi^4) \\
&= (2)(5)H_4 \quad \surd \\
\frac{dH_6}{d\xi} &= 1440\xi - 1920\xi^3 + 384\xi^5 = 12(120\xi - 160\xi^3 + 32\xi^5) \\
&= (2)(6)H_5\ . \quad \surd
\end{aligned}$$

**Solution (d):**

$$\frac{d}{dz}(e^{-z^2+2z\xi}) = (-2z + 2\xi)e^{-z^2+2z\xi};$$

putting in $z = 0$ gives

$$\boxed{H_0(\xi) = 2\xi\ .}$$

$$\left(\frac{d}{dz}\right)^2 (e^{-z^2+2z\xi}) = \frac{d}{dz}[(-2z + 2\xi)e^{-z^2+2z\xi}] = [-2 + (-2z + 2\xi)^2]e^{-z^2+2z\xi};$$

putting in $z = 0$ gives

$$\boxed{H_1(\xi) = -2 + 4\xi^2\ .}$$

$$\begin{aligned}
\left(\frac{d}{dz}\right)^3 (e^{-z^2+2z\xi}) &= \frac{d}{dz}\{[-2 + (-2z + 2\xi)^2]e^{-z^2+2z\xi}\} \\
&= \{2(-2z + 2\xi)(-2) + \\
&\quad [-2 + (-2z + 2\xi)^2](-2z + 2\xi)\}e^{-z^2+2z\xi}\ ;
\end{aligned}$$

putting in $z = 0$ gives

$$H_2(\xi) = -8\xi + (-2 + 4\xi^2)(2\xi) = \boxed{-12\xi + 8\xi^3\ .}$$

---

## F. The Free Particle

**1.** A **free particle** is simply one where $V(x) = 0$ for all $x$. The time-independent Schrödinger equation (TISE) becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi\ , \tag{III-132}$$

or

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \qquad \text{where } k \equiv \frac{\sqrt{2mE}}{\hbar}\ . \tag{III-133}$$

**a)** Instead of using sines and cosines, we will express the solution in exponential notation:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}\ . \tag{III-134}$$

**b)** Since there are no boundary conditions, $k$ (hence $E$) can take on *any* positive value $\Longrightarrow$ a **continuum** of possible energies.

**c)** Taking on the standard time dependence gives

$$\Psi(x,t) = Ae^{ik(x-\frac{\hbar k}{2m}t)} + Be^{-ik(x+\frac{\hbar k}{2m}t)}. \tag{III-135}$$

**2.** Any function of $x$ and $t$ that depends upon these variables in the special combination $(x \pm vt)$ (for some constant $v$) represents a wave of fixed profile, traveling in the $\mp x$-direction, at speed $v$.

**a)** As such, the first term in Eq. (III-135) represents a wave traveling to the *right*.

**b)** The second term, a wave traveling to the *left*.

**c)** Since the only difference between the 2 terms in Eq. (III-135) is the sign of $k$, we can write

$$\Psi_k(x,t) = A e^{ik(x - \frac{\hbar k}{2m} t)} , \tag{III-136}$$

and let $k$ run negative (as well as positive) to cover the case of waves traveling to the left:

$$k \equiv \pm \frac{\sqrt{2mE}}{\hbar}, \quad \text{with} \begin{cases} k > 0 \implies \text{traveling to the right,} \\ k < 0 \implies \text{traveling to the left.} \end{cases} \tag{III-137}$$

**3.** The speed of the wave is

$$v_{\text{quantum}} = \frac{\hbar |k|}{2m} = \sqrt{\frac{E}{2m}} . \tag{III-138}$$

**a)** On the other hand, the *classical* speed of a free particle with energy $E$ is given by $E = (1/2)mv^2$ (pure kinetic since $V = 0$), so

$$v_{\text{classical}} = \sqrt{\frac{2E}{m}} = 2 v_{\text{quantum}} . \tag{III-139}$$

**b)** The quantum mechanical wave function travels a *half* the speed of the particle it is suppose to represent!

**c)** *This wave function is <u>not</u> normalizable!* $\Longrightarrow$ in other words, there is no such thing as a free particle with a definite energy.

**4.** The general solution to the TISE is still a linear combination of separable solutions (only this time, it's an integral over the continuous variable $k$, instead of a sum over the discrete index $n$):

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m} t)} \, dk \ .} \tag{III-140}$$

**a)** Now *this* wave function *can* be normalized [for appropriate $\phi(k)$], but it necessarily carries a *range* of $k$'s, and hence a range of energies and speeds.

**b)** As such, this is called a **wave packet**.

**c)** The initial wave function is thus

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{ikx} \, dk \ . \tag{III-141}$$

**5.** This is a classic problem of Fourier analysis (see §III.C); the answer is provided by **Plancherel's theorem**:

$$\boxed{f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k) e^{ikx} \, dk \Longleftrightarrow F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-ikx} \, dx \ .} \tag{III-142}$$

**a)** $F(k)$ is called the **Fourier transform** of $f(x)$.

**b)** $f(x)$ is called the **inverse Fourier transform** of $F(k)$.

**c)** The necessary and sufficient condition on $f(x)$ is that $\int_{-\infty}^{+\infty} |f(x)|^2 \, dx$ be finite.

**6.** The solution to the generic, free-particle quantum problem is thus

$$\boxed{\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,0) e^{-ikx} \, dx \ .} \tag{III-143}$$

**a)** A wave packet is a sinusoidal function whose amplitude is modulated by $\phi$ (Figure III-3); it consists of *ripples* contained within an *envelope*.

**b)** What corresponds to the particle velocity is not the speed of the individual ripples (the so-called **phase velocity**), but rather the speed of the envelope (the **group velocity**)

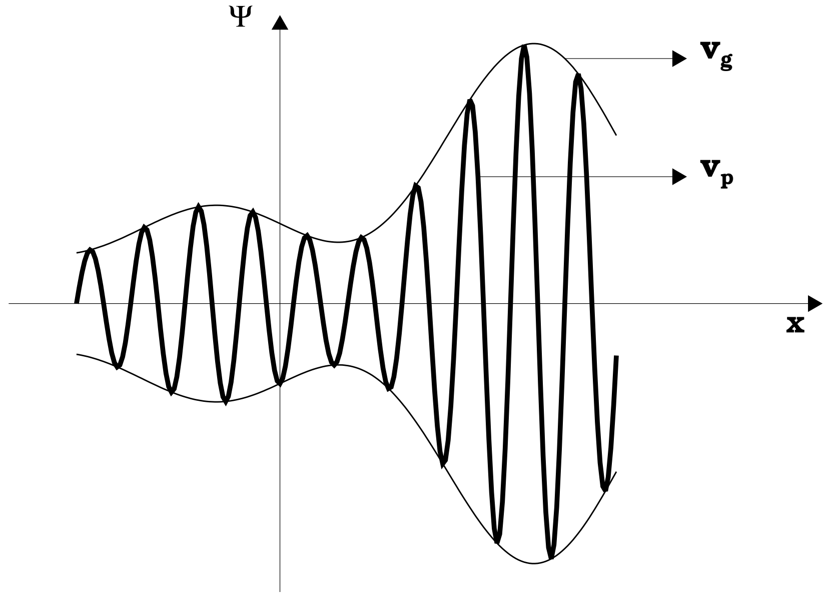



Figure III–3: A wave packet. The *envelope* travels at the group velocity; the *ripples* travel at the phase velocity.

