PHY 115A
Lecture Notes:
Time-Independent Schrödinger Equation
(Griffith's Chapter 2)

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Chapter 2

Time-Independent Schrödinger Equation

2.1 Stationary States

Here's our summary of Griffiths section 2.1:

We attempt to solve the Schrödinger Equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\,\Psi \tag{2.1}$$

in the case that the potential V(x) is not a function of t. We will try to find a solution under the assumption that $\Psi(x,t)$ is separable:

$$\Psi(x,t) = \psi(x)\,\phi(t) \tag{2.2}$$

which yields:

$$\begin{aligned}
i\hbar\,\psi \frac{d\phi}{dt} &= -\frac{\hbar^2}{2m}\,\phi \frac{d^2\psi}{dx^2} + V\,\Psi \\
i\hbar \frac{1}{\phi(t)} \frac{d\phi}{dt} &= -\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \frac{d^2\psi}{dx^2} + V(x)
\end{aligned}$$

As the LHS is a function of t only, and the RHS a function of x only, both sides must be constant wrt t and x respectively. We'll call that constant E, and solve for $\phi(t)$:

$$\begin{aligned}
i\hbar \frac{1}{\phi(t)} \frac{d\phi}{dt} &= E \\
\int \frac{d\phi}{\phi(t)} &= -\frac{iE}{\hbar} \int dt \\
\ln\phi &= -\frac{iEt}{\hbar} \\
\phi(t) &= \exp(-\frac{iEt}{\hbar})
\end{aligned}$$

The remaining equation is for $\psi(x)$ only

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\,\psi = E\psi$$

and is called the Time-Independent Schrödinger Equation (TISE), often just called the Schrödinger Equation when the meaning is clear.

In classical mechanics, the total energy (kinetic plus potential) is called the Hamiltonian:

$$H(x,p) = \frac{p^2}{2m} + V(x)$$

We can construct the corresponding operator in quantum mechanics by substituting

$$\begin{aligned} x &\rightarrow \hat{x} = x \\ p &\rightarrow \hat{p} = -i\hbar\frac{\partial}{\partial x} \end{aligned}$$

to calculate:

$$\hat{H} = H(\hat{x},\hat{p}) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \tag{2.3}$$

with which we can write the TISE as:

$$\hat{H}\,\psi(x) = E\,\psi(x) \tag{2.4}$$

We'll demonstrate later the following boundary conditions on $\psi(x)$:

- $\psi(x)$ is always continuous.
- $d\psi/dx$ is continuous except where the potential is infinite.

Note that these conditions do not apply to $\Psi(x,t)$ no $\partial\Psi/\partial x$ which need not be continuous. Some observations left as exercises (See Griffith's problems 2.1 and 2.2)

- For normalizable solutions, we must the separation constant E real.
- $\psi(x)$ can always be taken real.
- If $V(x)$ is an even function, than $\psi(x)$ can be taken as even or odd.
- E must be greater than the minimum value of $V(x)$.

The separable solutions are important solutions because:

- They represent **stationary states**: even though the "full" wave function

  $$\Psi(x,t) = \phi(t)\,\psi(x) = e^{-iEt/h}\,\psi(x)$$

  has a time dependence, the probability density is constant with time:

  $$\begin{aligned} |\Psi(x,t)|^2 &= \left(e^{-iEt/h}\,\psi(x)\right)^* \left(e^{-iEt/h}\,\psi(x)\right) \\ &= e^{iEt/h-iEt/h}\,\psi^*(x)\psi(x) \\ &= |\psi(x)|^2 \end{aligned}$$

  This means that every expectation value is constant wrt time as well. It also follows that:

  $$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1$$

- They represent **states of definite total energy:** the expectation value for the total energy of a separable solution is:

$$\begin{aligned}\langle E\rangle &= \int_{-\infty}^{+\infty} \Psi^*(x,t)\,\hat{H}\,\Psi(x,t)\;dx \\ &= \int_{-\infty}^{+\infty} \psi^*(x)\,\hat{H}\,\psi(x)\;dx \\ &= \int_{-\infty}^{+\infty} \psi^*(x)\,E\,\psi(x)\;dx \\ &= E\int_{-\infty}^{+\infty} |\psi(x)|\;dx \\ &= E\end{aligned}$$

  Remember that we just chose E as the symbol for the constant value when using separation of variables. This shows why we choose E, as that constant is the expectation value of the total energy. Now calculate in a similar fashion:

$$\begin{aligned}\langle E^2\rangle &= \int_{-\infty}^{+\infty} \Psi^*(x)\,\hat{H}^2\,\Psi(x)\;dx \\ &= E^2\end{aligned}$$

  From which it follows:

$$\sigma_H^2 = \langle E^2\rangle - \langle E\rangle^2 = E^2 - E^2 = 0$$

  This means that every measurement of the particles total energy will yield the result E.

- There is more, but (unlike Griffiths) we will leave those features for later.

2.2 Infinite Square Well

Next we will turn our attention to the infinite square well:

$$V(x) = \begin{cases} 0 & 0 \leq x \leq b \\ +\infty & \text{otherwise} \end{cases} \tag{2.5}$$

By setting $V(x) = +\infty$ outside the well, we just mean $\Psi(x,t) = 0$ in that region, and not anything more. We also see that for normalizable solutions, we must have $E > 0$.

We are looking for the stationary states that solve the TISE:

$$\hat{H}\,\psi(x) = E\,\psi(x)$$

Inside the well we have:

$$\begin{aligned}-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} &= E\,\psi(x) \\ \frac{d^2\psi}{dx^2} &= -k^2\psi\end{aligned}$$

where

$$k \equiv \frac{\sqrt{2mE}}{\hbar}$$

Taking $\psi(x)$ to be real, the solutions are:

$$\psi(x) = A\sin(kx) + B\cos(ks)$$

And the continuity requirements on $\psi(x)$ imply:

$$\psi(0) = \psi(b) = 0.$$

Why is there no continuity condition on $d\psi/dx$? Applying the conditions:

$$\psi(0) = A\sin(0) + B\cos(0) = B = 0$$

So now:

$$\psi(x) = A\sin(kx)$$

And applying the other condition:

$$\begin{aligned} \psi(b) &= A\sin(kb) = 0 \\ \sin(kb) &= 0 \end{aligned}$$

Where in the last step we have used $A \neq 0$ because $A = 0$ implies $\psi(x) = 0$ a non-normalizable solution. The sin function is zero for any integer value of pi, so:

$$\begin{aligned} kb &= n\pi \\ k_n &= \frac{n\pi}{b} \end{aligned}$$

where n is any integer.

The normalization condition is:

$$\int_{-\infty}^{+\infty} |\psi(x)|^2\, dx = 1$$

but keeping in mind that $\psi(x) = 0$ outside of the square well ($[0, b]$) this condition becomes:

$$\begin{aligned} 1 &= \int_0^a |A\,\sin(k_n x)|^2\, dx \\ 1 &= |A|^2 \int_0^b \sin^2(k_n x)\, dx \\ 1 &= |A|^2\,\frac{b}{2} \\ |A|^2 &= \frac{2}{b} \end{aligned}$$

As the phase of A doesn't matter for the purposes of normalization, we choose it to be positive real:

$$A = \sqrt{\frac{2}{b}}$$

So at last we have an infinite number of solutions to the TISE:

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{b}}\sin(k_n x) & 0 \leq x \leq b \\ 0 & \text{otherwise} \end{cases} \tag{2.6}$$

where

$$k_n = \frac{n\pi}{b}$$

In principle, n can be any integer, but for $n = 0$ we get the unnormalizable wave function $\psi(x) = 0$ and so we omit $n = 0$. We note also that:

$$\psi_{-n}(x) = \sqrt{\frac{2}{b}}\sin(k_{-n}x) = \sqrt{\frac{2}{b}}\sin(-k_n x) = -\sqrt{\frac{2}{b}}\sin(k_n x) = -\psi_n(x)$$

So ψ_{-n} differs from ψ_n only by a phase factor -1 and therefore adds nothing (recall that we simply chose A to be positive and real). If we need ψ_{-n} we can just use $-\psi_n$. So we can omit negative values of n as well. That leaves us with:

$$n = 1, 2, 3, \ldots$$

Recalling our definition for k, the definite total energy E_n of stationary state ψ_n is given by:

$$k_n = \frac{n\pi}{b} = \frac{\sqrt{2mE_n}}{\hbar} \tag{2.7}$$

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2mb^2} \tag{2.8}$$

2.3 The Fourier Series

In this section, we'll see how the Fourier Series can be interpreted in the context of a vector space with an inner product. Then we will see how it relates to stationary solutions of the infinite square-well potential which we have just determined.

2.3.1 Vector Spaces and Inner Product Spaces

The real numbers ((R)) and complex numbers ($\mathbb{C}$) are both examples of fields in mathematics: they are each a set on which the operations addition, subtraction, multiplication, and division are defined and follow their familiar rules. A vector space V over a scalar field S is a set whose elements are called vectors, for which an associative and commutative operation of addition and an associative and distributive operation of scalar multiplication are both defined. The complete set of properties which define a vector field are shown in Table 2.1.

An *inner product* is an operation which returns a scalar for any two vectors x and y. We write the inner product as $\langle x|y\rangle$. If a vector space V has an inner product defined which satisfies conditions I1-I5 in the table, it is an inner product space H as well. It is left as an exercise to show that the deducible properties D1-D4 listed in the table follow from the other properties.

Table 2.1: Here we define the properties of a vector space V over a scalar field S, and an inner product space H as well, using a compact mathematical notation. In this class the scalar field S will only be the real numbers ($\mathbb{R}$) or the complex numbers ($\mathbb{C}$). When $S = \mathbb{R}$, just ignore all complex conjugation below, e.g. take $\alpha^* = \alpha$.

Useful Math Symbols:

$\forall\, x \in V$	for all x in V (for any vector x)
$\forall\, \alpha \in S$	for all α in S (for any scalar α)
$\exists!\, y$	there exists unique y
s.t.	such that

Properties of Addition:

A1	**Closure**	$\forall x, y \in V$	$(x + y) \in V$
A2	**Commutative**	$\forall x, y \in V$	$x + y = y + z$
A3	**Associative**	$\forall x, y, z \in V$	$(x + y) + z = x + (y + z)$
A4	**Zero**	$\exists!\ 0$ s.t. $\forall x \in V$	$x + 0 = x$
A5	**Inverse**	$\forall x \in V \exists!\ (-x) \in V$ s.t.	$x + (-x) = 0$

Properties of Scalar Multiplication:

M1	**Closure**	$\forall x \in V$ and $\forall \alpha \in S$	$\alpha x \in V$
M2	**Identity**	$\forall x \in V$	$1x = x$
M3	**Associative**	$\forall x \in V$ and $\forall \alpha, \beta \in S$	$\alpha(\beta x) = (\alpha\beta)x$
M4	**Distributive**	$\forall x, y \in V$and $\forall \alpha \in S$	$\alpha(x + y) = \alpha x + \alpha y$
M5	**Distributive**	$\forall x \in V$and $\forall \alpha, \beta \in S$	$(\alpha + \beta)x = \alpha x + \beta x$

Deducible Properties:

D1	$\forall x \in V$	$0x = 0$
D2	$\forall x \in V$	$(-1)x = (-x)$

Properties of Inner Products:

I1	$\forall x, y \in H$	$\langle x\|y\rangle^* = \langle y\|x\rangle$
I2	$\forall x, y, z \in H$and $\forall \alpha \in S$	$\langle x\|\alpha y\rangle = \alpha \langle x\|y\rangle$
I3	$\forall x, y, z \in H$	$\langle x + y\|z\rangle = \langle x\|z\rangle + \langle y\|z\rangle$
I4	$\forall x \in H$	$\langle x\|x\rangle \geq 0$
I5	$\forall x \in H$	$\langle x\|x\rangle = 0$ if and only if $x = 0$

Deducible Properties:

D3	$\forall x, y \in H$and $\forall \alpha \in S$	$\langle \alpha x\|y\rangle = \alpha^* \langle x\|y\rangle$
D4	$\forall x, y, z \in H$	$\langle x\|y + z\rangle = \langle x\|y\rangle + \langle x\|z\rangle$

2.3.2 Euclidean Vector Space

Before turning to the Fourier Series, let's explore how the properties of an abstract vector space apply to the familiar Euclidean vectors. Such a vector is completely specified by its displacement in each spatial direction. Let's see how the axiomatic properties of Table 2.1 apply in this case. Note that the scalar field S is the real numbers ($\mathbb{R}$), so we'll just ignore all complex conjugation in the table for now.

