Griffith's QM Notes

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1 The Wave Function

Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi \tag{1.1}$$

It's often useful to isolate $\frac{\partial\Psi}{\partial t}$ and its conjugate in the Schrödinger equation

$$\frac{\partial\Psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} - \frac{i}{\hbar}V\Psi \tag{1.2}$$

$$\frac{\partial\Psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} + \frac{i}{\hbar}V\Psi^* \tag{1.3}$$

Normalization

Since $|\Psi|^2$ is a probability density function in space, then a valid wavefunction must satisfy:

$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 \mathrm{d}x = 1 \tag{1.4}$$

Additionally, this implies an expected value for position $\langle x\rangle$

$$\langle x\rangle = \langle\Psi|x|\Psi\rangle = \int_{-\infty}^{+\infty} x|\Psi(x,t)|^2 \mathrm{d}x \tag{1.5}$$

We can prove that the Schrödinger equation preserves normalization of the wave function with time by taking the derivative of (1.3) with respect to time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 \mathrm{d}x = \int_{-\infty}^{+\infty} \frac{\partial}{\partial t}|\Psi(x,t)|^2 \mathrm{d}x \tag{1.6}$$

note that

$$\frac{\partial}{\partial t}|\Psi(x,t)|^2 = \frac{\partial}{\partial t}(\Psi^*\Psi) = \Psi^*\frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t}\Psi \tag{1.7}$$

additionally, we can use the Schrödinger equation isolated for $\frac{\partial \Psi}{\partial t}$ and its complex conjugate in (1.2) and (1.3) and (1.6) to write the probability density in terms of x

$$\begin{aligned}\frac{\partial}{\partial t}(\Psi^*\Psi) &= \Psi^*\left(\frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} - \frac{i}{\hbar}V\Psi\right) \\ &\quad + \Psi\left(-\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + \frac{i}{\hbar}V\Psi^*\right) \\ &= \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \Psi\frac{\partial^2\Psi^*}{\partial x^2}\right) \qquad (1.8)\end{aligned}$$

There is a better way to write (1.8). First observe

$$\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x}\right) = \frac{\partial\Psi^*}{\partial x}\frac{\partial\Psi}{\partial x} + \Psi^*\frac{\partial^2\Psi}{\partial x^2} \tag{1.9}$$

$$\frac{\partial}{\partial x}\left(\Psi\frac{\partial\Psi^*}{\partial x}\right) = \frac{\partial\Psi}{\partial x}\frac{\partial\Psi^*}{\partial x} + \Psi\frac{\partial^2\Psi^*}{\partial x^2} \tag{1.10}$$

then by subtracting (1.10) from (1.9)

$$\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right) = \Psi^*\frac{\partial^2\Psi}{\partial x^2} - \Psi\frac{\partial^2\Psi^*}{\partial x^2} \tag{1.11}$$

we obtain an expression that can be substituted into (1.8) and allows the integral in (1.6) to be rewritten as:

$$\int_{-\infty}^{+\infty}\frac{i\hbar}{2m}\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right)\mathrm{d}x = \frac{i\hbar}{2m}\left[\ \Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right]_{x=-\infty}^{x=+\infty} \tag{1.12}$$

Normalized solutions of the Schrödinger equation must be zero when x tends to $\pm\infty$. Let it be known that this doesn't have to happen for any normalizable function, but in physics (i.e. with the the Schrödinger equation), it always will be this way. (We will have to make a slightly different argument in the next section)
Additionally, if Ψ tends to zero, then so will Ψ^*, so the entire expression on the right side of (1.12) is zero, and we find that the wavefunction is always normal throughout time.