— which, depending upon the nature of the waves, can be greater than, less than, or equal to the velocity of the ripples that go to make it up.

**c)** For a free particle in quantum mechanics, the group velocity is *twice* the phase velocity as shown in Eq. (III-139).

**7.** But what are the respective group and phase velocities of the wave packet with the general form

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{i(kx-\omega t)}\, dk \ ? \qquad \text{(III-144)}$$

**a)** Here the **dispersion relation**, that is, the formula for $\omega$ as a function of $k$, is $\omega = (\hbar k^2/2m)$.

**b)** The amplitude function $\phi(k)$ insures that the integrand in Eq. (III-144) is negligible except in the vicinity of $k_\circ$ (the position in $k$-space of the peak value of $\phi(k)$). As such, we can Taylor expand:

$$\omega(k) \cong \omega_\circ + \omega'_\circ(k - k_\circ) \ , \tag{III-145}$$

where $\omega'_\circ$ is the derivative of $\omega$ with respect to $k$ at point $k_\circ$.

**c)** Let $s \equiv k - k_\circ$, then

$$\Psi(x,t) \cong \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_\circ + s)\, e^{i[(k_\circ+s)x-(\omega_\circ+\omega'_\circ s)t]}\, ds \ . \tag{III-146}$$

**d)** At $t = 0$,

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_\circ + s)\, e^{i(k_\circ+s)x}\, ds \tag{III-147}$$

and at later times

$$\Psi(x,t) \cong \frac{1}{\sqrt{2\pi}} e^{i(-\omega_\circ t + k_\circ \omega'_\circ t)} \int_{-\infty}^{+\infty} \phi(k_\circ + s)\, e^{i(k_\circ+s)(x-\omega'_\circ t)}\, ds \ . \tag{III-148}$$

**e)** Except for the shift from $x$ to $(x - \omega'_\circ t)$, this last integral is the same as the one for $\Psi(x,0)$, thus

$$\Psi(x,t) \cong e^{i(-\omega_\circ t + k_\circ \omega'_\circ t)}\ \Psi(x - \omega'_\circ t, 0) \ . \tag{III-149}$$

**f)** Apart from the phase factor in front (which won't affect $|\Psi|^2$ in any event), the wave packet moves along at speed

$$v_{\text{group}} = \left.\frac{d\omega}{dk}\right|_{k_\circ} = \frac{\hbar k}{m} \ , \tag{III-150}$$

which is contrasted with the ordinary phase velocity

$$v_{\text{phase}} = \frac{\omega}{k} = \frac{\hbar k}{2m} \ . \tag{III-151}$$

**g)** Hence, the group velocity is twice as great as the phase velocity:

$$v_{\text{classical}} = v_{\text{group}} = 2 v_{\text{phase}}. \tag{III-152}$$

**Example III–6.** A free particle has the initial wave function

$$\Psi(x,0) = Ae^{-ax^2} \ ,$$

where $A$ and $a$ are constants ($a$ is real and positive).

**(a)** Normalize $\Psi(x,0)$.

**(b)** Show that $\Psi(x,t)$ can be written in the form

$$\Psi(x,t) = \left(\frac{2a}{\pi}\right)^{1/4} \frac{e^{-ax^2/[1+(2i\hbar at/m)]}}{\sqrt{1+(2i\hbar at/m)}} \ .$$

*Hint*: Integrals of the form

$$\int_{-\infty}^{+\infty} e^{-(ax^2+bx)}\, dx$$

can be handled by "completing the square." Let $y \equiv \sqrt{a}\,[x + (b/2a)]$, and note that $(ax^2 + bx) \equiv y^2 - (b^2/4a)$.

**(c)** Find $|\Psi(x,t)|^2$. Express your answer in terms of the quantity $w \equiv \sqrt{a/[1 + (2\hbar at/m)^2}$. Sketch $|\Psi|^2$ (as a function of $x$) at $t = 0$, and again for some very large $t$. Qualitatively, what happens to $|\Psi|^2$ as time goes on?

**(d)** Find $\langle x\rangle$, $\langle p\rangle$, $\langle x^2\rangle$, $\langle p^2\rangle$, $\sigma_x$, and $\sigma_p$. *Hint*: You will need to show that $\langle p^2\rangle = a\hbar^2$, but it may take some algebra to reduce it to this simple form.

**(e)** Does the uncertainty principle hold? At what time $t$ does the system come closest to the uncertainty limit?

**Solution (a):**

$$1 = |A|^2 \int_{\infty}^{+\infty} e^{-2ax^2}\, dx = |A|^2 \sqrt{\frac{\pi}{2a}}$$

or

$$\boxed{A = \left(\frac{2a}{\pi}\right)^{1/4} \ .}$$

**Solution (b):**

Using Eq. (III-143), we can write

$$\phi(k) = \frac{1}{\sqrt{2\pi}} A \int_{-\infty}^{+\infty} e^{-ax^2} e^{-ikx}\, dx = \frac{1}{\sqrt{2\pi}} A \int_{-\infty}^{+\infty} e^{-(ax^2+ikx)}\, dx \ .$$

Using the substitution variables in the question (*i.e.*, $y$ from the last page and let $b = ik$), the integral above as the functional form

$$\begin{aligned} \int_{-\infty}^{+\infty} e^{-(ax^2+bx)}\, dx &= \int_{-\infty}^{+\infty} e^{-y^2+(b^2/4a)} \frac{1}{\sqrt{a}}\, dy \\ &= \frac{1}{\sqrt{a}} e^{b^2/4a} \int_{-\infty}^{+\infty} e^{-y^2}\, dy = \sqrt{\frac{\pi}{a}} e^{b^2/4a} \ . \quad \textbf{(A)} \end{aligned}$$

So,

$$\begin{aligned} \phi(k) &= \frac{1}{\sqrt{2\pi}} \left(\frac{2a}{\pi}\right)^{1/4} \sqrt{\frac{\pi}{a}} e^{-k^2/4a} \\ &= \frac{1}{(2\pi a)^{1/4}}\, e^{-k^2/4a} \ . \end{aligned}$$

Now using $\phi(k)$ in Eq. (III-140), we can solve for $\Psi$,

$$\begin{aligned} \Psi(x,t) &= \frac{1}{\sqrt{2\pi}} \frac{1}{(2\pi a)^{1/4}} \int_{-\infty}^{+\infty} e^{-k^2/4a}\, e^{i(kx-\hbar k^2 t/2m)}\, dk \\ &= \frac{1}{\sqrt{2\pi}} \frac{1}{(2\pi a)^{1/4}} \int_{-\infty}^{+\infty} e^{-\frac{k^2}{4a}+ixk-\frac{i\hbar k^2 t}{2m}}\, dk \\ &= \frac{1}{\sqrt{2\pi}} \frac{1}{(2\pi a)^{1/4}} \int_{-\infty}^{+\infty} e^{-[k^2(\frac{1}{4a}+\frac{i\hbar t}{2m})-ixk]}\, dk \ . \end{aligned}$$