We have **vector addition** which satisfies properties A1-A5 of Table 2.1:

- **A1**: $\vec{u} + \vec{v} = \vec{w}$
- **A2**: $\vec{v} + \vec{w} = \vec{w} + \vec{v}$
- **A3**: $\vec{u} + (\vec{v} + \vec{w}) = (\vec{u} + \vec{v}) + \vec{w}$
- **A4**: There is the vector 0 with: $\vec{v} + 0 = \vec{v}$
- **A5**: For every $\vec{v}$ there is $(-\vec{v})$ s.t $\vec{v} + (-\vec{v}) = 0$

We also have **scalar multiplication** which satisfies properties M1-M5 and D1,D2:

- **M1:** $a\vec{v} = \vec{w}$
- **M2:** $1\vec{v} = \vec{v}$
- **M3:** $a(b\vec{v}) = (ab)\vec{v}$
- **M4:** $a(\vec{v} + \vec{w}) = a\vec{v} + a\vec{w}$
- **M5:** $(a + b)\vec{v} = a\vec{v} + b\vec{v}$
- **D1:** $(-1)\vec{v} = (-\vec{v})$
- **D2:** $0\vec{v} = 0$

In this vector space, the dot product:

$$\vec{v} \cdot \vec{w} = v_x w_x + v_y w_y + v_z w_z$$

is the inner product which satisfies properties I1-I5:

- **I1:** $\vec{v} \cdot \vec{w} = \vec{w} \cdot \vec{v}$
- **I2:** $\vec{v} \cdot (a\vec{w}) = a\vec{v} \cdot \vec{w}$
- **I3:** $(\vec{u} + \vec{v}) \cdot \vec{w} = \vec{u} \cdot \vec{w} + \vec{v} \cdot \vec{w}$
- **I4:** $\vec{v} \cdot \vec{v} \geq 0$
- **I5:** $\vec{v} \cdot \vec{v} = 0$ if and only if $\vec{v} = 0$
- **D3:** $(a\vec{v}) \cdot \vec{w} = a\,(\vec{v} \cdot \vec{w})$
- **D4:** $\vec{w} \cdot (\vec{u} + \vec{v}) = \vec{w} \cdot \vec{u} + \vec{w} \cdot \vec{v}$

We have a set of *basis vectors*: $\hat{x}$, $\hat{y}$, and $\hat{z}$. These basis vectors are orthogonal:

$$\hat{x} \cdot \hat{y} = \hat{y} \cdot \hat{z} = \hat{z} \cdot \hat{x} = 0$$

and normalized:

$$\hat{x} \cdot \hat{x} = \hat{y} \cdot \hat{y} = \hat{z} \cdot \hat{z} = 1.$$

When the basis vectors have both of these properties, we call them *orthonormal.*

For any possible vector $\vec{v}$, we can calculate its component in the direction of each basis vector by calculating the inner product:

$$\begin{aligned} v_x &= \vec{v} \cdot \hat{x} \\ v_y &= \vec{v} \cdot \hat{y} \\ v_z &= \vec{v} \cdot \hat{z} \end{aligned}$$

We say that the basis vectors $\hat{x}$, $\hat{y}$, and $\hat{z}$ are "complete", because specifying the values of v_x, v_y, and v_z completely describes the vector v. (Alternatively, we can say that the basis vectors span the vector space V.) The set of basis vectors $\hat{x}$ and $\hat{z}$ are orthonormal, but they are not complete in three dimensional space, because there are vectors which we cannot write using only these two directions. For instance, there are no possible values for v_x and v_z which make

$$\vec{v_1} = v_x\hat{x} + v_z\hat{z}$$

equal to the vector

$$\vec{v_2} = 3\hat{x} + 2\hat{y} + 7\hat{z}.$$

Orthogonality and completeness are intimately related. In Euclidean vector space, any three orthogonal vectors are a complete basis.

2.3.3 The Fourier Series

Using the language of inner product spaces, the Fourier Theorem states that the sines and cosines form a complete orthonormal basis for any periodic function. The vectors in this vector space are periodic functions. Addition of periodic functions $f(x)$ and $g(x)$ is another periodic function $f(x)+g(x)$. Scalar multiplication of a periodic function $f(x)$ by a real number a is another periodic function $af(x)$. The other properties of vector addition and scalar multiplication follow from the corresponding rules of ordinary addition and multiplication.

To obtain an inner product space, we need to define the inner product. If we restrict ourselves to **real** functions of x with period a, the inner product between any two functions $f(x)$ and $g(x)$ is defined to be the integral:

$$\langle f|g\rangle \equiv \int_{-\frac{a}{2}}^{\frac{a}{2}} f(x)\, g(x)\, dx \tag{2.9}$$

The basis vectors are the sine and cosine functions

$$s_n(x) \equiv \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi n}{a} x\right) \tag{2.10}$$

$$c_n(x) \equiv \sqrt{\frac{2}{a}} \cos\left(\frac{2\pi n}{a} x\right) \tag{2.11}$$

which are defined for

$$n = 1, 2, 3, ...$$

plus the constant function:

$$c_0(x) \equiv \sqrt{\frac{1}{a}} \tag{2.12}$$

Note that if it existed, $s_0(x) = 0$ would not be normalizable.

We leave it as an exercise to show that:

$$\begin{aligned} \langle s_n | s_m \rangle &= \delta_{nm} \\ \langle c_n | c_m \rangle &= \delta_{nm} \\ \langle s_n | c_m \rangle &= 0 \end{aligned} \tag{2.13}$$

for all n and m, but take care that c_0 exists while s_0 does not. For compact notation we use the Kronecker delta symbol:

$$\delta_{nm} = \begin{cases} 1 & \text{if } n = m \\ 0 & \text{otherwise} \end{cases}$$

We can write the orthonormality conditions out explicitly as integrals for $n > 0$ and $m > 0$ as:

$$\begin{aligned} \langle s_n | s_m \rangle &= \frac{2}{a} \int_{-\frac{a}{2}}^{\frac{a}{2}} \sin\left(\frac{2\pi n}{a} x\right) \sin\left(\frac{2\pi m}{a} x\right) dx = \delta_{nm} \\ \langle c_n | c_m \rangle &= \frac{2}{a} \int_{-\frac{a}{2}}^{\frac{a}{2}} \cos\left(\frac{2\pi n}{a} x\right) \cos\left(\frac{2\pi m}{a} x\right) dx = \delta_{nm} \\ \langle s_n | c_m \rangle &= \frac{2}{a} \int_{-\frac{a}{2}}^{\frac{a}{2}} \sin\left(\frac{2\pi n}{a} x\right) \cos\left(\frac{2\pi m}{a} x\right) dx = 0 \end{aligned} \tag{2.14}$$

leaving the special case for c_0 (and still keeping $n > 0$):

$$\begin{aligned} \langle c_n | c_0 \rangle &= \frac{\sqrt{2}}{a} \int_{-\frac{a}{2}}^{\frac{a}{2}} \cos\left(\frac{2\pi n}{a} x\right) dx = 0 \\ \langle s_n | c_0 \rangle &= \frac{\sqrt{2}}{a} \int_{-\frac{a}{2}}^{\frac{a}{2}} \sin\left(\frac{2\pi n}{a} x\right) dx = 0 \\ \langle c_0 | c_0 \rangle &= \frac{1}{a} \int_{-\frac{a}{2}}^{\frac{a}{2}} dx = 1 \end{aligned} \tag{2.15}$$

Fourier's Theorem states that these orthonormal basis functions are complete for the vector space of periodic functions with period a. That is, if $f(x)$ has the property that:

$$f(x) = f(x + a)$$

then $f(x)$ can be written as a sum of the orthonormal basis vectors:

$$f(x) = \sum_{n=0}^{\infty} A_n\, c_n(x) \quad + \quad \sum_{n=1}^{\infty} B_n\, s_n(x) \tag{2.16}$$

or explicitly in terms of sine and cosine functions:

$$f(x) = A_0\sqrt{\frac{1}{a}} + \sqrt{\frac{2}{a}}\sum_{n=1}^{\infty}\left[A_n \cos\left(\frac{2\pi n}{a}\,x\right) + B_n \sin\left(\frac{2\pi n}{a}\,x\right)\right] \tag{2.17}$$

The values A_n and B_n are called *Fourier coefficients*. The Nth term in the Fourier Series refers to the approximation for $f(x)$ from the first N terms in the infinite sum above, and we say that the Fourier Series converges to the function $f(x)$. The demonstration of completeness is optional reading, available in the Appendix.

We can write things a bit more neatly:

$$f(x) = a_0 + \sum_{n=1}^{\infty}\left[a_n \cos\left(\frac{2\pi n}{a}\,x\right) + b_n \sin\left(\frac{2\pi n}{a}\,x\right)\right] \tag{2.18}$$

where:

$$\begin{aligned} a_0 &= \sqrt{\frac{1}{a}}A_0 \\ a_n &= \sqrt{\frac{2}{a}}A_n \\ b_n &= \sqrt{\frac{2}{a}}B_n \end{aligned}$$

but at the cost of obscuring the role of the orthonormal basis functions.

For a visual example of the Fourier Series, the first terms of the Fourier Series for a step function are shown in Fig. 2.1.

2.3.4 Determining Fourier Coefficients

Just as in the Euclidean vector space, we can determine the Fourier coefficients of a function f by computing the inner products:

$$\begin{aligned} A_n &= \langle c_n | f \rangle \\ B_n &= \langle s_n | f \rangle \end{aligned}$$

or, in terms of the inner product integrals and sine and cosine functions:

$$\begin{aligned} A_0 &= \sqrt{\frac{1}{a}}\int_{-\frac{a}{2}}^{\frac{a}{2}} f(x)\,dx \\ A_n &= \sqrt{\frac{2}{a}}\int_{-\frac{a}{2}}^{\frac{a}{2}} \cos\left(\frac{2\pi n}{a}\,x\right)\, f(x)\,dx \\ B_n &= \sqrt{\frac{2}{a}}\int_{-\frac{a}{2}}^{\frac{a}{2}} \sin\left(\frac{2\pi n}{a}\,x\right)\, f(x)\,dx \end{aligned}$$

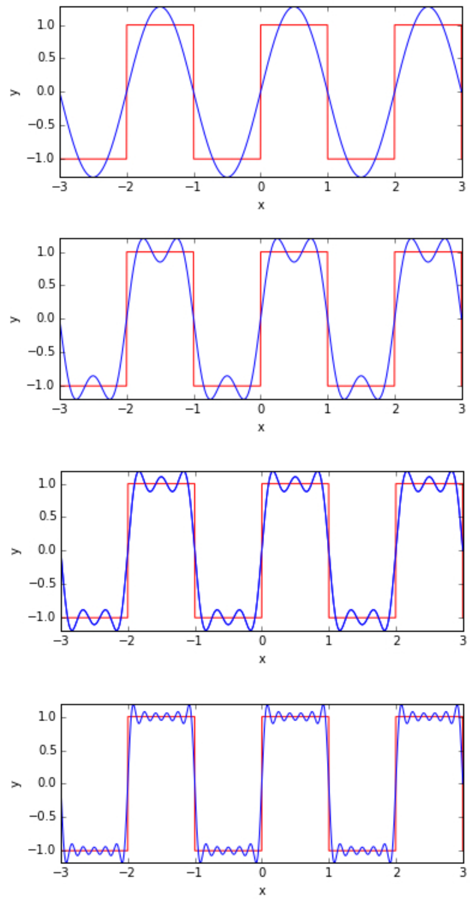

Figure 2.1: The Fourier Series for a step function including one term, three terms, five terms, and nineteen terms. The Fourier Theorem states that the series will converge, reproducing the original function, as the number of terms approaches infinity.

The inner product determines the correct coefficients only because the basis functions are complete and orthonormal. To see how this works, start with the completeness equation but replace n with m for clarity later:

$$f(x) \;=\; \sum_{m=0}^{\infty} A_m \, c_m(x) \;+\; \sum_{m=1}^{\infty} B_m \, s_m(x)$$

Then calculate:

$$\begin{aligned}
\langle c_n | f \rangle &= \langle c_n | \sum_{m=0}^{\infty} A_m \, c_m \;+\; \sum_{m=1}^{\infty} B_m \, s_m \rangle \\
&= \sum_{m=0}^{\infty} A_m \, \langle c_n | c_m \rangle \;+\; \sum_{m=1}^{\infty} B_m \, \langle c_m | s_m \rangle \\
&= \sum_{m=0}^{\infty} A_m \, \delta_{nm} \;+\; \sum_{m=1}^{\infty} B_m \; 0 \\
\langle c_n | f \rangle &= A_n
\end{aligned}$$

Note that the second step follows from properties I2 and D4 of Table 2.1. In the last step the only non-zero value in the sum across m is the term for $m = n$, because of the δ_{nm}. It is left as an exercise to work this out for $\langle s_n|f\rangle$. (It is also helpful to work through these same steps using the integral form of the orthogonality conditions. It's much more cumbersome notation, but much more explicit about what is going on. I highly recommend doing this if you are finding the abstract notation confusing at this point.)

2.3.5 Application of Fourier Series to Infinite Well

For the infinite potential well

$$V(x) = \begin{cases} 0 & 0 \le x \le b \\ +\infty & \text{otherwise} \end{cases} \tag{2.19}$$

we have a wave function $\psi(x)$ which meets the boundary conditions $\psi(0) = \psi(b) = 0$. We define a helper function:

$$f(x) = \begin{cases} \psi(x) & 0 \le x \le b \\ -\psi(-x) & -b \le x < 0 \end{cases}$$

It is an odd function by construction: $f(-x) = -f(x)$. Since f(b) = f(-b) = 0, we can consider it to be a periodic function with period $2b$. To evaluate it's Fourier series, we'll only need to evaluate it in the region $[-b, b]$ where it is defined[1]. When applying the formulas for the Fourier series, we will need to make the substitute $a \to 2b$ into the original formulas, because the period of $f(x)$ is $2b$.