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{+\infty}|\Psi|^2\mathrm{d}x = 0 \tag{1.13}$$

Momentum

Recall (1.5) where we gave the expected value for position among all particles in the state $|\Psi\rangle$.
One might be interested in seeing the rate of change in this value over time, as it might point to a quantum analog of velocity, or more importantly, momentum.
To do this, we can look at the definition of the value

$$\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{+\infty} x|\Psi(x,t)|^2 \mathrm{d}x = \int_{-\infty}^{+\infty} x\frac{\partial}{\partial x}(\Psi^*\Psi)\mathrm{d}x \text{ (with } \frac{\partial x}{\partial t} = 0) \tag{1.14}$$

$$\text{by (1.8), (1.11)} \qquad = \frac{i\hbar}{2m}\int_{-\infty}^{+\infty} x\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \Psi\frac{\partial \Psi^*}{\partial x}\right)\mathrm{d}x$$

$$\text{let } F(x,t) = \Psi^*\frac{\partial \Psi}{\partial x} - \Psi\frac{\partial \Psi^*}{\partial x} \text{ then } \quad \frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t} = \frac{i\hbar}{2m}\int_{-\infty}^{+\infty} x\frac{\partial}{\partial x}F(x,t)\mathrm{d}x$$

$$\text{then by using integration by parts} \qquad = \frac{i\hbar}{2m}\left[xF(x,t) - \int F(x,t)\mathrm{d}x\right]_{x=-\infty}^{x=+\infty}$$

$$\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t} = \frac{i\hbar}{2m}\left[\lim_{a\to\infty}\Bigg(aF(a,t) - (-a)F(-a,t)\Bigg) - \int_{-\infty}^{+\infty} F(x,t)\mathrm{d}x\right] \tag{1.15}$$

Because the wave function is normalized $\Psi \in L^2$, then F will tend to zero faster than a tends to $\pm\infty$

$$\begin{aligned}
\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t} &= \frac{i\hbar}{2m}\left(\lim_{a\to\infty}\cancelto{0}{\Bigg(aF(a,t) - (-a)F(-a,t)\Bigg)} - \int_{-\infty}^{+\infty} F(x,t)\mathrm{d}x\right) \\
&= -\frac{i\hbar}{2m}\int_{-\infty}^{+\infty}(\Psi^*\frac{\partial \Psi}{\partial x} - \Psi\frac{\partial \Psi^*}{\partial x})\mathrm{d}x \\
&= -\frac{i\hbar}{2m}\left(\int_{-\infty}^{+\infty}\Psi^*\frac{\partial \Psi}{\partial x}\mathrm{d}x - \int_{-\infty}^{+\infty}\Psi\frac{\partial \Psi^*}{\partial x}\mathrm{d}x\right) \\
\text{Then with integration by parts } &= -\frac{i\hbar}{2m}\left(\int_{-\infty}^{+\infty}\Psi^*\frac{\partial \Psi}{\partial x}\mathrm{d}x - \left[\Psi^*\Psi - \int\Psi^*\frac{\partial \Psi}{\partial x}\mathrm{d}x\right]_{x=-\infty}^{x=+\infty}\right)
\end{aligned} \tag{1.16}$$

$\Psi^*\Psi$ is also an element of L^2, so it vanishes, and we are left with

$$\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t} = -\frac{i\hbar}{m}\int_{-\infty}^{+\infty}\Psi^*\frac{\partial \Psi}{\partial x}\mathrm{d}x \tag{1.17}$$

and by defining the momentum as $\langle p\rangle = m\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t}$ and using (1.17) we obtain the following elegant formula:

$$\langle p\rangle = \int_{-\infty}^{+\infty} \Psi^*(-i\hbar\frac{\partial}{\partial x})\Psi \mathrm{d}x \tag{1.18}$$

This is incredibly useful. Due to the principles of Hamilton, we can now express any physical quantity as a function of $\langle x\rangle$ and $\langle p\rangle$, written as $\langle Q(x,p)\rangle$.
Looking back at (1.18), notice that the form of $\langle p\rangle$ is not much different from $\langle x\rangle$, which can be re-written in the following form:

$$\langle x\rangle = \int_{-\infty}^{+\infty} \Psi^* x \Psi \mathrm{d}x$$

This way, x is not only a scalar, but is abstracted to a *position operator* that acts as a scalar. Clearly, this also applies to $-i\hbar\frac{\partial}{\partial x}$, which can be called the *momentum operator*. Thus, it is correct to assume that the operator $Q(x, -i\hbar\frac{\partial}{\partial x})$ will allow us to find $\langle Q(x,p)\rangle$, which is demonstrated below.