At this point, let

$$\beta = \left(\frac{1}{4a} + \frac{i\hbar t}{2m}\right) \quad \text{and} \quad \gamma = -ix \ .$$

Then making use of Eq. (A) above, the integral in the equation above becomes

$$\int_{-\infty}^{+\infty} e^{-[k^2(\frac{1}{4a}+\frac{i\hbar t}{2m})-ixk]}\, dk = \int_{-\infty}^{+\infty} e^{-(\beta k^2+\gamma k)}\, dk$$

$$= \sqrt{\frac{\pi}{\beta}}\, e^{\gamma^2/4\beta}$$

$$= \frac{\sqrt{\pi}}{\sqrt{\frac{1}{4a} + \frac{i\hbar t}{2m}}}\, e^{-x^2/4(\frac{1}{4a}+\frac{i\hbar t}{2m})} \;.$$

Substituting this integral solution into the equation for $\Psi$ above, we get

$$\Psi(x,t) \;=\; \frac{1}{\sqrt{2\pi}(2\pi a)^{1/4}} \frac{\sqrt{\pi}}{\sqrt{\frac{1}{4a} + \frac{i\hbar t}{2m}}}\, e^{-x^2/4(\frac{1}{4a}+\frac{i\hbar t}{2m})}$$

$$= \boxed{\left(\frac{2a}{\pi}\right)^{1/4} \frac{e^{-ax^2/(1+2i\hbar at/m)}}{\sqrt{1+2i\hbar at/m}}\;.}$$

**Solution (c):** Let $\theta = 2\hbar at/m$, then

$$|\Psi|^2 = \sqrt{\frac{2a}{\pi}}\, \frac{e^{-ax^2/(1+i\theta)}\, e^{-ax^2/(1-i\theta)}}{\sqrt{(1+i\theta)(1-i\theta)}} \;.$$

The exponent is

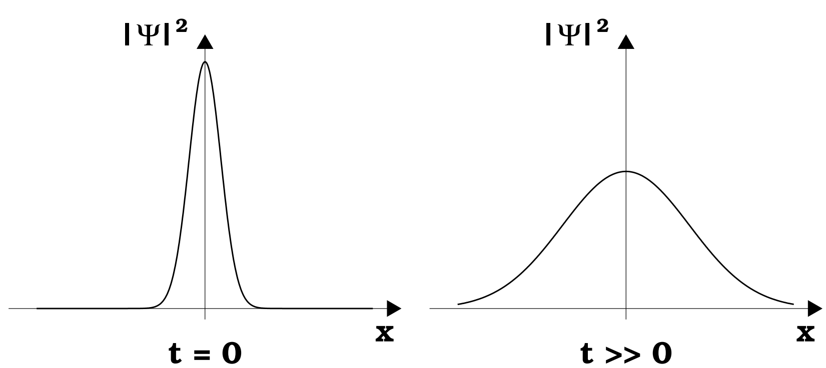
$$-\frac{ax^2}{(1+i\theta)} - \frac{ax^2}{(1-i\theta)} = -ax^2 \frac{(1-i\theta+1+i\theta)}{(1+i\theta)(1-i\theta)} = \frac{-2ax^2}{1+\theta^2} \;,$$

and

$$|\Psi|^2 = \sqrt{\frac{2a}{\pi}}\, \frac{e^{-2ax^2/(1+\theta^2)}}{\sqrt{(1+\theta^2)}} \;.$$

Or, with $w \equiv \sqrt{\frac{a}{1+\theta^2}}$, we get

$$\boxed{|\Psi|^2 = \sqrt{\frac{2}{\pi}}\, w\, e^{-2w^2x^2} \;.}$$




As $t$ increases, the graph of $|\Psi|^2$ flattens out and broadens, as can be seen by examining $w$ (*i.e.*, proportional to the peak of the probability) as $t \gg 0$,

$$\begin{aligned} w &= \sqrt{\frac{a}{1+\theta^2}} = \sqrt{\frac{a}{1+(2\hbar a t/m)^2}} \\ &\approx \sqrt{\frac{a}{(2\hbar a t/m)^2}} = \sqrt{\frac{m^2}{4\hbar^2 a t^2}} = \frac{m}{2\hbar t\sqrt{a}} \ . \end{aligned}$$

As $t$ gets very large, $w$ goes to zero.

**Solution (d):**

$$\begin{aligned} \langle x \rangle &= \int_{-\infty}^{+\infty} x\,|\Psi|^2\,dx = \int_{-\infty}^{+\infty} x\sqrt{\frac{2}{\pi}}\,w\,e^{-2w^2x^2}\,dx = \boxed{0} \quad \text{(odd integrand)} \\ \langle p \rangle &= m\,\frac{d\langle x\rangle}{dt} = \boxed{0} \\ \langle x^2 \rangle &= \sqrt{\frac{2}{\pi}}\,w\int_{-\infty}^{+\infty} x^2 e^{-2w^2x^2}\,dx = \sqrt{\frac{2}{\pi}}\,w\,\frac{1}{4w^2}\sqrt{\frac{\pi}{2w^2}} = \boxed{\frac{1}{4w^2}} \\ \langle p^2 \rangle &= -\hbar^2\int_{-\infty}^{+\infty} \Psi^*\frac{d^2\Psi}{dx^2}\,dx \ . \end{aligned}$$

Write $\Psi = Be^{-bx^2}$, where $B \equiv \left(\frac{2a}{\pi}\right)^{1/4}\frac{1}{\sqrt{1+i\theta}}$ and $b \equiv \frac{a}{1+i\theta}$. Then

$$\begin{aligned} \frac{d^2\Psi}{dx^2} &= B\frac{d}{dx}(-2bxe^{-bx^2}) = -2bB(1-2bx^2)\,e^{-bx^2} \\ \Psi^*\frac{d^2\Psi}{dx^2} &= -2b|B|^2(1-2bx^2)\,e^{-(b+b^*)x^2}; \\ b+b^* &= \frac{a}{1+i\theta}+\frac{a}{1-i\theta} = \frac{2a}{1+\theta^2} = 2w^2 \ . \\ |B|^2 &= \sqrt{\frac{2a}{\pi}}\,\frac{1}{\sqrt{1+\theta^2}} = \sqrt{\frac{2}{\pi}}\,w \ . \end{aligned}$$

So

$$\begin{aligned} \Psi^*\frac{d^2\Psi}{dx^2} &= -2b\sqrt{\frac{2}{\pi}}\,w\,(1-2bx^2)\,e^{-2w^2x^2} \\ \langle p^2 \rangle &= 2b\hbar^2\sqrt{\frac{2}{\pi}}\,w\int_{-\infty}^{+\infty}(1-2bx^2)\,e^{-2w^2x^2}\,dx \end{aligned}$$

$$
\begin{aligned}
&= 2b\hbar^2\sqrt{\frac{2}{\pi}}\,w\left\{\sqrt{\frac{\pi}{2w^2}} - 2b\,\frac{1}{4w^2}\sqrt{\frac{\pi}{2w^2}}\right\} \\
&= 2b\hbar^2\left(1 - \frac{b}{2w^2}\right) \ .
\end{aligned}
$$