For $f(x)$ the Fourier coefficients of the cosines all vanish:

$$\begin{aligned} A_0 &= \sqrt{\frac{1}{2b}} \int_{-b}^{b} f(x)\, dx = 0 \\ A_n &= \sqrt{\frac{1}{b}} \int_{-b}^{b} \cos\left(\frac{\pi n}{b}\, x\right) f(x)\, dx = 0 \end{aligned}$$

and so the Fourier Series for $f(x)$ contains only sines:

$$\begin{aligned} f(x) &= \sqrt{\frac{1}{b}} \sum_{n=1}^{\infty} B_n \sin\left(\frac{\pi n}{b}\, x\right) \\ &= \sum_{n=1}^{\infty} \left(\frac{B_n}{\sqrt{2}}\right) \left[\sqrt{\frac{2}{b}} \sin\left(\frac{\pi n}{b}\, x\right)\right] \end{aligned}$$

Where we have arranged the factors of $\sqrt{2}$ so that the function in square brackets $[\ldots]$ has unit normalization on $[0, b]$. We determine the Fourier coefficients for the sines from:

$$B_n = \sqrt{\frac{1}{b}} \int_{-b}^{b} \sin\left(\frac{\pi n}{b}\, x\right) f(x)\, dx = 0$$

[1] If you prefer, you can imagine making the helper function truly periodic by just stamping out a copy of $f(x)$ from $[-a, a]$ into $[a, 3a]$, and so on. It will have no effect in what follows.

but since the integrand is now even, the integral does not vanish, and in fact, we need only integrate in $[0, b]$ and multiply by a factor of two:

$$B_n = 2 \times \sqrt{\frac{1}{b}} \int_0^b \sin\left(\frac{\pi n}{b}\, x\right)\, f(x)\, dx = 0$$

$$c_n \equiv \frac{B_n}{\sqrt{2}} = \int_0^b \left(\sqrt{\frac{2}{b}} \sin\left(\frac{\pi n}{b}\, x\right)\right) f(x) dx$$

And since we are now integrating only from $[0, b]$ then

$$f(x) = \psi(x)$$

and we can rewrite these equations in terms of

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{b}}\, \sin(k_n x) & 0 \leq x \leq b \\ 0 & \text{otherwise} \end{cases} \tag{2.20}$$

where

$$k_n = \frac{n\pi}{b}$$

Any wave function in [0,b] can be expressed as a linear combination of these basis functions:

$$\psi(x) = \sum_{n=1}^{\infty} c_n \psi_n(x) \tag{2.21}$$

and

$$c_n = \langle \psi_n | \psi \rangle = \int_0^b \psi_n(x)\, \psi(x)\, dx$$

2.4 Insights from the Infinite Square Well

Let's recap what we have learned so far. By assuming that we could find solutions of the form

$$\Psi(x, t) = \psi(x)\, \phi(t)$$

we have indeed found an infinite number of solutions to the TISE for the Infinite Square Well potential:

$$\hat{H}\, \psi_n(x) = E_n\, \psi_n(x)$$

for $n = 1, 2, 3, \ldots$. Each of these solutions has an associated time dependent "wiggle factor":

$$\phi_n(t) = \exp(-\frac{iE_n t}{\hbar})$$

so that the total wave equation is:

$$\Psi_n(x, t) = \exp(-\frac{iE_n t}{\hbar})\, \psi_n(x)$$

We saw that these are **stationary states** (the expectation values are constant in time) and they are **states of definite energy** (every measurement of their energy will yield the results E_n).

The wave functions $\Psi_n(x,t)$ are solutions to the (time dependent) SE. It's instructive to see exactly how that works:

$$\begin{aligned}
\hat{H}\,\Psi_n(x,t) &= -i\hbar\frac{\partial \Psi}{\partial t} \\
\exp(-\frac{iE_nt}{\hbar})\ \hat{H}\ \psi_n(x) &= -i\hbar\psi_n(x)\,\frac{d}{dt}\exp(-\frac{iE_nt}{\hbar}) \\
\exp(-\frac{iE_nt}{\hbar})\ E_n\ \psi_n(x) &= -i\hbar\psi_n(x)\,\frac{-iE_n}{\hbar}\exp(-\frac{iE_nt}{\hbar}) \\
E_n\Psi(x,t) &= E_n\Psi(x,t)
\end{aligned}$$

The recognition of stationary states as the Fourier series gives us a crucial additional insight. The $\psi_n(x)$ are also a complete orthonormal basis (the Fourier series) for any function that meets the boundary conditions for this problem. That means that we have in fact already found the *general solution* to this problem.

Let's see how this works. Suppose the initial state of a particle is $\Psi(x,0) \equiv \psi_i(x)$. This can be absolutely any function so long as it vanishes outside of $[0,a]$ and it is properly normalized. Our job is to find $\Psi(x,t)$ that satisfies the SE for all future times. We calculate the Fourier coefficients of $\psi_i(x)$ as:

$$c_n = \langle\psi_n|\psi_i\rangle = \int_0^a \psi_n(x)\,\psi_i(x)\,dx$$

and by Fourier's theorem, we know that:

$$\Psi(x,0) = \sum_{n=0}^{\infty} c_n\,\psi_n(x)$$

But what about $\Psi(x,t)$? It really couldn't be any simpler:

$$\Psi(x,t) = \sum_{n=0}^{\infty} c_n\,\Psi_n(x,t) = \sum_{n=0}^{\infty} c_n\,\exp(-\frac{iE_nt}{\hbar})\,\psi_n(x)$$

It is left as an exercise to show explicitly that $\Psi(x,t)$ as defined here does satisfy the time-dependent SE and is equal to $\psi_i(x)$ at $t=0$.

There is still some insight to be gleamed from this simple example. We specified that $\Psi(x,0)$ is normalized, and we showed that the SE preserves normalization, so we know that $\Psi(x,t)$ is normalized as well:

$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2\,dx = 1$$

And plugging in the Fourier series for $\Psi(x,t)$:

$$\begin{aligned}
1 &= \int_{-\infty}^{+\infty} \Psi^*(x,t)\Psi(x,t)\ dx \\
&= \int_{-\infty}^{+\infty} \left(\sum_{n=1}^{\infty} c_n^* \Psi_n^*(x,t)\right)\left(\sum_{m=1}^{\infty} c_m \Psi_m(x,t)\right)\ dx \\
&= \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} c_n^* c_m \ \exp\left(\frac{i(E_n - E_m)t}{\hbar}\right) \int_{-\infty}^{+\infty} \psi_n^*(x)\psi_m(x)\ dx \\
&= \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} c_n^* c_m \ \exp\left(\frac{i(E_n - E_m)t}{\hbar}\right) \delta_{nm}
\end{aligned}$$

so that

$$\sum_{n=1}^{\infty} |c_n|^2 = 1 \tag{2.22}$$

We can also calculate:

$$\begin{aligned}
\langle H\rangle &= \int_{-\infty}^{+\infty} \Psi^*(x,t)\hat{H}\Psi(x,t)\ dx \\
&= \int_{-\infty}^{+\infty} \left(\sum_{n=1}^{\infty} c_n^* \Psi_n^*(x,t)\right)\hat{H}\left(\sum_{m=1}^{\infty} c_m \Psi_m(x,t)\right)\ dx \\
&= \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} c_n^* c_m \ \exp\left(\frac{i(E_n - E_m)t}{\hbar}\right) \int_{-\infty}^{+\infty} \psi_n^*(x)\hat{H}\psi_m(x)\ dx \\
&= \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} c_n^* c_m \ \exp\left(\frac{i(E_n - E_m)t}{\hbar}\right) \int_{-\infty}^{+\infty} \psi_n^*(x)E_m\psi_m(x)\ dx \\
&= \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} c_n^* c_m \ \exp\left(\frac{i(E_n - E_m)t}{\hbar}\right) E_m \int_{-\infty}^{+\infty} \psi_n^*(x)\psi_m(x)\ dx \\
&= \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} c_n^* c_m \ \exp\left(\frac{i(E_n - E_m)t}{\hbar}\right) E_m\delta_{nm}
\end{aligned}$$

so that

$$\langle H\rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n \tag{2.23}$$

Recall from our review of statistics that:

$$\langle H\rangle = \sum_{n=1}^{\infty} P(n) E_n \tag{2.24}$$

where $P(n)$ is the probability of observing the particle in state n. This allows us to identify $|c_n|^2$ as the probability of observing the particle with energy E_n.

At this point, it would be reasonable to assume that these results apply only to the infinite square well potential. In fact, there is a generalization to the Fourier series called the Spectral Theorem which shows that these results apply more more widely. The stationary solutions to the TISE will always be a complete orthonormal basis for the general solution, exactly as here.

2.5 Commutators

Let's review the situation. The state of a quantum system is contained entirely in a wave function $\Psi(x,t)$ which is a function of the position x but not momentum p. To calculate quantities involving momentum, instead of a variable, we must use the momentum operator:

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

But note that while:

$$x\,\hat{p}\;\Psi(x,t) = -i\hbar\,x\frac{\partial\Psi}{\partial x}$$

because of the chain rule, we have:

$$\hat{p}\,x\;\Psi(x,t) = -i\hbar\Psi(x,t) - i\hbar\,x\frac{\partial\Psi}{\partial x}$$

and:

$$(x\,\hat{p} - \hat{p}\,x)\;\Psi(x,t) = i\hbar\,\Psi(x,t)$$

This might seems like it is all a silly mistake... like maybe we should just be more careful with our parenthesis in our notation and apply operators only to the part we want without getting anything extra. But no, this non-commutative behavior and its physical consequences are far reaching and impossible to avoid.

When using operators we encounter terms like $x\hat{p} - \hat{p}x$ so often that we have a special notation for them. The commutator of A and B is written and defined as:

$$\left[\hat{A},\hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A} \tag{2.25}$$

Using this notation, and noting $\hat{x} = x$, we can rewrite our result about as:

$$[\hat{x},\hat{p}]\;\Psi(x,t) = i\hbar\,\Psi(x,t)$$

or more simply:

$$[\hat{x},\hat{p}] = i\hbar \tag{2.26}$$

This small little equation is called the **canonical commutation relation** and as we will see, it is a central feature of quantum mechanics.

2.6 The Harmonic Oscillator

The classical harmonic oscillator is a mass m connected to a spring which follows Hooke's law:

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

with oscillatory solutions

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

where:

$$\omega = \sqrt{\frac{k}{m}}$$

The potential energy is

$$V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2$$

The classical harmonic oscillator is *widely* applicable, at least as an approximation, because any potential is approximately a parabola near a local minimum in the potential:

$$\begin{aligned} V(x) &= V(x_0) + V'(x_0)\,(x - x_0) + \frac{1}{2}\,V''(x_0)\,(x - x_0)^2 + \ldots \\ V(x) &= V_0 + \frac{1}{2}\,V''(x_0)\,(x - x_0)^2 + \ldots \\ V(x) &\approx -\frac{1}{2}\,V''(x_0) \end{aligned}$$

where we have used the fact that $V'(x_0) = 0$ at the minimum and the constant offset V_0 can be taken as zero.

In this section, we will turn our attention to the widely applicable quantum harmonic oscillator, and find the solutions to the TISE for:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2x^2$$

We are first going to solve this the hard way, through the power series solution, and then solve it using an elegant algebraic method.

2.6.1 Power Series Solutions

We are solving this equation:

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

but if we leave it in that form we will spend all our time dealing with constants and not make any progress. Instead our idea is two multiply through by:

$$\frac{2}{\hbar\omega}$$

as this will make the coefficient of the RHS dimensionless, and get rid of the factors of 1/2 on the LHS. This gives us:

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

and we can see the progress we've made if we put:

$$x_0 \equiv \sqrt{\frac{\hbar}{m\omega}}$$

and

$$\epsilon \equiv \frac{2E}{\hbar\omega}$$

Our equation becomes:

$$-x_0^2\,\frac{d^2\psi}{dx^2} \;+\; \frac{x^2}{x_0^2}\,\psi(x) \;=\; \epsilon\,\psi(x)$$

which is already looking less tedious. But note that we can define a dimensionless variable u to replace x as:

$$u \equiv \frac{x}{x_0}$$

and noting that:

$$\frac{d}{dx} = \frac{du}{dx}\frac{d}{du} = a\frac{d}{du}$$

we have at last:

$$-\frac{d^2\psi}{du^2} + u^2\,\psi(u) \;=\; \epsilon\,\psi(x)$$

or:

$$\frac{d^2\psi}{du^2} \;=\; (u^2 - \epsilon)\,\psi(u)$$

the same equation with the tedious constants hidden in our variable definitions.