$$\langle Q(x,p)\rangle = \int_{-\infty}^{+\infty} \Psi^* Q(x, -i\hbar\frac{\partial}{\partial x})\Psi \mathrm{d}x \tag{1.19}$$

Now we can determine expressions like kinetic energy, since $T = \frac{p^2}{2m}$, which is associated with the operator $\frac{1}{2m}(-i\hbar\frac{\partial}{\partial x})^2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

$$\langle T\rangle = -\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty} \Psi^* \frac{\partial^2}{\partial x^2}\Psi \mathrm{d}x \tag{1.20}$$

2 Time-Independent Schrödinger equation

2.1 Stationary States

Our goal is to solve the Schrödinger equation for a fixed distribution for V. Starting with the time-dependent Schrödinger equation :

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

Assume a separable solution:

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

Then:

$$\frac{\partial\Psi}{\partial t} = \psi(x)\,\frac{d\phi}{dt}, \tag{2.2}$$

$$\frac{\partial^2\Psi}{\partial x^2} = \phi(t)\,\frac{d^2\psi}{dx^2}. \tag{2.3}$$

Substitute into the Schrödinger equation while letting V constant in time but not in space, so that the solution is stationary:

$$i\hbar\psi(x)\frac{d\phi}{dt} = -\frac{\hbar^2}{2m}\phi(t)\frac{d^2\psi}{dx^2} + V(x)\Psi. \tag{2.4}$$

Divide through by $\Psi = \psi(x)\phi(t)$:

$$i\hbar\frac{1}{\phi(t)}\frac{d\phi}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi}{dx^2} + V(x). \tag{2.5}$$

Since the left-hand side depends only on t and the right-hand side only on x, both sides must equal a constant E:

$$i\hbar\frac{1}{\phi(t)}\frac{d\phi}{dt} = E, \tag{2.6}$$

$$\Rightarrow \quad \frac{1}{\phi(t)}\frac{d\phi}{dt} = -\frac{iE}{\hbar}. \tag{2.7}$$

Integrate:

$$\ln\big(\phi(t)\big) = -\frac{iE}{\hbar}t, \tag{2.8}$$

so that

$$\phi(t) = C\,e^{-\frac{iE}{\hbar}t}. \tag{2.9}$$

We will not make attempts to solve the equation for ψ as it is problem-dependent for now, and since ψ may absorb the constant C, we can write:

$$\Psi(x,t) = \psi(x)\,e^{-\frac{iE}{\hbar}t}. \tag{2.10}$$

Hamiltonian

The Hamiltonian is defined by:

$$H(x,p) = \frac{p^2}{2m} + V(x). \tag{2.11}$$

Since the momentum operator is

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

then we can construct an operator for the Hamiltonian

$$H(x,p) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x). \tag{2.12}$$

Thus the Hamiltonian operator is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x), \tag{2.13}$$

and the time-independent Schrödinger equation re-emerges as the following, equivalent to its form in (2.5):

$$\hat{H}\psi = E\psi. \tag{2.14}$$

Some Notable Facts

It's worth mentioning that the time-dependent factor of Ψ doesn't affect the probability density; the proof is simple:

$$\Psi^*\Psi = (\psi^* e^{iEt/\hbar})(\psi e^{-iEt/\hbar})$$
$$\Psi^*\Psi = \psi^*\psi$$

Take a look at the expectation value of H. We can substitute the factor $\hat{H}\psi$ in the integrand for $E\psi$ by the time-independent Schrödinger equation .

$$\langle H\rangle = \int_{-\infty}^{+\infty} \psi^*\,\hat{H}\,\psi\,\mathrm{d}x = \int_{-\infty}^{+\infty} \psi^*\,E\psi\,\mathrm{d}x \tag{2.15}$$

and since ψ is normalized

$$\langle H\rangle = E. \tag{2.16}$$

thus,

$$\langle H\rangle^2 = E^2. \tag{2.17}$$

and,

$$\hat{H}^2\psi = \hat{H}(\hat{H}\psi) = \hat{H}(E\psi) \quad\Rightarrow\quad E\,\hat{H}\psi = E^2\psi. \tag{2.18}$$