But

$$
\begin{aligned}
1 - \frac{b}{2w^2} &= 1 - \left(\frac{a}{1+i\theta}\right)\left(\frac{1+\theta^2}{2a}\right) \\
&= 1 - \frac{1-i\theta}{2} = \frac{1+i\theta}{2} = \frac{a}{2b} \ ,
\end{aligned}
$$

so

$$
\langle p^2\rangle = 2b\hbar^2\frac{a}{2b} = \boxed{\hbar^2 a \ .}
$$

The uncertainty for $x$ and $p$ is thus

$$
\sigma_x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \boxed{\frac{1}{2w} \ ;}
$$

and

$$
\sigma_p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \boxed{\hbar\sqrt{a} \ .}
$$

**Solution (e):**

$$
\begin{aligned}
\sigma_x\,\sigma_p &= \frac{1}{2w}\,\hbar\sqrt{a} = \frac{\hbar}{2}\sqrt{1+\theta^2} \\
&= \frac{\hbar}{2}\sqrt{1 + \left(\frac{2\hbar a t}{m}\right)^2} \geq \frac{\hbar}{2} \ . \quad \checkmark
\end{aligned}
$$

The closest that this system gets to the Heisenberg uncertainty limit occurs at $\boxed{t = 0}$, at which time it is right <u>at</u> the uncertainty limit.

---

## G. The Delta-Function Potential.

**1.** In *classical* mechanics, there are two distinct states associated with a particle in a potential field:

a) **Bound state**: The particle is *stuck* in the potential well and oscillates back and forth between the **turning points** (a, b) where $E = V(a) = V(b)$, $E > V(x), a < x < b$, and $E < V(x)$, for $x < a$, and $x > b$ (*e.g.*, harmonic oscillator).

b) **Scattering state**: $E > V(x)$ on one side of a given point and $E < V(x)$ on the other side. Then, a particle approaches the turning point where $E = V$ from infinity, then bounces and returns to infinity.

c) Some potential fields permit both of kinds states.

**2.** We have just derived the *quantum* mechanics analogies to these two states:

a) A linear combination (*i.e.*, summation) of normalizable, stationary states of *specific* energy $E_n$ (*i.e.*, infinite potential well, harmonic oscillators) $\Longrightarrow$ **bound states**.

b) An integral over non-normalizable, continuous values of $k$-states (*i.e.*, free particles) $\Longrightarrow$ **scattering states**.

c) Because of the quantum effect of **tunneling** (see below), allows a *bound* particle to "leak" through a finite potential barrier, the type of state a particle is actually in is only a function of the potential at infinity:

$$\begin{cases} E < V(-\infty) \text{ and } V(+\infty) & \Longrightarrow \text{ bound state} \\ E > V(-\infty) \text{ or } V(+\infty) & \Longrightarrow \text{ scattering state} \end{cases} \tag{III-153}$$

d) Since most potentials in physics go to zero at infinity, the criterion is simplified even further:

$$\begin{cases} E < 0 & \Longrightarrow \text{ bound state} \\ E > 0 & \Longrightarrow \text{ scattering state} \end{cases} \tag{III-154}$$

e) Because the infinite potential well and harmonic oscillator potentials go to infinity as $x \to \pm\infty$, they admit only bound states.

f) Because the free particle potential is zero everywhere, it allows only scattering states.

3. The **Dirac delta function**, $\delta(x)$, gives rise to both kinds of states and is informally defined as

$$\delta(x) = \left\{ \begin{array}{ll} 0, & \text{if } x \neq 0 \\ \infty & \text{if } x = 0 \end{array} \right\}, \text{ with } \int_{-\infty}^{+\infty} \delta(x)\, dx = 1. \qquad \text{(III-155)}$$

It is an infinitely high, infinitesimally narrow spike at the origin, whose *area* is 1.

a) Technically, it is not a function at all, since it is not finite at $x = 0$ (mathematicians call it a **generalized function**, or **distribution**).

b) It can be thought of as the *limit* of a *sequence* of functions, such as rectangles (or triangles) of ever-increasing height and ever-decreasing width.

c) It is an extremely useful construct in theoretical physics $\Longrightarrow$ in electrodynamics, the charge density of a point charge is a delta function.

d) Notice that $\delta(x - a)$ would be a spike of area 1 at the point $a$.

e) The delta function interacts with other functions as follows:

$$f(x)\,\delta(x - a) = f(a)\,\delta(x - a), \qquad \text{(III-156)}$$

because the product is zero anyway except at point $a$. In particular,

$$\int_{-\infty}^{+\infty} f(x)\,\delta(x-a)\,dx = f(a)\int_{-\infty}^{+\infty}\delta(x-a)\,dx = f(a). \qquad \text{(III-157)}$$

Under the integral sign, the delta function serves to *pick out* the value of $f(x)$ at the point $a$.

**4.** Let's consider the potential of the form

$$V(x) = -\alpha\delta(x), \qquad \text{(III-158)}$$

where $\alpha$ is some constant. The TISE then is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha\delta(x)\psi = E\psi. \qquad \text{(III-159)}$$

**a)** This potential yields both bound states ($E < 0$) and scattering states ($E > 0$).

**b)** In the region $x < 0, V(x) = 0$, so

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = \kappa^2\psi, \qquad \text{(III-160)}$$

where

$$\kappa \equiv \frac{\sqrt{-2mE}}{\hbar} \quad (E < 0). \qquad \text{(III-161)}$$

**c)** The solution to Eq. (III-160) is

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x}, \qquad \text{(III-162)}$$

but the first term blows up as $x \to -\infty$, so $A$ must be zero:

$$\psi(x) = Be^{\kappa x} \quad (x < 0). \qquad \text{(III-163)}$$

**d)** For $x > 0, V(x) = 0$ once again and from the same logic above (except now $\psi(x)$ blows up as $x \to +\infty$), we get

$$\psi(x) = Fe^{-\kappa x} \quad (x > 0). \qquad \text{(III-164)}$$

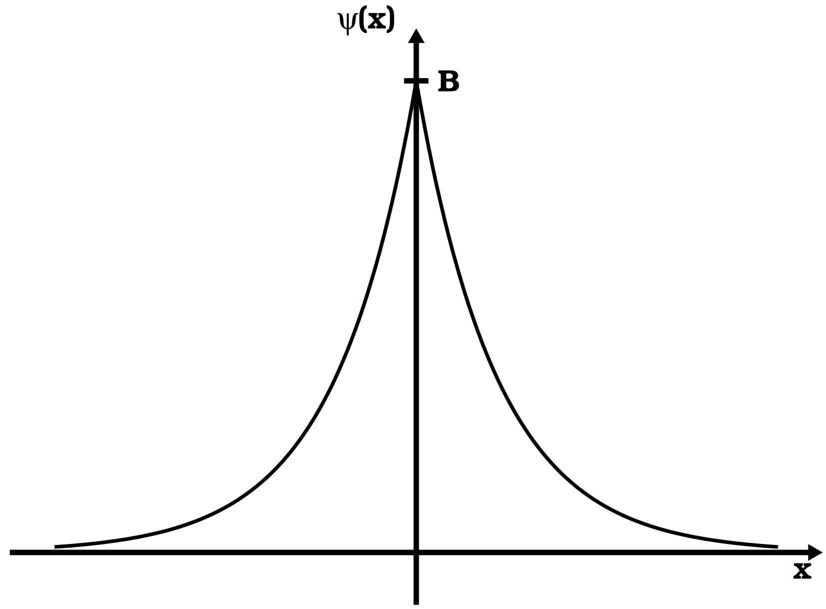



Figure III–4: The wave function for a $\delta$ function potential.