Next we consider the behavior of ψ at large u (which is also large x). In this case, the differential equation becomes:

$$\frac{d^2\psi}{du^2} \approx u^2\psi(u)$$

Noticing that the derivatives cause the power of u to increase leads us to try something like:

$$\psi(u) = \exp\left(\frac{\alpha u^2}{2}\right)$$

for some α, because each derivative will bring down a factor of u. But as we'll see, even something like:

$$\psi(u) = u^k\ \exp\left(\frac{\alpha u^2}{2}\right)$$

will do the trick. Trying it out:

$$\frac{d\psi}{du} = \left(\alpha u^{k+1} + k\,u^{k-1}\right)\,\exp\left(\frac{\alpha u^2}{2}\right)$$

and

$$\frac{d^2\psi}{du^2} = \alpha^2 u^{k+2}\exp\left(\frac{\alpha u^2}{2}\right)\,\left(1 + \mathcal{O}(1/u^2)\right)$$

where the symbol $\mathcal{O}(1/u^2)$ means terms of order $1/u^2$ and smaller. Because u is large, we can neglect these higher order terms relative to the leading 1, and get:

$$\frac{d^2\psi}{du^2} = \alpha^2 u^2 \psi$$

which satisfies the differential equation if $\alpha^2 = 1$, i.e.:

$$\psi(u) = Au^k\exp(-u^2/2) + Bu^k\exp(+u^2/2)$$

but we cannot hope to normalize the wave function unless the B term is zero. So we conclude that the limiting behavior of the wave function we want is:

$$\psi(u) = Au^k\exp(-u^2/2)$$

This leads us to try a solution of the form:

$$\psi(u) = h(u)\exp(-u^2/2)$$

where $h(u)$ is any function of u. Note that we are no longer making any approximation. We can express any wave function this way. We are just hopeful the differential equation for $h(u)$ will be easier to solve than the differential equation for $\psi(u)$, because the asymptotic behavior has been factored out. Trying it out:

$$\frac{d\psi}{du} = \left(\frac{dh}{du} - u\,h(u)\right)\,e^{-u^2/2}$$

and

$$\frac{d^2\psi}{du^2} = \left(\frac{d^2h}{du^2} - 2u\frac{dh}{du} + (u^2-1)h(u)\right)\,e^{-u^2/2}$$

the TISE becomes:

$$\begin{aligned}\left(\frac{d^2h}{du^2} - 2u\frac{dh}{du} + (u^2-1)h(u)\right)\,e^{-u^2/2} &= (u^2-\epsilon)\\ \left(\frac{d^2h}{du^2} - 2u\frac{dh}{du} + (\epsilon-1)h(u)\right)\,e^{-u^2/2} &= 0\end{aligned}$$

but $e^{-u^2/2}$ is nowhere zero, so we are left with the TISE for $h(u)$ as:

$$\frac{d^2h}{du^2} - 2u\frac{dh}{du} + (\epsilon-1)h(u) = 0 \tag{2.27}$$

We will solve it with everyones least favorite method: power series. We assume:

$$h(u) = \sum_{m=0}^{\infty} a_m u^m$$

then calculate:

$$\frac{dh}{du} = \sum_{m=0}^{\infty} m a_m u^{m-1}$$

and

$$\frac{d^2h}{du^2} = \sum_{m=0}^{\infty} m(m-1)a_m u^{m-2}$$

Then we start collecting terms from the LHS of the Equation 2.27:

$$(\epsilon-1)\;h(u) = \sum_{m=0}^{\infty}(\epsilon-1)\;a_m u^m$$

and:

$$-2u\,\frac{dh}{du} = \sum_{m=0}^{\infty} -2\,m\,a_m\,u^m$$

which to our good fortune have the same power of u for each value of m. But that is not the case for the second derivative, which we will reproduce here as:

$$\frac{d^2h}{du^2} = \sum_{n=2}^{\infty} n(n-1)a_n u^{n-2}$$

with the index in the sum changed to n (for simplicity below) and where the first two terms have been omitted from the sum as they are both zero. To line up nicely with the first two series, we need to have the term m be a power u^m so substituting $m = n - 2$ we get:

$$\frac{d^2h}{du^2} = \sum_{m=0}^{\infty}(m+2)(m+1)a_{m+2}u^m$$

and the TISE for $h(u)$ becomes:

$$\sum_{m=0}^{\infty}\left[(\epsilon - 1)\, a_m - 2\, m\, a_m + (m+2)(m+1)a_{m+2}\right] u^m = 0$$

to be zero everywhere, the coefficients of every power of u must vanish, leading to:

$$(\epsilon - 1)\, a_m - 2\, m\, a_m + (m+2)(m+1)a_{m+2} = 0$$

which can be written as the recursion relationship:

$$a_{m+2} = \frac{2m + 1 - \epsilon}{(m+2)(m+1)}\, a_m$$

which appears on a first glance to solve the problem. This recursion relation will give all the even a_m starting from a_0 and all the odd a_m starting from a_1. Noting that:

$$h(0) = a_0$$

and

$$h'(0) = a_1$$

it seems that given two initial conditions, we obtain the corresponding solution $h(u)$ as a series. We can break this solution into two solutions, an even solution and an odd solution:

$$h(u) = h_{\text{even}}(u) + h_{\text{odd}}$$

with:

$$h_{\text{even}}(u) = a_0 + a_2\, u^2 + a_4\, u^4 + \ldots$$

and

$$h_{\text{odd}}(u) = a_1\, u + a_3\, u^3 + a_5\, u^5 + \ldots$$

But on a closer look, it seems we are in deep trouble for two reason. First, we expected (as in the infinite square well) to find that we had solutions only for certain values of the energy (*epsilon* here) but these recursion relations give a solution for any value of ϵ. Secondly, for large m the recursion relationship becomes:

$$a_{m+2} \approx \frac{2}{j}\, a_m$$

which looks like **bad news**. Let's start with $h_{\text{even}}(u)$. Picking some large even number $2n$ and defining (you see why shortly):

$$C \equiv a_{2n} n!$$

we have:

$$a_{2(n+1)} \approx \frac{1}{n}\, a_{2n} \approx \frac{1}{n+1}\, a_{2n} = \frac{C}{(n+1)!}$$

and it keeps going:

$$a_{2(n+2)} \approx \frac{C}{(n+2)!}$$

So the asymptotic behavior of h_{even} is:

$$h_{\text{even}}(u) \approx \sum_{n=0}^{\infty} \frac{C}{n!} u^{2n} = C \exp(u^2)$$

and so:

$$\psi(u) \approx h_{\text{even}}(u) \exp(-u^2/2) \approx C \exp(u^2/2)$$

which we cannot possibly normalize. In fact, this is **exactly** the unusable solution to the TISE at large u that we threw away, coming back to us. You might hope that $h_{\text{odd}}(u)$ can save the day, but we can pick a large odd number $2n+1$ and proceed in exact same manner to find that $h_{\text{odd}}(u)$

There is only one way out of this predicament. The series must terminate at some coefficient a_n. Looking back at Equation **??** we see that if:

$$2n + 1 - \epsilon = 0$$

then $a_{n+2} = 0$. Recalling our definition for ϵ we see that:

$$E = \hbar\omega \left(n + \frac{1}{2} \right) \tag{2.28}$$

The highest power term in the series defining $h(u)$ will be u^n, with the asymptotic before of $\psi(u)$ now:

$$\psi(u) \;\approx\; h(u)\, \exp(-u^2/2) \;\approx\; C\, u^n\, \exp(-u^2/2)\, dx$$

this is precisely the nice behavior we choose at the very start.

We can work out explicit solutions. It's convenient to rewrite the recursion formula in terms of the quantum number n instead of $\epsilon = 2n+1$:

$$a_{m+2} = \frac{-2(n-m)}{(m+2)(m+1)}\, a_m \tag{2.29}$$

For $n = 0$, the last term is a_0, so we have simply $h_0(u) = a_0$ and so

$$\psi_0(u) = a_0 e^{-u^2/2}$$

For $n = 1$, the last term is a_1, and so $h_1 = a_1 u$ and

$$\psi_1(u) = a_1 u e^{-u^2/2}$$

For $n = 2$, the last term is a_2, with $a_2 = -2a_0$ and so and so $h_2 = a_0\,(1 - 2u^2)$ and

$$\psi_2(u) = a_0\,(1 - 2u^2)\, e^{-u^2/2}$$

The polynomials are know as the Hermite polynomials $H_n(u)$. They can be most "easily" obtained from the Taylor expansion of the generating function:

$$\exp(-z^2 + 2zu) = \sum_{n=0}^{\infty} \frac{z_n}{n!} H_n(u)$$

with this convention, the normalized stationary states for the harmonic oscillator are:

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(u) e^{-u^2/2}$$

where

$$u \equiv \sqrt{\frac{m\omega}{\hbar}}\, x$$

.

2.6.2 Algebraic Method

We write the Hamiltonian for the harmonic oscillator in terms of the position and momentum operators:

$$\hat{H} = \frac{1}{2m}\left[\hat{p}^2 + (m\omega\hat{x})^2\right]$$

In this problem, the only parameter is ω, the frequency of the classical harmonic oscillator, and so $\hbar\omega$ has units of energy. It's reasonable to consider the dimensionless quantity:

$$\frac{\hat{H}}{\hbar\omega} = \frac{\hat{p}^2 + (m\omega\hat{x})^2}{2\hbar m\omega} = \frac{1}{2}\left(\left(\frac{\hat{p}}{p_0}\right)^2 + \frac{m\omega\hat{x}^2}{\hbar}\right)$$

As before, we define:

$$x_0 \equiv \sqrt{\frac{\hbar}{m\omega}}$$

and also:

$$p_0 \equiv \frac{\hbar}{x_0} = \sqrt{\hbar m\omega}$$

so:

$$\frac{\hat{H}}{\hbar\omega} = \frac{1}{2}\left[\left(\frac{\hat{p}}{p_0}\right)^2 + \left(\frac{\hat{x}}{x_0}\right)^2\right]$$

The algebraic solution we will use here is based on the observation that we can factor the dimensionless product in square brackets. If these were ordinary real numbers we would have:

$$\alpha^2 + \beta^2 = (\alpha + i\beta)(\alpha - i\beta)$$

so we'll define:

$$\begin{aligned} \hat{a}_- &\equiv \frac{1}{\sqrt{2}}\left(i\frac{\hat{p}}{p_0} + \frac{\hat{x}}{x_0}\right) \\ \hat{a}_+ &\equiv \frac{1}{\sqrt{2}}\left(-i\frac{\hat{p}}{p_0} + \frac{\hat{x}}{x_0}\right) \end{aligned}$$

there are other possible choices for the sign and which term is made imaginary, and these would work as well in what follows, but this choice will give us the most conventional notation for our results. We calculate:

$$\begin{aligned} \hat{a}_+\,\hat{a}_- &= \frac{1}{2}\left[\left(\frac{\hat{p}}{p_0}\right)^2 + \left(\frac{\hat{x}}{x_0}\right)^2 + i\,\frac{\hat{x}\hat{p} - \hat{p}\hat{x}}{x_0\,p_0}\right] \\ &= \frac{\hat{H}}{\hbar\omega} + i\,\frac{[\hat{x},\hat{p}]}{\hbar} \end{aligned}$$

where we have noted that $x_0 p_0 = \hbar$. Using the canonical commutation relation $[\hat{x},\hat{p}] = i\hbar$:

$$\hat{a}_+\,\hat{a}_- = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2}$$

and a similar calculation gives:

$$\hat{a}_-\,\hat{a}_+ \;=\; \frac{\hat{H}}{\hbar\omega} \;+\frac{1}{2}$$

so that:

$$[\hat{a}_-, \hat{a}_+] \;=\; \hat{a}_-\,\hat{a}_+ - \hat{a}_+, \hat{a}_- \;=\; 1 \tag{2.30}$$

and

$$\hat{H} = \hbar\omega \left(\hat{a}_+\hat{a}_- + \frac{1}{2} \right) \tag{2.31}$$

These two equations contain everything that we need. Let's start by calculating:

$$\begin{aligned}
[\hat{H}\,,\, \hat{a}_+] &= \hbar\omega\, [\hat{a}_+\hat{a}_-, \hat{a}_+] \\
&= \hbar\omega\, \left(\hat{a}_+\hat{a}_-\hat{a}_+ - \hat{a}_+\hat{a}_+\hat{a}_-\right) \\
&= \hbar\omega\, \hat{a}_+(\hat{a}_-\hat{a}_+ - \hat{a}_+\hat{a}_-) \\
&= \hbar\omega\, \hat{a}_+[\hat{a}_-, \hat{a}_+] \\
&= \hbar\omega\, \hat{a}_+
\end{aligned}$$

Similarly

$$[\hat{H}, \hat{a}_-] = -\hbar\omega\hat{a}_-$$

So now suppose we have a solution to the TISE, so that:

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

then we also have:

$$\begin{aligned}
\hat{H}\,(\hat{a}_+\Psi) &= \left(\hat{H}\hat{a}_+\right)\,\Psi \\
&= \left(\hat{H}\hat{a}_+ \;-\; \hat{a}_+\hat{H} \;+\; \hat{a}_+\hat{H}\right)\,\Psi \\
&= \left([\hat{H}, \hat{a}_+] \;+\; \hat{a}_+\hat{H}\right)\,\Psi \\
&= \left(\hbar\omega\,\hat{a}_+ \;+\; \hat{a}_+\hat{H}\right)\,\Psi \\
&= \left(\hbar\omega\,\hat{a}_+ \;+\; \hat{a}_+\,E\right)\,\Psi \\
&= \left(E \;+\; \hbar\omega\right)\,\left(\hat{a}_+\,\Psi\right)
\end{aligned}$$

which shows that $\hat{a}_+\Psi$ is a new solution to the TISE with energy $E + \hbar\omega$. A similar calculation shows that:

$$\hat{H}\,(\hat{a}_-\Psi) = (E - \hbar\omega)\,(\hat{a}_-\Psi)$$

that is $\hat{a}_-\Psi$ is a new solution to the TISE with energy $E + \hbar\omega$.