Then the expectation value of H^2 is:

$$\langle H^2 \rangle = \int_{-\infty}^{+\infty} \psi^* \, \hat{H}^2 \psi \, dx = \int_{-\infty}^{+\infty} \psi^* \, E^2 \psi \, dx \tag{2.19}$$

$$= E^2 \int_{-\infty}^{+\infty} |\psi|^2 dx = E^2. \tag{2.20}$$

which helped us find the variance of H

$$\sigma_H^2 = \langle H^2 \rangle - \langle H \rangle^2 \tag{2.21}$$

$$= E^2 - E^2 = 0. \tag{2.22}$$

Generalized solution

Now we can confirm that there is a unique energy E_n measured for every associated time-independent solution to the Schrödinger equation (i.e. $\sigma_H^2 = 0$), and for each ψ_n we can construct a generalized solution due to linearity of the DE:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \underbrace{\psi_n(x) e^{-iE_n t/\hbar}}_{=\Psi_n} \tag{2.23}$$

each c_n is arbitrary, but must keep Ψ normalized, and so:

$$\sum_{n=1}^{\infty} |c_n|^2 = 1 \tag{2.24}$$

where each $|c_n|^2$ is the probability of measuring the state with energy E_n, meaning that:

$$\langle H \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n \tag{2.25}$$

2.2 The Infinite Square Well

If we construct a potential V so that

$$V(x) = \begin{cases} 0 & \text{if } 0 \le x \le a \\ \infty & \text{otherwise} \end{cases} \tag{2.26}$$

making it impossible for the wavefunction to exist outside the interval $[0, a]$, only causing the time-dependent Schrödinger equation to be relevant on the same interval where $V = 0$.

This is called the infinite square well problem, and gives us the following DE:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi \tag{2.27}$$

if we let a value $k = \sqrt{2mE}/\hbar$, then (2.27) vaguely resembles the classical simple harmonic oscillator, and so the solution is:

$$\psi(x) = A\sin(kx) + B\cos(kx) \tag{2.28}$$

However, since V imposes the boundary conditions: $\psi(0) = 0$ and $\psi(a) = 0$

$$B = 0 \tag{2.29}$$

$$0 = A\sin(ka) \tag{2.30}$$

meaning that either $A = 0$ or $\sin(ka) = 0$. If we choose the primary, ψ becomes the degenerate solution identical to zero, but the latter requires that

$$ka = 0, \pm\pi, \pm 2\pi, \cdots \tag{2.31}$$

$ka = 0$ gives us the degenerate solution again, but the rest can be used to solve for k, providing the means to make the nontrivial solutions associated with:

$$k_n = \frac{n\pi}{a} \tag{2.32}$$

However, something still feels fishy. The constant A wasn't determined from the boundary condition as is usual, but instead restricted us to valid values of k. Instead of coming from the boundary conditions, we actually determine A via the normalization condition:

$$\begin{aligned} 1 = \int_{-\infty}^{+\infty} \psi^*\psi \mathrm{d}x &= \int_0^a |A|^2 \sin^2(kx)\mathrm{d}x \\ &= |A|^2\frac{a}{2} \\ \frac{2}{a} &= |A|^2 \end{aligned} \tag{2.33}$$

Now we have infinitely many solutions for A, but notice that if we express $A = Re^{i\theta}$, (2.33) becomes:

$$R = \pm\sqrt{\frac{2}{a}} \tag{2.34}$$

Since the positive and negative values yield the same magnitude for A, and we do not lose generality for the wavefunction by specifying a phase, we can just take $\theta = 0$, giving us

$$A = \sqrt{\frac{2}{a}} \tag{2.35}$$

finally allowing us to write

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) & \text{if } 0 \le x \le a \\ 0 & \text{otherwise} \end{cases} \tag{2.36}$$