**e)** We now use the **standard boundary conditions** for $\psi$:

$$\boxed{\left\{\begin{array}{ll} 1. & \psi \text{ is always continuous, and} \\ 2. & d\psi/dx \text{ is continuous except at points} \\ & \text{where the potential is infinite.} \end{array}\right.} \quad \text{(III-165)}$$

**f)** In this case, the first boundary condition tells us that $B = F$, so

$$\psi(x) = \begin{cases} Be^{\kappa x} & (x \leq 0), \\ Be^{-\kappa x} & (x \geq 0). \end{cases} \quad \text{(III-166)}$$

The 2nd boundary condition tells us nothing in this case.

**g)** This solution for the wave function has a discontinuity in the derivative at $x = 0$ as shown in Figure III-4. The $\delta$ function must determine the discontinuity in the derivative of $\psi$ at $x = 0$.

**i)** First, integrate the TISE from $-\epsilon$ to $\epsilon$, then take the limit as $\epsilon \to 0$:

$$-\frac{\hbar^2}{2m} \int_{-\epsilon}^{\epsilon} \frac{d^2\psi}{dx^2}\, dx + \int_{-\epsilon}^{\epsilon} V(x)\, \psi(x)\, dx = E \int_{-\epsilon}^{\epsilon} \psi(x)\, dx \; . \quad \text{(III-167)}$$

The first term in this equation can be rewritten as

$$\begin{aligned}\int_{-\epsilon}^{\epsilon} \frac{d^2\psi}{dx^2}\,dx &= \int_{-\epsilon}^{\epsilon} \frac{d}{dx}\left(\frac{d\psi}{dx}\right)\,dx = \int_{-\epsilon}^{\epsilon} d\left(\frac{d\psi}{dx}\right) \\ &= \left.\frac{d\psi}{dx}\right|_{-\epsilon}^{\epsilon} = \Delta\left(\frac{d\psi}{dx}\right) \; . \qquad \text{(III-168)}\end{aligned}$$

The integral on the RHS of the TISE equation above is zero,

$$\lim_{\epsilon\to 0} \int_{-\epsilon}^{\epsilon} \psi(x)\,dx = 0 \; , \qquad \text{(III-169)}$$

since this integral is the area of a *sliver* with vanishing width and finite height. As such under these circumstances, Eq. (III-167) becomes

$$\Delta\left(\frac{d\psi}{dx}\right) = \frac{2m}{\hbar^2} \lim_{\epsilon\to 0} \int_{-\epsilon}^{\epsilon} V(x)\,\psi(x)\,dx \; . \qquad \text{(III-170)}$$

**ii)** The potential energy integral on the RHS of Eq. (III-170) can be determined with the help of Eqs. (III-157) and (III-158):

$$\begin{aligned}\int_{-\epsilon}^{\epsilon} V(x)\,\psi(x)\,dx &= \int_{-\epsilon}^{\epsilon} \left[-\alpha\delta(x)\right]\,\psi(x)\,dx \\ &= -\alpha \int_{-\epsilon}^{\epsilon} \delta(x)\psi(x)\,dx \\ &= -\alpha\,\psi(0) \; , \qquad \text{(III-171)}\end{aligned}$$

which is independent of $\epsilon$, hence taking the limit will not change the form of this solution.

**iii)** We next need to take the derivative of Eq. (III-166):

$$\frac{d\psi}{dx} = \begin{cases} B\kappa e^{\kappa x} & (x < 0), \\ -B\kappa e^{-\kappa x} & (x > 0). \end{cases} \qquad \text{(III-172)}$$

So, if we let these derivatives get infinitesimally close to $x = 0$, we see that

$$\begin{aligned}(d\psi/dx)|_+ &= -B\kappa \\ (d\psi/dx)|_- &= +B\kappa \; , \end{aligned} \qquad \text{(III-173)}$$

hence

$$\Delta\left(\frac{d\psi}{dx}\right) = \left(\frac{d\psi}{dx}\right)\Big|_{+} - \left(\frac{d\psi}{dx}\right)\Big|_{-} = -2B\kappa \ . \quad \text{(III-174)}$$

**iv)** Meanwhile $\psi(0) = B$, so using Eqs. (III-171) and (III-174) in Eq. (III-170) gives

$$-2B\kappa = -\frac{2m}{\hbar^2}\,\alpha B$$

or

$$\kappa = \frac{m\alpha}{\hbar^2} \ , \qquad \text{(III-175)}$$

which gives an energy (via Eq. III-161) of

$$E = -\frac{\hbar^2\kappa^2}{2m} = -\frac{m\alpha^2}{2\hbar^2} \ . \qquad \text{(III-176)}$$

**h)** Finally, normalizing $\psi$ gives:

$$\int_{-\infty}^{+\infty} |\psi(x)|^2\,dx = 2|B|^2 \int_0^{\infty} e^{-2\kappa x}\,dx = \frac{|B|^2}{\kappa} = 1 \ , \qquad \text{(III-177)}$$

or

$$B = \sqrt{\kappa} = \frac{\sqrt{m\alpha}}{\hbar} \ . \qquad \text{(III-178)}$$

**i)** Hence, the delta-function well, regardless of its *strength* $\alpha$, has exactly one bound state:

$$\boxed{\psi(x) = \frac{\sqrt{m\alpha}}{\hbar}\,e^{-m\alpha|x|/\hbar^2}; \qquad E = -\frac{m\alpha^2}{2\hbar^2} \ .} \qquad \text{(III-179)}$$

**5.** For scattering states with $E > 0$ and $x < 0$, the TISE reads

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\,\psi = -k^2\psi \ , \qquad \text{(III-180)}$$

where

$$k \equiv \frac{\sqrt{2mE}}{\hbar} \quad (E > 0). \qquad \text{(III-181)}$$

**a)** The solution to Eq. (III-180) is

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad (x < 0), \tag{III-182}$$

which is a trigonometric function $\Longrightarrow$ neither term blows up.