So evidently, given even one solution to the TISE, we can find an infinite number of new states at higher energy by successive applications of $\hat{a}_+$. But what of $\hat{a}_-$? We know that the energy of a normalizable wave function must be greater than zero. So there must be a ground state, let's call it Ψ_0 such that:

$$\hat{a}_-\Psi_0 = 0 \tag{2.32}$$

What is the energy of the ground state? We can "ask" the Hamiltonian:

$$\begin{aligned}\hat{H}\psi_0 &= \hbar\omega\left(a_+a_- + \frac{1}{2}\right)\psi_0 \\ &= \frac{\hbar\omega}{2}\psi_0 + \hbar\omega a_+\left(a_-\psi_0\right) \\ &= \frac{\hbar\omega}{2}\psi_0\end{aligned}$$

So the ground state has energy $E_0 = \hbar\omega/2$ and we have:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \qquad\qquad n = 0, 1, 2, \ldots \tag{2.33}$$

Take a look back at what a different way of doing business this has been. We have determined the entire energy spectrum from Equations 2.30 and 2.31 using nothing but algebra.

Let's see how far we can take this.

$$\begin{aligned}\hat{H}\psi_n &= E_n\psi_n \\ \hbar\omega\left(a_+a_- + \frac{1}{2}\right)\psi_n &= \hbar\omega\left(n + \frac{1}{2}\right)\psi_n \\ \hat{a}_+\hat{a}_-\psi_n &= n\psi_n\end{aligned}$$

Also:

$$\begin{aligned}\hat{a}_-\hat{a}_+\psi_n &= \left(\hat{a}_+\hat{a}_- + [\hat{a}_-, \hat{a}_+]\right)\psi_n \\ &= (n+1)\psi_n\end{aligned}$$

From their definition, we have:

$$\hat{x} = \frac{x_0}{\sqrt{2}}\left(a_+ + a_-\right)$$

and

$$\hat{p} = \frac{i\,p_0}{\sqrt{2}}\left(a_+ - a_-\right)$$

So we can calculate:

$$x^2 = \frac{x_0^2}{2}\left(a_+^2 + a_+a_- + a_-a_+ + a_-^2\right)$$

and so:

$$V(x) = \frac{1}{2}m\omega^2x^2 = \frac{\hbar\omega}{4}\left(a_+^2 + a_+a_- + a_-a_+ + a_-^2\right)$$

with

$$\langle V\rangle = \frac{\hbar\omega}{4}\int_{-\infty}^{+\infty}\psi_n^*\left(a_+^2 + a_+a_- + a_-a_+ + a_-^2\right)\psi_n\,dx$$

This integral vanishes:

$$\int_{-\infty}^{+\infty}\psi_n^* a_+^2\psi_n dx = k\int_{-\infty}^{+\infty}\psi_n^*\psi_{n-2}dx = 0$$

as does the integral involving a_-^2 leaving only:

$$\langle V\rangle = \frac{\hbar\omega}{4}(n+n+1) = \frac{\hbar\omega}{2}\left(n + \frac{1}{2}\right) = \frac{E_n}{2}$$

In principle we can calculate any classical dynamical variable in terms of the a's.

2.7 The Free Particle

We now consider the free particle, for which

$$V(x) = 0$$

and the TISE is:

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

which can be written as:

$$\frac{d^2\psi}{dx^2} = -k^2\psi(x), \qquad\qquad k \equiv \frac{\sqrt{2mE}}{\hbar}.$$

This so far looks exactly like the infinite square well, except that there are no restrictions on the allowed energies beyond $E > 0$. (Why must $E > 0$?) We know well the solutions to this differential equation but in this context we prefer the complex exponentials

$$\psi(x) = A\,e^{ikx} \;+\; B\,e^{-ikx}$$

over the sines and cosines, because the former will combine conveniently with the wiggle factor[2] To determine the wiggle factor we note that:

$$E = \frac{\hbar^2 k^2}{2m}, \qquad\qquad \frac{E}{\hbar} = \frac{\hbar k^2}{2m} \equiv \omega$$

and so

$$\phi(t) \;=\; e^{-iEt/\hbar} \;=\; e^{-i\omega t}$$

which we use to get the full wave function:

$$\Psi(x,t) = A\,e^{i(kx-\omega t)} + B\,e^{-i(kx+\omega t)}$$

For visualization, it is useful to consider the real part of $\Psi(x,t)$:

$$\mathrm{Re}(\Psi(x,t)) = A\,\cos(kx-\omega t) + B\cos(kx+\omega t)$$

Any function $f(x \pm |v|t)$ is a traveling wave. Suppose for convenience that $f(x)$ has some distinctive feature (like a local minimum) at $x = 0$, then for $f(x \pm |v|t)$, at some later time t this feature will be located where:

$$x \pm |v|\,t = 0, \qquad\qquad x = \mp|v|t$$

The same analysis for any feature of $f(x)$ leads to the same conclusion, and so $f(x)$ is simply translated unchanged left or right along the x axis over time with speed $|v|$.

In this case, the speed is $|v| = \omega/k$. Note that as defined $\omega > 0$ and $k > 0$. Note, however, that our two solutions (with coefficients A and B) just differ by the sign in front of k. So we might as well take k as a signed parameter and consider only one exponential function:

$$\Psi_k(x,t) = Ae^{i(kx-\omega t)} \tag{2.34}$$

where

$$k = \pm\frac{\sqrt{2mE}}{\hbar} \tag{2.35}$$

[2]Why can't the wiggle factor be a sine or cosine? Have a look back at how we determined it!

and the sign of k indicates the direction of the traveling wave:

$$\begin{aligned} k > 0 \quad &\Longrightarrow \quad \text{wave is traveling right} \\ k < 0 \quad &\Longrightarrow \quad \text{wave is traveling left} \end{aligned}$$

The quantity ω/k is signed now as well, so it is a velocity, which we call the phase velocity:

$$v_{\text{phase}} = \frac{\omega}{k} \tag{2.36}$$

There are few more important things to notice about the free particle solution in Equation 2.34:

- The wave completes one cycle when x advances by one wave length λ, so $k(\lambda - 0) = 2\pi$, and:

$$k = \pm\frac{2\pi}{\lambda}$$

- The wave competes one cycle when the time advances by one period T, so $\omega(T - 0) = 2\pi$, and:

$$\omega = \frac{2\pi}{T}$$

- The phase velocity is:

$$v_{\text{phase}} = \frac{\omega}{k} = \pm\frac{\lambda}{T}$$

We have found that for the free particle:

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

As we have established that the sign of k indicates the direction of the particle, we conclude:

$$p = \hbar k \tag{2.37}$$

and

$$|p| = \hbar|k| = \frac{2\pi\hbar}{\lambda} \tag{2.38}$$

This the de Broglie formula that relates a particles momentum to its wavelength. We assumed the SE and derived the de Broglie formula. But one can instead start from the de Broglie formula and deduce the SE.

We can calculate:

$$|\Psi_k(x,t)|^2 = \left(Ae^{i(kx-\omega t)}\right)\left(Ae^{i(kx-\omega t)}\right)^* = |A|^2$$

which shows that Ψ_k has no time dependence, as expected for a stationary state. But it can't be normalized:

$$\int_{-\infty}^{+\infty} |\Psi_k(x,t)|^2 dx = |A|^2 \int_{-\infty}^{+\infty} dx = \infty$$

We'll need some more mathematical tools to tackle this problem...

2.8 Fourier Series for Complex Functions

The Fourier series for a periodic function with period a can be expressed in terms of the complex exponential by noting that:

$$\sin\theta = \frac{e^{i\theta}-e^{-i\theta}}{2i}$$
$$\cos\theta = \frac{e^{i\theta}+e^{-i\theta}}{2}$$

In the Appendix, we determine the Fourier series in terms of complex exponentials, and how to calculate the Fourier coefficients, by plugging Euler's Identities into the Fourier series for sines and cosines and working carefully through the bookkeeping to arrive at the corresponding formula's for the complex exponential. This is satisfying and instructive to see, but a bit on the tedious side. Let's see if we can cut right to chase instead, using our insights from vector space.

First off, note that the periodic complex functions with period a form a vector space just as well as periodic real functions. Next, note that a periodic complex functions $\psi(x)$ has a Fourier series, as we can just write:

$$\psi(x) = f(x) + ig(x)$$

for real periodic functions $f(x)$ and $g(x)$, which each have a Fourier series. And each sine and cosine can be written in terms of complex exponentials. So we've concluded that Fourier's Theorem combined with the Euler Identities leads to conclusion that and complex periodic function with period a has a Fourier series representation in terms of complex exponentials, that is:

$$\psi(x) = \sum_{n=-\infty}^{\infty} c_n\, e_n(x) \tag{2.39}$$

where

$$e_n(x) \equiv A\exp\left(i\,\frac{2\pi n x}{a}\right)$$

and A is some normalization factor. Notice that the Fourier coefficients now extend to $-\infty$, that's because Euler's identities contain $e^{i\theta}$ and $e^{-i\theta}$. (Remember, this is all worked out carefully in the Appendix if you find this too hand wavy.)

So all that we need is to show that these new $e_n(x)$ are orthonormal. And here we encounter our first problem:

$$\int_{-a/2}^{a/2} e_n(x)e_n(x)dx \;=\; A^2\int_{-a/2}^{a/2}\exp\left(i\,\frac{4\pi n x}{a}\right)dx \;\propto\; \exp(2\pi n)-\exp(-2\pi n) = 0$$

What is going on here? It's zero because the complex exponential is periodic, with equal parts positive and negative, and so the integral is vanishing. But this didn't happen for our sines and cosines, because e.g.:

$$\int_{-a/2}^{a/2}\sin^2\left(\frac{2\pi n x}{a}\right)dx = \frac{a}{2}$$

The difference is that $\sin\theta$ is a real valued function, so $\sin^2\theta$ is non-negative. But $(e^{i\theta})^2$ can be negative, because $e^{i\theta}$ is a complex number. For example, $e^{i\pi/2} = i$, so $\left(e^{i\pi/2}\right)^2 = -1$. With this understood, we know exactly what we have to do, we want the integral to be:

$$\int_{-a/2}^{a/2}|e_n(x)|^2dx \;=\; \int_{-a/2}^{a/2}e_n^*(x)e_n(x)dx \;=\; |A|^2\int_{-a/2}^{a/2}1dx = |A|^2a \tag{2.40}$$

since we want to set this normalization integral to one, we conclude $|A|^2 = 1/a$. We might as well choose the positive real solution, so:

$$e_n(x) \equiv \sqrt{\frac{1}{a}} \exp\left(i \frac{2\pi n x}{a}\right) \tag{2.41}$$

But we need to modify our inner product so that we obtain the normalization integral in Equation 2.40 when we take the inner product of $e_n(x)$ with itself. That is easily accomplished by defining the inner product of **complex** valued functions $f(x), g(x) \in \mathbb{C}$ as:

$$\langle f|g\rangle = \int_{-\frac{a}{2}}^{\frac{a}{2}} f^*(x) g(x) dx \tag{2.42}$$

It is left as an exercise to show that using this definition of inner product, we have:

$$\langle e_n|e_m\rangle = \delta_{nm} \tag{2.43}$$

And thus we can determine the Fourier coefficients in the usual way via Fourier's trick:

$$\begin{aligned}
\psi(x) &= \sum_{m=-\infty}^{\infty} c_m \, e_m(x) \\
\langle e_n|\psi\rangle &= \langle e_n| \sum_{m=-\infty}^{\infty} c_m \, e_m\rangle \\
&= \sum_{m=-\infty}^{\infty} c_m \, \langle e_n|e_m\rangle \\
&= \sum_{m=-\infty}^{\infty} c_m \delta_{nm} \\
&= c_n
\end{aligned}$$

That is:

$$c_n = \langle e_n|f\rangle \tag{2.44}$$

2.9 Fourier Transform

The Fourier series for a periodic complex valued function $\psi(x)$ with period a is:

$$\psi(x) = \sum_n c_n e_n(x)$$

Here it will be useful to define the wave number

$$k_n \equiv \frac{2\pi n}{a} \tag{2.45}$$

with

$$e_n(x) = \sqrt{\frac{1}{a}} \exp(i \, k_n \, x)$$

As always the Fourier coefficients are determined as

$$c_n = \langle e_n|\psi\rangle = \int_{-\frac{a}{2}}^{\frac{a}{2}} e_n^*(x)\psi(x)dx$$

Consider the function:

$$\phi(x) = \begin{cases} \psi(x) & -\frac{a}{2} \leq x \leq \frac{a}{2} \\ \psi\left(\frac{a}{2}\right) & \text{otherwise} \end{cases} \tag{2.46}$$

and convince yourself of two things:

- $\phi(x)$ need not be a periodic function (and in fact $\phi(x)$ is a very trivial function if it is).
- Nonetheless, we can calculate it's Fourier coefficients in the usual way:

  $$c_n = \langle e_n, \phi\rangle$$

  and they will work perfectly well:

  $$\phi(x) = \sum_n c_n e_n(x)$$

  as long as we restrict ourselves to:

  $$-\frac{a}{2} \leq x \leq \frac{a}{2}$$

  .