Properties of Stationary States

Even though we didn't need the value of A to determine the energies, it is worth mentioning now that upon finding k_n, we were able to write them in the following form by using (2.27)

$$\begin{aligned} k_n &= \frac{\sqrt{2mE_n}}{\hbar} \\ \text{and by (2.32)} \qquad \frac{n\pi}{a} &= \frac{\sqrt{2mE_n}}{\hbar} \\ E_n &= \frac{n^2\pi^2\hbar^2}{2ma^2} \end{aligned} \tag{2.37}$$

Finally, this gives us the energy associated with each stationary state ψ_n. Before we get into finding Ψ in terms of an initial function, it is worth noting some properties of the collection of ψ_n's:

(1) If ψ_j is an even function then ψ_{j+1} is an odd function

(2) ψ_j has $j-1$ nodes (zeros)

(3) They are mutually orthogonal, forming an orthonormal basis.

The first two are trivial, but before proving (3), I will emphasize here that we are defining the inner product as

$$\langle f|g\rangle = \int_{-\infty}^{+\infty} f^*(x)g(x)\mathrm{d}x \tag{2.38}$$

Proof of (3):

$$\langle \psi_m|\psi_n\rangle = \int_{-\infty}^{+\infty} \psi_m^*\psi_n \mathrm{d}x = \frac{2}{a}\int_0^a \sin\left(\frac{m\pi}{a}x\right)\sin\left(\frac{n\pi}{a}x\right)\mathrm{d}x \tag{2.39}$$

also recall

$$\cos(\alpha+\beta) = \cos(\alpha)\cos(\beta) - \sin(\alpha)\sin(\beta)$$
$$\cos(\alpha-\beta) = \cos(\alpha)\cos(\beta) + \sin(\alpha)\sin(\beta)$$

And by subtracting the second identity from the first, we get:

$$\frac{1}{2}(\cos(\alpha+\beta) - \cos(\alpha-\beta)) = \sin(\alpha)\sin(\beta) \tag{2.40}$$

if $\alpha = \frac{m\pi}{a}x$ and $\beta = \frac{n\pi}{a}x$ and we plug (2.40) into (2.39) then

$$\begin{aligned}\int_{-\infty}^{+\infty} \psi_m^* \psi_n \mathrm{d}x &= \frac{1}{a}\int_0^a \left(\cos\left(\frac{m-n}{a}\pi x\right) - \cos\left(\frac{m+n}{a}\pi x\right)\right)\mathrm{d}x \\ &= \left[\frac{1}{(m-n)\pi}\sin\left(\frac{m-n}{a}\pi x\right) - \frac{1}{(m+n)\pi}\sin\left(\frac{m+n}{a}\pi x\right)\right]_0^a \\ &= \cancelto{0}{\frac{\sin((m-n)\pi)}{(m-n)\pi}} - \cancelto{0}{\frac{\sin((m+n)\pi)}{(m+n)\pi}} = 0 \end{aligned} \tag{2.41}$$

However, this argument fails when $m = n$ since one of the denominators in (2.41) become 0. When this happens, know that the initial definition of the inner product just becomes the norm of ψ, which is equal to 1, and reveals that:

$$\int_{-\infty}^{+\infty} \psi_m^* \psi_n \mathrm{d}x = \delta_{mn} \tag{2.42}$$

where δ_{mn} is the Kronecker Delta, and since $\delta_{mn} = 0$ for any $m \neq n$, the set of every ψ_n is orthonormal and constructs a basis for every function under the inner product stated initially that satisfies the same boundary conditions as ψ. QED

Now with (1), (2), and (3) being true, we can say that any function $f(x)$ that satisfies the boundary conditions can be constructed via the infinite series in (2.23) at $t = 0$ with a precise selection for every c_n. This is useful when setting up the initial condition $\Psi(x, 0)$, especially since in the case of the infinite square well, the series becomes a Fourier series, and each c_n can be found via Fourier's trick for a given $f(x)$ as follows:

$$\begin{aligned}\text{First,}\quad f(x) &= \sum_{n=1}^{\infty} c_n \psi_n(x) \\ \int_{-\infty}^{+\infty} \psi_m^* f \mathrm{d}x &= \sum_{n=1}^{\infty} c_n \underbrace{\int_{-\infty}^{+\infty} \psi_m^* \psi_n \mathrm{d}x}_{=\delta_{mn}} \\ \int_{-\infty}^{+\infty} \psi_m^* f \mathrm{d}x &= \sum_{n=1}^{\infty} \delta_{mn} c_n \\ \int_{-\infty}^{+\infty} \psi_m^* f \mathrm{d}x &= c_n \end{aligned} \tag{2.43}$$