**b)** Similarly for $x > 0$,

$$\psi(x) = Fe^{ikx} + Ge^{-ikx} \quad (x > 0). \tag{III-183}$$

**c)** Continuity of $\psi(x)$ at $x = 0$ requires that

$$F + G = A + B \ . \tag{III-184}$$

**d)** The derivatives are

$$\begin{aligned} \frac{d\psi}{dx} &= ik\left(Fe^{ikx} - Ge^{-ikx}\right), \quad \text{for } (x > 0) \\ \frac{d\psi}{dx} &= ik\left(Ae^{ikx} - Be^{-ikx}\right), \quad \text{for } (x < 0). \end{aligned} \tag{III-185}$$

Let $x \longrightarrow 0$ on either side of zero, then

$$\begin{aligned} \frac{d\psi}{dx}|_{+} &= ik(F - G) \\ \frac{d\psi}{dx}|_{-} &= ik(A - B) \ , \end{aligned} \tag{III-186}$$

and hence $\Delta(d\psi/dx) = ik(F - G - A + B)$.

**e)** Meanwhile, $\psi(0) = (A + B)$, so the second boundary condition says

$$ik(F - G - A + B) = -\frac{2m\alpha}{\hbar^2}(A + B) \ , \tag{III-187}$$

or more compactly

$$F - G = A(1 + 2i\beta) - B(1 - 2i\beta), \quad \text{where } \beta \equiv \frac{m\alpha}{\hbar^2 k} \ . \tag{III-188}$$

**f)** Having imposed the boundary conditions, we are left with 2 equations (*i.e.*, Eqs. III-184 & III-188) with 4 unknowns — 5 if you count $k$.

**i)** Normalization won't help since this isn't a normalizable state.

**ii)** Remember that the term $e^{ikx}$ corresponds to particles propagating to the *right* in Eqs. (III-182 & III-183) and $e^{-ikx}$ to particles traveling to the *left*.

**iii)** It follows that $A$ corresponds to the amplitude of a wave coming <u>from</u> the left, and $B$ is the amplitude of the wave <u>returning</u> to the left in Eq. (III-182).

**iv)** Likewise, $F$ is the amplitude of the wave traveling off <u>to</u> the right, and $G$ is the amplitude of the wave coming in <u>from</u> the right in Eq. (III-183).

**g)** Let's insist that in our scattering experiment, we only fire particles in from the *left*, then

$$G = 0 \quad \text{(for scattering from the left)}. \tag{III-189}$$

**i)** $A$ is then the amplitude of the **incident wave**.

**ii)** $B$ is the amplitude of the **reflected wave**.

**iii)** $F$ is the amplitude of the **transmitted wave**.

**h)** Solving Eqs. (III-184) & (III-188) for $B$ and $F$ we get

$$B = \frac{i\beta}{1 - i\beta} A \,, \qquad F = \frac{1}{1 - i\beta} A \,. \tag{III-190}$$

**i)** The probability of finding the particle at a specified location is given by $|\Psi|^2$, so the *relative* probability that an incident particle will be reflected back is

$$R \equiv \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1+\beta^2} \ , \tag{III-191}$$

where $R$ is called the reflection coefficient.

**j)** The probability of transmission is given by the **transmission coefficient**:

$$T \equiv \frac{|F|^2}{|A|^2} = \frac{1}{1+\beta^2} \ , \tag{III-192}$$

and, as you can see, the total probability of finding a particle *somewhere* is then $T + R = 1$.

**k)** In terms of energy

$$\boxed{R = \frac{1}{1+(2\hbar^2 E/m\alpha^2)} \ , \quad T = \frac{1}{1+(m\alpha^2/2\hbar^2 E)} \ .} \tag{III-193}$$

The higher the energy, the greater the probability of transmission.

**l)** This is not the end of the story, however, since this potential gives a wave function that is not normalizable, so they don't represent possible particle states.

**i)** The resolution to this problem is to form normalizable linear combinations of the stationary states (as in the case of the free particle).

**ii)** However, the math is extremely complicated and it will not be reproduced here. It is best solved numerically with a computer.

**iii)** Since it is impossible to create a normalizable free particle wave function without involving a range of energies, $R$ and $T$ should be interpreted as the *approximate* reflection and transmission probabilities for particles in a narrow energy range about $E$.

**m)** Note that unlike classical mechanics, having $E < V_{\rm max}$ will result in $T > 0 \Longrightarrow$ in quantum mechanics some of the particles get past the barrier. This phenomenon is called **tunneling**.

## H. The Finite Square Well.

**1.** As was introduced for the "free particle" (§III.F), the wave function for **traveling waves** can always be described by

$$\psi(x) = A\, e^{i\alpha x} + B\, e^{-i\alpha x} \ .$$

**a)** Here, the $A$-coefficient term corresponds to a wave traveling to the right.

**b)** The $B$-coefficient term corresponds to a wave traveling to the left.

**2.** Meanwhile, a **standing wave** is characterized by the following wave function:

$$\psi(x) = C\, \sin(\alpha x) + D\, \cos(\alpha x) \ .$$

Here, the sine and the cosine terms do not have any specific directional information associated with them, which is easy to understand since we are talking about a standing wave.

**Exercise:** Mathematically prove the statement just made about the directionality about the sine and cosine terms in the equation above. *Hint:* Note that

$$\begin{aligned} e^{\pm i\alpha} &= \cos\alpha \pm i\, \sin\alpha \ , \\ \sin\alpha &= \frac{e^{i\,\alpha} - e^{-i\,\alpha}}{2i} \ , \text{ and} \end{aligned}$$

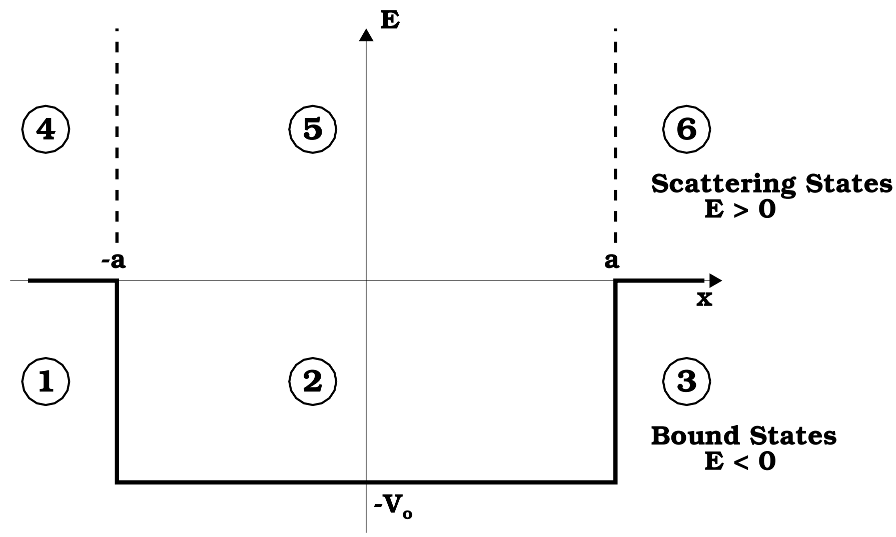



Figure III–5: The finite square well potential (Eq. III-196).

$$\cos\alpha = \frac{e^{i\alpha}+e^{-i\alpha}}{2} \, .$$

**3.** With this information in mind, consider the finite square well:

$$V(x) = \begin{cases} -V_\circ, & \text{for } -a < x < a, \\ 0, & \text{for } |x| > a, \end{cases} \tag{III-194}$$

where $V_\circ$ is a (positive) constant as shown in Figure III-5.

a) **Bounds states** will occur when $E < 0$ (as indicated by Regions 1, 2, and 3 in Figure III-5).

b) **Scattering states** will occur when $E > 0$ (as indicated by Regions 4, 5, and 6 in Figure III-5).