We are going to extend the Fourier series to apply to any function $\psi(x)$ for which $\psi(x) \to 0$ as $x \to \pm\infty$.

- In the limit $a \to \infty$, then

  $$\psi(-a/2) \to 0, \qquad \psi(a/2) \to 0,$$

  so

  $$\psi(-a/2) \to \psi(a/2)$$

  and so $\psi(x)$ has a Fourier series valid in

  $$[-a/2, a/2] \to [-\infty, \infty].$$

- In the limit $a \to \infty$

  $$k_{n+1} - k_n = \frac{2\pi}{a} \to 0$$

  so we can now pick any value of k_n we want, without concern for n, so we write:

  $$k_n \to k$$

  k has become a continuous variable.

Next we will turn our attention to the Fourier coefficients:

$$c_n = \frac{1}{\sqrt{a}} \int_{-a/2}^{a/2} \psi(x)\, e^{-ik_n x} dx$$

In the limit $a \to \infty$

$$k_n \to k$$

and considering just the integral:

$$\int_{-a/2}^{a/2} \psi(x)\, e^{-ik_n x} dx \quad \to \quad C(k) \quad \equiv \quad \int_{-\infty}^{\infty} \psi(x)\, e^{-ikx} dx$$

where, as is our right as physicists, we bravely assume $C(k)$ is a well defined integral. Now evidently in this limit:

$$c_n \to \frac{C(k)}{\sqrt{a}} = 0$$

which is not very useful. The Fourier coefficients as we defined them carried a normalization factor that vanishes as $a \to \infty$. More useful will be the quantity

$$\left(\sqrt{a}\; c_n\right) \;\to\; C(k)$$

which will show up again below.

Next we consider the Fourier series itself:

$$\psi(x) = \sum_n c_n e_n(x) = \frac{1}{\sqrt{a}} \sum_n c_n e^{ik_n x}$$

and recalling:

$$k_{n+1} - k_n = \frac{2\pi}{a}$$

so that we can write:

$$\psi(x) = \frac{1}{2\pi} \sum_n (\sqrt{a}\, c_n)\; e^{ik_n x}\; (k_{n+1} - k_n)$$

Now in the limit $a \to \infty$ the quantity

$$k_{n+1} - k_n$$

becomes infinitesimal and the sum becomes an integral:

$$\psi(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} C(k)\; e^{ik_n x}\; dk$$

For a symmetric definition we define the Fourier transform of $\psi(x)$ as:

$$\widetilde{\psi}(k) \equiv \frac{C(k)}{\sqrt{2\pi}}$$

so that:

$$\widetilde{\psi}(k) \;=\; \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x)\; e^{-ikx}\; dx \qquad (2.47)$$

$$\psi(x) \;=\; \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{\psi}(k)\; e^{ikx}\; dk \qquad (2.48)$$

2.10 Wave Packet

We saw before that the stationary soluctions to the Schrodinger equation from the free particle are non-normalizable: they cannot represent the actual physics state of a particle. But we can still create a physically realizable state as the superposition of many stationary solutions, by making use of the Fourier Transform. Let's see how that works.

We are given a wave function at $\Psi(x, 0)$ at $t = 0$ describing the initial state. This function must be normalized. We calculate it's Fourier transform:

$$\widetilde{\Psi}(k, 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x, 0)\, e^{-ikx}\, dx$$

and so then we can write $\Psi(x, 0)$ as a integral of traveling waves:

$$\Psi(x, 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{\Psi}(k, 0)\, e^{ikx}\, dk$$

The beautiful thing is, we know the time dependence for each traveling wave e^{ikx} that appears in the integral. These are stationary solution the TISE, so they each have a wiggle factor:

$$\phi(t) = \exp\left(-i\frac{E_k t}{\hbar}\right) = \exp\left(-i\frac{\hbar k^2}{2m}t\right)$$

where we have used:

$$E_k = \frac{\hbar^2 k^2}{2m}$$

so we have:

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{\Psi}(k, 0)\, \exp\left[ik\left(x - \frac{\hbar k}{2m}t\right)\right]\, dk$$

It is left as an exercise to show that this is indeed a solution to the SE. Just note that $\hat{H}$ and $-i\hbar\frac{\partial}{\partial t}$ both happily move inside the integral. Since it is a solution to the SE, it preserves its normalization. So as $\Psi(x, 0)$ must be normalized, $\Psi(x, t)$ is normalized as well.

The classical free particle has velocity

$$v_{\text{classical}} = \pm\sqrt{\frac{2E}{m}}$$

But the phase velocity is:

$$v_{\text{phase}} = \frac{\omega}{k} = \frac{E}{\hbar k} = \frac{E}{\sqrt{2mE}} = \sqrt{\frac{E}{2m}}$$

so:

$$v_{\text{phase}} = \frac{1}{2} v_{\text{classical}}$$

the wave is traveling at one half the speed of the corresponding classical particle.

But we already know that individual travelling waves do not represent physical states. It we want to describe a particle with a position and velocity, we need to build a wave packet: a burst of localized wave action. Your homework will include a very good example of a Gaussian wave packet, but we don't need to be so explicit here. Let's assume that the Fourier transform $\widetilde{\psi}(k, 0)$ of the wave packet is nonzero only close to a single value of k which we will call k_0. If this were not true, different parts of the wave packet will travel at different speeds, and the notion of the velocity of the particle will be poorly defined.

We'll write our wave packet like this:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{\Psi}(k,0)\, e^{i(kx - \omega(k)t)}\, dk$$

Now in our specific case:

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

but we are keeping things more general here. Since our wave packet is zero unless k is near k_0, we can Taylor expand $\omega(k)$ about k_0:

$$\omega(k) = \omega(k_0) + \omega'(k_0)(k - k_0)$$

And so we can write:

$$\begin{aligned}
\Psi(x,t) &= \frac{1}{\sqrt{2\pi}} e^{i(k_0 x - \omega(k_0)t)} \int_{-\infty}^{\infty} \widetilde{\Psi}(k,0)\, e^{i(k-k_0)(x - \omega'(k_0)t)}\, dk \\
&= e^{i(k_0 x - \omega(k_0)t)}\, F(x - \omega'(k_0)t)
\end{aligned}$$

for some complex function F. The first term in the product is a travelling wave moving at the phase velocity:

$$v_{\text{phase}} = \left.\frac{\omega(k)}{k}\right|_{k_0}$$

and the second is an envelope, that locally sets the amplitude of the travelling wave. It is moving at what is called the group velocity:

$$v_{\text{group}} = \omega'(k_0) = \left.\frac{d\omega}{dk}\right|_{k_0}$$

For the free particle:

$$\omega = \frac{E}{\hbar} = \frac{\hbar k^2}{2m}$$

So:

$$v_{\text{group}} = 2 v_{\text{phase}} = v_{\text{classical}}$$

That is, the wave packet travels at the classical speed of the particle.

2.11 Hermetian Adjoints and Hermetian Operators

The normalizable wave functions are a vector space over the complex numbers, with an inner product:

$$\langle f|g\rangle \equiv \int_{-\infty}^{\infty} f^*(x)\, g(x)\, dx \tag{2.49}$$

We can now recognize the normalization condition as a requirement on the inner product of the wave function with itself:

$$\langle \Psi|\Psi\rangle \equiv \int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1 \tag{2.50}$$

Expectation values are inner products as well:

$$\langle O\rangle = \langle\Psi|\hat{O}\Psi\rangle \equiv \int_{-\infty}^{\infty} \Psi^*(x,t)\hat{O}\Psi(x,t)dx \tag{2.51}$$

For an operator $\hat{O}$ we[3] define it's Hermitian adjoint (or conjugate) $\hat{O}^\dagger$ by the property:

$$\langle f|\hat{O}^\dagger g\rangle = \langle\hat{O}f|g\rangle \tag{2.52}$$

That is $\hat{O}^\dagger$ operating on g (i.e. in the "usual place") gives a result equivalent to the original operator $\hat{O}$ acting on f (i.e. in the "unusual place"). Explicitly in terms of the integral definition of the inner product:

$$\int_{-\infty}^{\infty} f^*(x,t)\hat{O}^\dagger g(x,t)dx = \int_{-\infty}^{\infty} \left(\hat{O}f(x,t)\right)^* g(x,t)dx \tag{2.53}$$

So, to find the Hermetian adjoint of an operator $\hat{O}$, operate $\hat{O}$in the "unusual spot", then perform whatever manipulations are required to bring the operator over to the "usual spot". Then read off the operator $\hat{O}^\dagger$.

For the operator $\hat{x}$:

$$\int_{-\infty}^{\infty} f^*(x)\hat{x}^\dagger g(x)dx = \int_{-\infty}^{\infty} (xf(x))^* g(x)dx = \int_{-\infty}^{\infty} xf^*(x)g(x)dx = \int_{-\infty}^{\infty} f^*(x)xg(x)dx$$

So:

$$\hat{x}^\dagger = \hat{x} \tag{2.54}$$

For a complex number z:

$$\int_{-\infty}^{\infty} f^*(x)z^\dagger g(x)dx = \int_{-\infty}^{\infty} (zf(x))^* g(x)dx = \int_{-\infty}^{\infty} z^*f^*(x)g(x)dx = \int_{-\infty}^{\infty} f^*(x)z^*g(x)dx$$

So:

$$z^\dagger = z^* \tag{2.55}$$

For a single derivative:

$$\int_{-\infty}^{\infty} f^*(x)\left(\frac{\partial}{\partial x}\right)^\dagger g(x)dx = \int_{-\infty}^{\infty} \left(\frac{\partial f}{\partial x}\right)^* g(x)dx = -\int_{-\infty}^{\infty} f^*(x)\frac{\partial g}{dx}dx$$

where we used integration by parts in the last step (and assumed f and g vanish at the boundaries.

$$\left(\frac{\partial}{\partial x}\right)^\dagger = -\frac{\partial}{\partial x} \tag{2.56}$$

It is left as an exercise to show:

$$\hat{p}^\dagger = \hat{p} \tag{2.57}$$

When an operator has the property $\hat{o}^\dagger = \hat{o}$ we say that it is hermetian.

$$\langle o\rangle = \langle\Psi|\hat{o}\Psi\rangle = \langle\Psi|\hat{o}^\dagger\Psi\rangle = \langle\hat{o}\Psi|\Psi\rangle = \overline{\langle\Psi|o\Psi\rangle} = \langle o\rangle^* \tag{2.58}$$

Expectations values of hermetian operators are real, and so we associate physical observables with hermetian operators.

It is left as an exercise to show that our definition is equivalent to Griffith's and others:

$$\langle f|\hat{O}g\rangle = \langle\hat{O}^\dagger f|g\rangle$$

Hint: just take the complex conjugate of both sides of the equation.

[3]Some authors (most?) define this differently, but you'll show that our definition is equivalent.

2.12 Orthogonality of the Stationary Solutions

It is left as an exercise, to show that the Hamiltonian is a Hermetian operator:

$$\hat{H}^\dagger = \hat{H}$$

Now suppose we have two solutions to the TISE $\psi_n(x)$ and $\psi_m(x)$ with:

$$\hat{H}\psi_n(x) = E_n\psi_n(x), \qquad \hat{H}\psi_m(x) = E_m\psi_m(x)$$

Now notice that:

$$\begin{aligned} \langle\psi_m|\hat{H}\psi_n\rangle &= \langle\psi_m|E_n\psi_n\rangle \\ &= E_n \langle\psi_m|\psi_n\rangle \end{aligned}$$

but also, as $\hat{H}^\dagger = \hat{H}$, we have:

$$\begin{aligned} \langle\psi_m|\hat{H}\psi_n\rangle &= \langle\hat{H}\psi_m|\psi_n\rangle \\ &= \langle E_m\psi_m|\psi_n\rangle \\ &= E_m \langle\psi_m|\psi_n\rangle \end{aligned}$$

Why isn't it E_m^* in the last step? So now we have:

$$(E_m - E_n)\langle\psi_m|\psi_n\rangle = 0$$

That is, if $E_m \neq E_n$,

$$\langle\psi_m|\psi_n\rangle = 0 \tag{2.59}$$

For the cases we've seen so far, $E_n \neq E_m$ for $n \neq m$, so we see that our assumption that the stationary solutions are orthogonal was sound. We'll handle the case of degeneracy (different states having same energy) later.

2.13 Ladder Operators Revisited

Recall our ladder operators:

$$\begin{aligned} \hat{a}_- &\equiv \frac{1}{\sqrt{2}}\left(i\frac{\hat{p}}{p_0} + \frac{\hat{x}}{x_0}\right) \\ \hat{a}_+ &\equiv \frac{1}{\sqrt{2}}\left(-i\frac{\hat{p}}{p_0} + \frac{\hat{x}}{x_0}\right) \end{aligned}$$

where:

$$x_0 \equiv \sqrt{\frac{\hbar}{m\omega}}, \qquad \text{and} \qquad p_0 \equiv \frac{\hbar}{x_0} = \sqrt{\hbar m\omega}.$$

with:

$$[\hat{a}_-, \hat{a}_+] = 1$$

and:

$$\hat{H} = \hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right)$$

We leave it as an exercise to show that $\hat{a}_-$ is the Hermetian adjoint of $\hat{a}_+$ and vice-versa, i.e.:

$$\begin{aligned} \hat{a}_- &= \hat{a}_+^\dagger \\ \hat{a}_+ &= \hat{a}_-^\dagger \end{aligned}$$

We showed that these operators act as raising and lowering operators:

$$\begin{aligned} \hat{a}_+\psi_n &= c_n\psi_{n+1} \\ \hat{a}_-\psi_n &= d_n\psi_{n-1} \end{aligned}$$

where:

$$\hat{H}\psi_n = E_n\psi_n$$

for:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

But we don't know the constants c_n and d_n yet, which is the only thing between us and rolling this machinery out to find the complete set of wave functions explicitly. We do have:

$$\begin{aligned} \hat{a}_+\hat{a}_-\psi_n &= n\,\psi_n \\ \hat{a}_-\hat{a}_+\psi_n &= (n+1)\,\psi_n \end{aligned}$$

The trick to determining c_n is to work out the expectation value for $\langle a_+a_-\rangle$ for the stationary state ψ_n in two different ways. First:

$$\begin{aligned} \langle a_+a_-\rangle &= \langle\psi_n|a_+a_-\psi_n\rangle \\ &= \langle\psi_n|n\psi_n\rangle \\ &= n\,\langle\psi_n|\psi_n\rangle \\ &= n \end{aligned}$$

and second, using $\hat{a}_+^\dagger = \hat{a}_-$:

$$\begin{aligned} \langle a_+a_-\rangle &= \langle\psi_n|\hat{a}_+\hat{a}_-\psi_n\rangle \\ &= \langle\hat{a}_+^\dagger\psi_n|\hat{a}_-\psi_n\rangle \\ &= \langle\hat{a}_-\psi_n|\hat{a}_-\psi_n\rangle \\ &= \langle c_n\psi_n|c_n\psi_n\rangle \\ &= c_n^*c_n\,\langle\psi_n|\psi_n\rangle \\ &= |c_n|^2 \end{aligned}$$

so we conclude that:

$$|c_n|^2 = n$$

A similar calculation shows:

$$|d_n|^2 = n+1$$

But there is (one!) arbitrary phase factor. It is left as an exercise to show that:

$$
\begin{aligned}
c_n &= \sqrt{n} \\
d_n &= \sqrt{n+1}
\end{aligned}
$$

are a mutually consistent choice of phase, and they keep the spatial wave functions real.

Now we can produce the explicit solutions by solving the (simple!) differential equation for the ground state:

$$\hat{a}_- \psi_0 = 0$$

to find $\psi_0(x)$ and then use:

$$\psi_n(x) = \frac{1}{n!} (\hat{a}_+)^n \psi_0$$

to get the rest!

2.14 The Dirac Delta Function

Note that the Fourier Transform of the Dirac delta function is:

$$\widetilde{\delta}(k) = \langle e_k, \delta \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \delta(x) e^{-ikx} dx = \frac{e^{-ik0}}{\sqrt{2\pi}} = \frac{1}{\sqrt{2\pi}}$$

and so we can write the Dirac delta function as:

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk$$

and so also:

$$\delta(x - x') = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x')} dk$$

and (by changing variables):

$$\delta(k - k') = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k-k')x)} dx$$

2.15 The Fourier Transform Revisited

Our inner product now extends between positive and negative infinity:

$$\langle \Psi, \phi \rangle \equiv \int_{-\infty}^{\infty} \Psi^*(x) \phi(x) \, dx \tag{2.60}$$

Our basis functions, which are now defined for any value of k,

$$e_k = \frac{1}{\sqrt{2\pi}} \exp(ikx) \tag{2.61}$$

are still orthonormal, but the condition looks a bit different in the continuum case:

$$\langle e_k, e_{k'} \rangle = \delta(k - k')$$

See the appendix for more details on the Dirac delta function $\delta(x)$, which is zero everywhere but at $x = 0$, where it is infinite. It is the continuous version of δ_{nm}.

Our basis functions are also still complete. In the discrete case we have a complex Fourier coefficient for every integer n. Now we have a complex Fourier coefficient for any real value of k. In place of Fourier coefficients, we have instead a function of k which we call the Fourier transform: $\widetilde{\Psi}(k)$. Instead of a sum over discrete terms, we now have to integrate over all values of k:

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{\Psi}(k) \exp(ikx)\, dk. \tag{2.62}$$

Just as in the discrete case, we determine the Fourier transform from the inner product:

$$\widetilde{\Psi}(k) = \langle e_k, \Psi \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x) \exp(-ikx)\, dx \tag{2.63}$$

Equation 2.63 is generally referred to as the *Fourier Transform*, while Equation 2.62 is referred to as the *Inverse Fourier Transform.*

2.16 The Fourier Transform in Quantum Mechanics

So far we have been considering the Fourier transform with respect to position x and wave-number k. A much more useful pair of variables for Quantum Mechanics turns out to be momentum p and position x. To relate p to k we need only apply the DeBroglie relation to the wavelength in the definition of the wavenumber:

$$k \equiv \frac{2\pi}{\lambda} = \frac{2\pi p}{h} = \frac{p}{\hbar}$$

We could therefore make the substitution $k \to p/\hbar$ (and $dk \to dp/\hbar$)) in Equations 2.62 and 2.63. It turns out that a marginally more useful equation results if we make the normalization factors symmetric, by splitting the normalization factor of $1/\hbar$ across both equations with $1/\sqrt{\hbar}$ applied to each:

$$\Psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \widetilde{\Psi}(p) \exp(ipx/\hbar)\, dp \tag{2.64}$$

$$\widetilde{\Psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x) \exp(-ipx/\hbar)\, dx \tag{2.65}$$

The major benefit of this symmetric form is that the normalization of $\Psi(x)$ and $\widetilde{\Psi}(p)$ in this case turns out to be the same:

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 dx = \int_{-\infty}^{\infty} |\widetilde{\Psi}(p)|^2 dp = 1$$

Because we can always calculate $\Psi(x)$ from $\widetilde{\Psi}(p)$ either one completely describes the quantum mechanical state. We call $\widetilde{\Psi}(p)$ the momentum wave function. Whereas $|\Psi(x)|^2$ gives us the probability density for the quanton to be at position x, $|\Psi(p)|^2$ gives us the probability density for the quanton to have momentum p.

2.17 Ladder Operators Revisited

Appendix A

Fourier Series for Complex Functions

The Fourier series for a periodic function with period a can be expressed in terms of the complex exponential by noting that:

$$\begin{aligned}\sin\theta &= \frac{e^{i\theta}-e^{-i\theta}}{2i}\\ \cos\theta &= \frac{e^{i\theta}+e^{-i\theta}}{2}\end{aligned}$$

so:

$$\begin{aligned}s_n(x) &= \sqrt{\frac{2}{a}}\,\sin\left(\frac{2\pi nx}{a}\right) = \frac{e_n(x)-e_n^*(x)}{i\sqrt{2}}\\ c_n(x) &= \sqrt{\frac{2}{a}}\,\cos\left(\frac{2\pi nx}{a}\right) = \frac{e_n(x)+e_n^*(x)}{\sqrt{2}}\end{aligned}$$

where:

$$e_n(x) \equiv \frac{1}{\sqrt{a}}\exp\left(i\,\frac{2\pi nx}{a}\right) \tag{A.1}$$

and note that:

$$c_0(x) = e_0(x)$$

So now the Fourier series for f(x) can be written:

$$\begin{aligned}f(x) &= A_0c_0(x) + \sum_{n=1}^{\infty}\{A_n\,c_n(x) + B_n\,s_n(x)\}\\ &= A_0e_0(x) + \sum_{n=1}^{\infty}\left\{A_n\,\frac{e_n(x)+e_n^*(x)}{\sqrt{2}} + B_n\,\frac{e_n(x)-e_n^*(x)}{i\sqrt{2}}\right\}\\ &= A_0e_0(x) + \sum_{n=1}^{\infty}\left\{\frac{A_n-iB_n}{\sqrt{2}}\,e_n(x) + \frac{A_n+iB_n}{\sqrt{2}}\,e_n^*(x)\right\}\end{aligned}$$

If we define the complex Fourier Coefficient

$$c_n \equiv \frac{A_n-iB_n}{\sqrt{2}} \qquad\qquad n = 1,2,3,\ldots$$

and put $c_0 \equiv A_0$ then we have:

$$f(x) = c_0 e_0(x) + \sum_{n=1}^{\infty} \{c_n\, e_n(x) + c_n^*\, e_n^*(x)\}$$

Furthermore, if we note that:

$$e_{-n}(x) = e_n^*(x)$$

and define:

$$c_{-n} \equiv c_n^* \tag{A.2}$$

we can write this all quite compactly:

$$f(x) = \sum_{n=-\infty}^{\infty} c_n\, e_n(x)$$

Now we need only work out how to calculate the complex Fourier coefficients c_n. For $n > 0$ we had

$$\begin{aligned} c_n &\equiv \frac{A_n - iB_n}{\sqrt{2}}. \\ &= \frac{1}{\sqrt{2}} \left\{ \sqrt{\frac{2}{a}} \int_{-\frac{a}{2}}^{\frac{a}{2}} f(x) \cos\left(\frac{2\pi n x}{a}\right) dx - i\frac{2}{a} \int_{-\frac{a}{2}}^{\frac{a}{2}} f(x) \sin\left(\frac{2\pi n x}{a}\right) dx \right\} \\ &= \frac{1}{\sqrt{a}} \int_{-\frac{a}{2}}^{\frac{a}{2}} f(x) \left\{ \cos\left(\frac{2\pi n x}{a}\right) - i \sin\left(\frac{2\pi n x}{a}\right) \right\} dx \\ &= \int_{-\frac{a}{2}}^{\frac{a}{2}} f(x)\, \frac{1}{\sqrt{a}} \exp\left(-i\frac{2\pi n x}{a}\right) dx \end{aligned}$$

or finally:

$$c_n = \int_{-\frac{a}{2}}^{\frac{a}{2}} f(x)\, e_n^*(x)\, dx$$

What's going on? It seems that to calculate the Fourier coefficient of the $e_n(x)$ we have to use it's complex conjugate $e_n^*(x)$ in the integral with $f(x)$. But we also expect to obtain these coefficients from the inner product of $f(x)$ and $e_n(x)$. The conclusion is that the definition of the inner product for a vector space of a complex scalar field must include complex conjugation. For $f(x), g(x) \in \mathbb{C}$ we have:

$$\langle f|g\rangle = \int_{-\frac{a}{2}}^{\frac{a}{2}} f^*(x) g(x) dx \tag{A.3}$$

With this definition of the inner product, we can determine the Fourier coefficient as expected:

$$c_n = \langle e_n|f\rangle \tag{A.4}$$

Exercise: Show that the definition of the inner product in Equation A.3 satisfies properties I1 and I4 of Table 2.1

Exercise: Using the definition of the inner product in Equation A.3, show that:

$$\langle e_n|e_m\rangle = \delta_{nm}$$

Exercise: Show that for a real function f, according to Equation A.4, then $c_{-n} = c_n^*$ as required in Equation A.2.

Exercise: Show that for a periodic function f

$$c_0\, e_0(x) = \langle e_0|f\rangle\, e_0(x) = \frac{1}{a}\int_{-a}^{a} f(x)dx$$

That is, the $n = 0$ term in the Fourier series is just the average value of the function.

Together these results show that this definition correctly and consistently covers all n, not just $n > 0$ for which it was derived.

Exercise: We've not yet considered the Fourier series of a complex periodic function $\psi(x)$. Suppose that real periodic functions $f(x)$ and $g(x)$ with period a have Fourier series:

$$f(x) = \sum_n a_n e_n(x)$$

and:

$$g(x) = \sum_n b_n e_n(x)$$

And suppose:

$$\psi(x) \equiv f(x) + ig(x)$$

Calculate the complex Fourier coefficients:

$$c_n = \langle e_n, \psi\rangle$$

and show that:

$$\sum_n c_n e_n(x) = f(x) + ig(x) \equiv \psi(x)$$

.