**4.** **Bound States** ($E < 0$) of the finite square well.

a) **Region 1:** For bound states in the region $x < -a$, $V(x) = 0$ and the TISE becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi, \quad \text{or} \quad \frac{d^2\psi}{dx^2} = \kappa^2\psi \ , \tag{III-195}$$

where

$$\kappa \equiv \frac{\sqrt{-2mE}}{\hbar} \qquad \text{(III-196)}$$

is real and positive. The general solution is identical to Eq. (III-149) but, as before, the first term blows up (as $x \rightarrow -\infty$), so $A = 0$ and

$$\psi(x) = Be^{\kappa x}, \quad \text{for } (x < -a). \qquad \text{(III-197)}$$

b) **Region 2:** In the region $-a < x < a$, $V(x) = -V_\circ$ and the TISE becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_\circ \psi = E\psi \ , \quad \text{or} \ \frac{d^2\psi}{dx^2} = -\ell^2\psi \ , \qquad \text{(III-198)}$$

where

$$\ell \equiv \frac{\sqrt{2m(E+V_\circ)}}{\hbar} \ , \qquad \text{(III-199)}$$

hence, $E + V_\circ$ is the energy that the wave is above the minimum potential.

**i)** Although $E$ is negative, for a bound state, it must be greater than $-V_\circ$, otherwise, the bound-state wave function would not be normalizable $\Longrightarrow$ as such, $\ell$ is also real and positive.

**ii)** The general solution is

$$\psi(x) = C\sin(\ell x) + D\cos(\ell x) \ , \quad \text{for } (-a < x < a), \qquad \text{(III-200)}$$

where $C$ and $D$ are arbitrary constants.

**Exercise:** Prove Eq. (III-200) by taking its double derivative and plugging $\psi$ and $d^2\psi/dx^2$ back into Eq. (III-198).

c) **Region 3:** For bound states in the region $x > a$, the potential is again zero and the general solution has the form of $\psi(x) = Fe^{-\kappa x} + Ge^{\kappa x}$, but the second term blows up (as $x \to \infty$), so

$$\psi(x) = F e^{-\kappa x}, \quad \text{for } (x > a). \tag{III-201}$$

**d)** **The final solution for the bound states ($E < 0$) of the finite square well:** Imposing the standard boundary conditions: $\psi$ and $d\psi/dx$ continuous at $-a$ and $a$. Also, realizing that the potential is an even function, the wave function will either be odd or even, and we only need to look at the boundary conditions only on one side (say, at $+a$) — the other side is automatic since $\psi(-x) = \pm\psi(x)$. We will do the even solutions here and do the odd solutions in the next exercise (note that the cosine is an even function, and the sine, an odd function. The even solution for $\mathbf{E < 0}$ is

$$\psi(x) = \begin{cases} F e^{-\kappa x}, & \text{for } (x > a), \\ D\cos(\ell x), & \text{for } (0 < x < a), \\ \psi(-x), & \text{for } (x < 0). \end{cases} \tag{III-202}$$

**i)** The continuity of $\psi(x)$, at $x = a$, says

$$F e^{-\kappa a} = D\cos(\ell a) \; . \tag{III-203}$$

**ii)** The continuity of $d\psi/dx$ says

$$-\kappa F e^{-\kappa a} = -\ell D \sin(\ell a) \; . \tag{III-204}$$

**iii)** Dividing Eq. (III-204) by (III-203) gives

$$\kappa = \ell \tan(\ell a) \; . \tag{III-205}$$

**e)** Since $\ell$ and $\kappa$ are both functions of $E$, we can determine a formula for $E$ by letting

$$z \equiv \ell a, \quad \text{and} \;\; z_\circ \equiv \frac{a}{\hbar}\sqrt{2mV_\circ} \; . \tag{III-206}$$

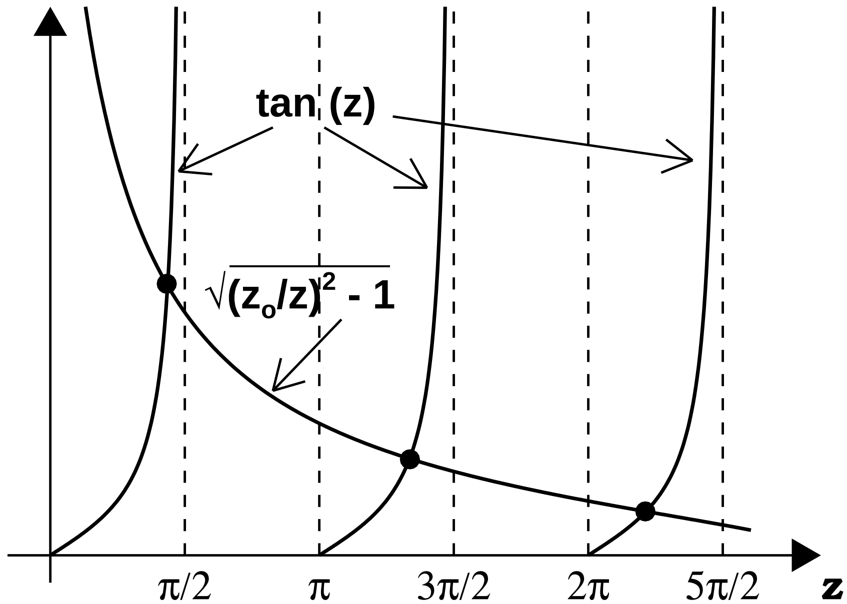



Figure III–6: Graphical solution to Eq. (III-209) for $z_\circ = 8$ (*even* states). Black dots indicate intersection points.

Then according to Eqs. (III-196) and (III-199), $(\kappa^2 + \ell^2) = 2mV_\circ/\hbar^2$, so $\kappa a = \sqrt{z_\circ^2 - z^2}$ and Eq. (III-205) becomes

$$\tan z = \sqrt{(z_\circ/z)^2 - 1} \; . \qquad \text{(III-207)}$$

**i)** This is a transcendental equation for $z$ (and hence for $E$) as a function of $z_\circ$ (which is a measure of the *size* of the well).

**ii)** It can be solved numerically by plotting $\tan z$ and $\sqrt{(z_\circ/z)^2 - 1}$ on the same grid and looking for points of intersection (see Figure III-6).

**f)** Two limiting cases are of special interest:

**i)** **Wide, deep well:** If $z_\circ$ is very large, the intersections occur just slightly below $z_\circ = n\pi/2$, with $n$ odd; it follows that

$$E_n + V_\circ \cong \frac{n^2 \pi^2 \hbar^2}{2m(2a)^2} \; . \qquad \text{(III-208)}$$

- Here, $(E_n + V_\circ)$ is the energy above the bottom of the well.
- On the right, we have the solution for an infinite square well energies of width $2a$, or rather, *half* of them, since $n$ is odd.