The previous exercise shows that these results hold for a complex valued periodic function $\psi(x)$. Specifically the Fourier series for $\psi(x)$ is

$$\psi(x) = \sum_n c_n e_n(x) \tag{A.5}$$

where the limits on n are implicitly $-\infty$ to ∞ and

$$c_n = \langle e_n, \psi\rangle \tag{A.6}$$

Exercise: For

$$\psi(x) = \sum_m c_m e_m(x)$$

show by explicit calculation that:

$$\langle e_n, \psi\rangle = c_n$$

Do not compute any integrals: use the inner product notation only.
Exercise: Now that our Equations A.5 and A.6 apply to complex valued function $\psi(x)$, find an example $\psi(x)$ for which:

$$c_{-n} \neq c_n^*$$

for some n.

A.1 Fourier Transform

The Fourier series for a periodic complex valued function $\psi(x)$ with period a is:

$$\psi(x) = \sum_n c_n e_n(x)$$

Here it will be useful to define the wave number

$$k_n \equiv \frac{2\pi n}{a} \tag{A.7}$$

with

$$e_n(x) = \exp(i\, k_n\, x)$$

As always the Fourier coefficients are determined as

$$c_n = \langle e_n, \psi \rangle = \int_{-\frac{a}{2}}^{\frac{a}{2}} \psi(x) e_n^*(x)$$

Consider the function:

$$\phi(x) = \begin{cases} \psi(x) & -\frac{a}{2} \leq x \leq \frac{a}{2} \\ \psi\left(\frac{a}{2}\right) & \text{otherwise} \end{cases} \tag{A.8}$$

and convince yourself of two things:

- $\phi(x)$ need not be a periodic function (and in fact $\phi(x)$ is a very trivial function if it is).
- Nonetheless, we can calculate it's Fourier coefficients in the usual way:

  $$c_n = \langle e_n, \phi \rangle$$

  and they will work perfectly well:

  $$\phi(x) = \sum_n c_n e_n(x)$$

  as long as we restrict ourselves to:

  $$-\frac{a}{2} \leq x \leq \frac{a}{2}$$

  .

We are going to extend the Fourier series to apply to any function $\psi(x)$ for which $\psi(x) \to 0$ as $x \to \pm\infty$.

- In the limit $a \to \infty$, then

  $$\psi(-a/2) \to 0, \qquad\qquad \psi(a/2) \to 0,$$

  so

  $$\psi(-a/2) \to \psi(a/2)$$

  and so $\psi(x)$ has a Fourier series valid in

  $$[-a/2, a/2] \to [-\infty, \infty].$$

- In the limit $a \to \infty$

$$k_{n+1} - k_n = \frac{2\pi}{a} \to 0$$

so we can now pick any value of k_n we want, without concern for n, so we write:

$$k_n \to k$$

k has become a continuous variable.

Next we will turn our attention to the Fourier coefficients:

$$c_n = \frac{1}{\sqrt{a}} \int_{-a/2}^{a/2} \psi(x)\, e^{-ik_n x} dx$$

In the limit $a \to \infty$

$$k_n \to k$$

and considering just the integral:

$$\int_{-a/2}^{a/2} \psi(x)\, e^{-ik_n x} dx \quad \to \quad C(k) \quad \equiv \quad \int_{-\infty}^{\infty} \psi(x)\, e^{-ikx} dx$$

where, as is our right as physicists, we bravely assume $C(k)$ is a well defined integral. Now evidently in this limit:

$$c_n \to \frac{C(k)}{\sqrt{a}} = 0$$

which is not very useful. The Fourier coefficients as we defined them carried a normalization factor that vanishes as $a \to \infty$. More useful will be the quantity

$$\left(\sqrt{a}\, c_n\right) \;\to\; C(k)$$

which we will show up again below.

Next we consider the Fourier series itself:

$$\psi(x) = \sum_n c_n e_n(x) = \frac{1}{\sqrt{a}} \sum_n c_n e^{ik_n x}$$

and recalling:

$$k_{n+1} - k_n = \frac{2\pi}{a}$$

so that we can write:

$$\psi(x) = \frac{1}{2\pi} \sum_n (\sqrt{a}\, c_n)\, e^{ik_n x}\, (k_{n+1} - k_n)$$

Now in the limit $a \to \infty$ the quantity

$$k_{n+1} - k_n$$

becomes infinitesimal and the sum becomes an integral:

$$\psi(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} C(k)\, e^{ik_n x}\, dk$$

For a symmetric definition we define the Fourier transform of $\psi(x)$ as:

$$\widetilde{\psi}(k) \equiv \frac{C(k)}{\sqrt{2\pi}}$$

so that:

$$\widetilde{\psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x)\, e^{-ikx}\, dx \tag{A.9}$$

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{\psi}(k)\, e^{ikx}\, dk \tag{A.10}$$

Appendix B

Proofs of Completeness of Trigonometric Functions

B.0.1 The Dirac Delta Function

These proofs make extensive use of the Dirac delta function, $\delta(x)$, which is zero everywhere but at $x = 0$, where it is infinite. Mathematically, the delta function only makes formal sense inside an integral, where it has the following defining properties:

$$\int_{-\infty}^{\infty} f(x')\,\delta(x-x')\,dx' = f(x) \tag{B.1}$$

$$\int_{-\infty}^{\infty} \delta(x)\,dx = 1 \tag{B.2}$$

The delta function simply picks out from the integral the one value of the integrand which makes the argument of the delta function zero. This makes intuitive sense, because the delta function is zero everywhere else. The second equation shows the normalization of the delta function, which follows from the first if you take $f(x) = 1$.

B.0.2 The completeness of the sines and cosines

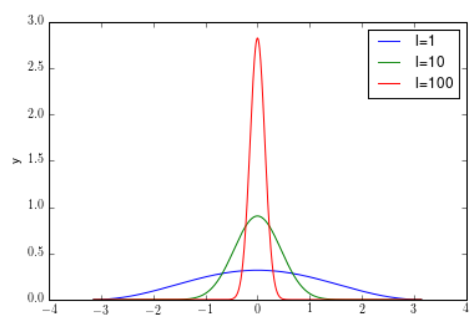

Figure B.1: The function $h_\ell(x)$ for increasingly large values of ℓ.

To demonstrate the completeness of sines and cosines[1] we construct a peculiar but useful set of

[1]This proof taken from http://web.mit.edu/jorloff/www/18.03-esg/notes/fourier-complete.pdf

functions defined for $\ell = 1, 2, 3, ...$:

$$h_\ell(x) = c_\ell \left(\frac{1 + \cos(x)}{2} \right)^\ell$$

We chose each factor c_ℓ such that:

$$\int_{-\pi}^{\pi} h_\ell(x) = 1$$

The shape of h_ℓ is shown in Fig. B.1. As ℓ increases, h_ℓ becomes more and more narrow at $x = 0$, while the normalization is as in Equation B.2. It looks more and more like the delta function:

$$\lim_{\ell \to \infty} h_\ell(x) = \delta(x)$$

It has one other important feature: $h_\ell(x)$ is simply a sum of cosines of nx with coefficients that don't depend on x. To see how this can be, note that we can always turn a product of cosines into a sum via the trigonometric identity:

$$\cos\alpha\cos\beta = \frac{1}{2}\{\cos(\alpha - \beta) + \cos(\alpha + \beta)\}.$$

So, for instance, we can write:

$$\begin{aligned} h_2(x) &= \frac{c_2}{4} + \frac{c_2\cos(x)}{2} + \frac{c_2\cos^2(x)}{4} \\ &= \frac{c_2}{4} + \frac{c_2\cos(x)}{2} + \frac{c_2\cos(2x)}{8} \end{aligned}$$

This property implies that the function $h_\ell(x - a)$ for some constant a is simply a sum of *both* sines and cosines of nx with coefficients that don't depend on x, as:

$$\cos(nx - na) = \cos(nx)\cos(na) + \sin(nx)\sin(na).$$

With this technology in hand we are ready to demonstrate the completeness of the sines and cosines. For simplicity, it suffices to consider only functions with period $L = 2\pi$ (i.e. $k_n = n$). The general case can then be inferred by transformation of coordinates. Consider a real function $f(x)$ which is periodic for $L = 2\pi$. For now just define the function $F(x)$ to be the infinite series:

$$F(x) \equiv a_0 + \sum_{n=1}^{\infty} \{a_n \cos(nx) + b_n \sin(nx)\}. \tag{B.3}$$

This is the compact form of the Fourier Series for this special case $L = 2\pi$, so $k_n = n$. We assume the coefficients are determined in the usual way:

$$\begin{aligned} a_n &= \frac{2}{L}\int_{-\frac{L}{2}}^{\frac{L}{2}} f(x)\cos(nx)\,dx \\ b_n &= \frac{2}{L}\int_{-\frac{L}{2}}^{\frac{L}{2}} f(x)\sin(nx)\,dx. \end{aligned}$$

We need to show that $F(x) = f(x)$, or

$$g(x) = F(x) - f(x) = 0$$

The proof hinges on the fact that $F(x)$ and $f(x)$ have the same Fourier coefficients, so that:

$$\begin{aligned}
\int_{-\pi}^{\pi} g(x)\sin(nx)dx &= \int_{-\pi}^{\pi} F(x)\sin(nx)dx - \int_{-\pi}^{\pi} f(x)\sin(nx)dx \\
&= b_n - b_n \\
&= 0 \\
\int_{-\pi}^{\pi} g(x)\cos(nx)dx &= \int_{-\pi}^{\pi} F(x)\cos(nx)dx - \int_{-\pi}^{\pi} f(x)\cos(nx)dx \\
&= a_n - a_n \\
&= 0
\end{aligned}$$

This shows that the integral of $g(x)$ times any sine or cosine is zero. But our special function $h_\ell(x-a)$ function is just a sum of sines and cosines of nx for any value of a. This means that:

$$\int_{-\pi}^{\pi} h_\ell(x-a)g(x)dx = 0$$

If we take the limit as $\ell \to \infty$, we obtain:

$$\begin{aligned}
\int_{-\pi}^{\pi} \delta(x-a)g(x)dx &= 0 \\
g(a) &= 0
\end{aligned}$$

Since this is true for any value of a, we have $g(x) = 0$ and so $F(x) = f(x)$.

B.0.3 The orthogonality and completeness of the complex exponential function

The first thing we need to show is that:

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} \exp(ikx)\,dk = \delta(x) \tag{B.4}$$

To see this we first calculate:

$$\begin{aligned}
\frac{1}{2\pi}\int_{-a}^{a} \exp(ikx)\,dk &= \frac{1}{2\pi}\frac{\exp(iax)-\exp(-iax)}{ix} \\
&= \frac{1}{\pi}\frac{\sin(ax)}{x} \\
&= \frac{a}{\pi}\operatorname{sinc}(ax)
\end{aligned}$$

An integration shows that:

$$\int_{-\infty}^{\infty} \frac{a}{\pi}\operatorname{sinc}(ax)\,dx = 1 \tag{B.5}$$

exactly as needed for Equation B.2.

Fig. B.2 shows that this function peaks at zero and becomes more and more narrow for progressively larger values of a. Since it has the correct normalization, we conclude that:

$$\begin{aligned}\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp(ikx)\,dk &= \lim_{a\to\infty}\frac{1}{2\pi}\int_{-a}^{a}\exp(ikx)\,dk \\ &= \lim_{a\to\infty}\frac{a}{\pi}\operatorname{sinc}(ax) \\ &= \delta(x)\end{aligned}$$

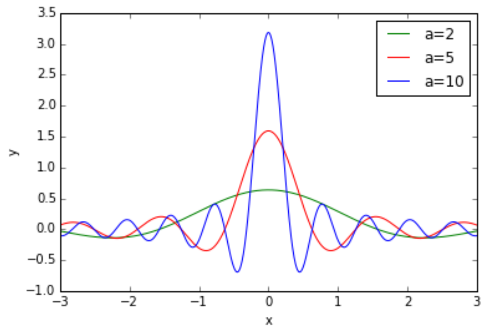

Figure B.2: The function $a\,\operatorname{sinc}(ax)/\pi$ for progressively larger values of a. As $a\to\infty$, this function approaches the delta function $\delta(x)$.

We are now fully equip to show that the complex exponential functions:

$$e_k = \frac{1}{\sqrt{2\pi}}\exp(ikx)$$

are orthonormal. Calculating the inner product

$$\begin{aligned}\langle e_k, e_{k'}\rangle &= \int_{-\infty}^{\infty}\frac{1}{\sqrt{2\pi}}\exp(-ikx)\frac{1}{\sqrt{2\pi}}\exp(ik'x)\,dx \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\{i(k'-k)x\}\,dx \\ &= \delta(k-k')\end{aligned}$$

where we have used Equation B.5 but with the roles of x and k exchanged. To prove completeness, we can now show that:

$$\begin{aligned}\Psi(x) &= \int_{-\infty}^{\infty}\Psi(x')\,\delta(x-x')\,dx' \\ &= \int_{-\infty}^{\infty} f(x')\left\{\frac{1}{2\pi}\int_{-\infty}^{+\infty}\exp\{ik(x-x')\}\,dk\right\}\,dx' \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left\{\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} f(x')\exp(-ikx')\,dx'\right\}\exp(ikx)\,dk \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\widetilde{\Psi}(k)\exp(ikx)\,dk\end{aligned}$$

where:

$$\widetilde{\Psi}(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Psi(x)\,\exp(-ikx)\,dx$$