- So a finite square well goes to an infinite square well as $V_\circ \to \infty$. However, for any *finite* $V_\circ$ there are only a finite number of bound states.

**ii) Shallow narrow well:** As $z_\circ$ decreases, there are fewer and fewer bound states, until finally (for $z_\circ < \pi/2$, where the lowest *odd* state disappears) only one remains.

- Note that there is always, at least, one bound state despite how *weak* the well becomes.

**5. Scattering States** $(E > 0)$ of the finite square well.

**a) Region 4:** For the scattering $(E > 0)$ states, to the left, where $V(x) = 0$, we have

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \;, \quad \text{for } (x < -a), \tag{III-209}$$

where

$$k \equiv \frac{\sqrt{2mE}}{\hbar} \;. \tag{III-210}$$

**Exercise:** Prove Eq. (III-209) by taking its double derivative and plugging $\psi$ and $d^2\psi/dx^2$ back into Eq. (III-198). (Remember, $V = 0$ here.)

**b) Region 5:** Inside the well, where $V(x) = -V_\circ$,

$$\psi(x) = C\sin(\ell x) + D\cos(\ell x) \;, \quad \text{for } (-a < x < a), \tag{III-211}$$

where

$$\ell \equiv \frac{\sqrt{2m(E+V_\circ)}}{\hbar} \; . \qquad \text{(III-212)}$$

**Exercise:** Prove Eq. (III-211) by taking its double derivative and plugging $\psi$ and $d^2\psi/dx^2$ back into Eq. (III-198). Explain why the $C$ and $D$ terms do not correspond to waves traveling in any specific direction.

**c)** **Region 6:** To the right, assuming no incoming wave from that region, we have

$$\psi(x) = Fe^{ikx} \; . \qquad \text{(III-213)}$$

**d)** As described at the beginning of this subsection, in Equations (III-209) and (III-213), $A$ is the incident amplitude, $B$ is the reflected amplitude, and $F$ is the transmitted amplitude of a wave traveling in the vicinity of this finite square well.

**e)** There are 4 boundary conditions for these three equations (Eqs. III-209, III-211, and III-213):

**i)** Continuity of $\psi(x)$ at $-a$ gives

$$Ae^{-ika} + Be^{ika} = -C\sin(\ell a) + D\cos(\ell a) \; . \qquad \text{(III-214)}$$

**ii)** Continuity of $d\psi/dx$ at $-a$ gives

$$ik[Ae^{-ika} - Be^{ika}] = \ell[C\cos(\ell a) + D\sin(\ell a)] \; . \qquad \text{(III-215)}$$

**iii)** Continuity of $\psi(x)$ at $+a$ gives

$$C\sin(\ell a) + D\cos(\ell a) = Fe^{ika} \; . \qquad \text{(III-216)}$$

**iv)** Continuity of $d\psi/dx$ at $+a$ gives

$$\ell[C\cos(\ell a) - D\sin(\ell a)] = ikFe^{ika} \ . \qquad \text{(III-217)}$$

**f)** We can use two of these to eliminate $C$ and $D$, and solve the remaining two for $B$ and $F$:

$$B = i\frac{\sin(2\ell a)}{2k\ell}\,(\ell^2 - k^2)\,F, \qquad \text{(III-218)}$$

$$F = \frac{e^{-2ika}\,A}{\cos(2\ell a) - i[\sin(2\ell a)/2k\ell]\,(k^2 - \ell^2)} \qquad \text{(III-219)}$$

**g)** The transmission coefficient ($T = |F|^2/|A|^2$) is then

$$T^{-1} = 1 + \frac{V_\circ^2}{4E(E+V_\circ)}\,\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_\circ)}\right) \ . \qquad \text{(III-220)}$$

**Exercise:** Show how Eq. (III-220) results from Eq. (III-219).

**h)** Notice that $T = 1$ (*i.e.*, the well becomes *transparent*) whenever the argument of the sine is zero, or

$$\frac{2a}{\hbar}\sqrt{2m(E+V_\circ)} = n\pi \ , \qquad \text{(III-221)}$$

where $n$ is any integer.

**i)** The energies for perfect transmission are given by

$$E_n + V_\circ = \frac{n^2\pi^2\hbar^2}{2m(2a)^2} \ , \qquad \text{(III-222)}$$

which happens to be precisely the allowed energies for the infinite square well.

**Example III–7.** Analyze the *odd* bound-state wave functions for the finite square well. Derive the transcendental equation for the allowed energies, and solve it graphically. Examine the two limiting cases. Is there always at least one odd bound state?

**Solution:**

In place of Eq. (III-202), we have

$$\psi(x) = \begin{cases} Fe^{-\kappa x}, & \text{for } (x > a), \\ D\sin(\ell x), & \text{for } (0 < x < a), \\ -\psi(-x), & \text{for } (x < 0). \end{cases}$$

Continuity of $\psi(x)$ gives:

$$Fe^{-\kappa a} = D\sin(\ell a) \; ;$$

Continuity of $d\psi/dx$ gives:

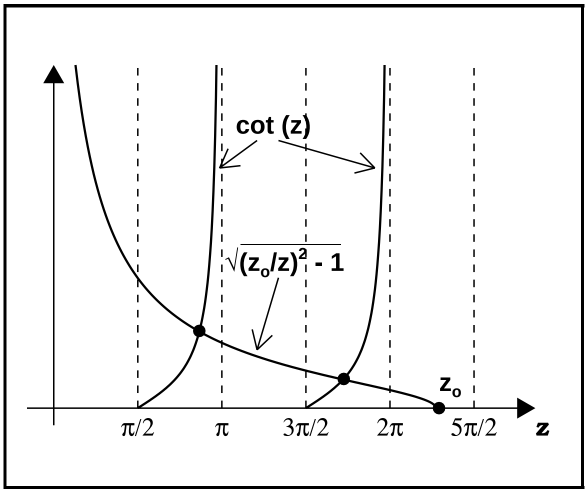
$$-\kappa F e^{-\kappa a} = D\ell\cos(\ell a) \; .$$

Dividing these two gives:

$$\begin{aligned} -\kappa &= \ell\cot(\ell a), \quad \text{or} \\ -\kappa a &= \ell a\cot(\ell a) \quad \Longrightarrow \\ \sqrt{z_\circ^2 - z^2} &= -z\cot z \; , \end{aligned}$$

or

$$\boxed{\cot z = \sqrt{(z_\circ/z)^2 - 1} \; .}$$




Wide, deep well: Intersections are at $\pi, 2\pi, 3\pi$, etc. Energies are the same as Eq. (III-208), but now for $n$ even. This fills the rest of the states for the infinite square well.

Shallow, narrow well: If $z_\circ < \pi/2$, there is no odd bound state. The corresponding condition on $V_\circ$ is $\boxed{V_\circ < \dfrac{\pi^2\hbar^2}{8ma^2}}$.