By using (2.43) we can now write every c_n in terms of the initial condition:

$$c_n = \sqrt{\frac{2}{a}}\int_0^a \sin\left(\frac{n\pi}{a}x\right)\Psi(x, 0)\mathrm{d}x \tag{2.44}$$

giving us:

$$\Psi(x,t) = \sqrt{\frac{2}{a}} \sum_{n=0}^{\infty} \int_0^a \sin\Big(\frac{n\pi}{a}x\Big) \Psi(x,0) \mathrm{d}x \sin\Big(\frac{n\pi}{a}x\Big) e^{-i(n^2\pi^2\hbar/2ma^2)t} \tag{2.45}$$

and completely solving the infinite square well problem.

A Note on the c_n Constants

We still haven't proven that the c_n constants introduced in (2.23) will always be able to keep Ψ normalized via their convergence to 1 in (2.24).
Starting by expanding the norm for Ψ as follows:

$$\begin{aligned}
\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 \mathrm{d}t &= \int_{-\infty}^{+\infty} \left(\sum_{m=1}^{\infty} c_m \psi_m e^{-iE_m t/\hbar}\right)^* \left(\sum_{n=1}^{\infty}\sum_{n=1}^{\infty} c_n \psi_n e^{-iE_n t/\hbar}\right) \mathrm{d}x \\
&= \int_{-\infty}^{+\infty} \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} c_m^* c_n \psi_m^* \psi_n e^{-it(E_n-E_m)/\hbar} \mathrm{d}x \\
\text{by (2.42)} \qquad &= \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} c_m^* c_n \underbrace{\int_{-\infty}^{+\infty} \psi_m^* \psi_n e^{-it(E_n-E_m)/\hbar} \mathrm{d}x}_{=\delta_{mn}} \\
&= \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} c_m^* c_n \delta_{mn} \\
&= \sum_{m=1}^{\infty} c_m^* c_m = \sum_{n=1}^{\infty} |c_n|^2 = 1
\end{aligned}$$

which is useful, especially since you can easily construct a similar proof for the expected value of energy $\langle H \rangle$.

2.3 The Harmonic Oscillator

In the example of the infinite square well, we encountered a form of the Schrödinger equation that resembled the equation for a simple harmonic oscillator in x. Know that this is distinct from the equation for a true harmonic oscillator, which is instead in t. This is especially useful, as a harmonic oscillator can help us approximate behavior around local minima within a more complex potential.

The formalism behind this comes from the Taylor expansion of the potential about its local minimum, called x_0:

$$V(x) = V(x_0) + V'(x_0)(x-x_0) + \frac{1}{2}V''(x_0)(x-x_0)^2 + \cdots \tag{2.46}$$

The first derivative at a local minimum is zero, so the second term disappears, and we will ignore the first term by using the intuition that it wouldn't affect the classical equation of motion. For a "soft" local minimum, the terms with an order greater than two are negligible and can also be ignored. Therefore:

$$V(x) \approx \frac{1}{2}V''(x_0)(x - x_0)^2 \tag{2.47}$$

Now we will assert that $V''(x_0) > 0$ since x_0 is a local minimum, and that without loss of generality that $x_0 = 0$. We can then formulate a potential by writing the coefficient $V''(x_0)$ in terms of ω and m by intuition from the classical Hooke's law. This gives us:

$$V(x) = \frac{1}{2}m\omega^2 x^2 \tag{2.48}$$

Then by plugging this into the time-independent Schrödinger equation :

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi \tag{2.49}$$

Note that we can factor the left-hand side of the above equation into the form that gives us the Hamiltonian:

$$\underbrace{\frac{1}{2m}\left(\hat{p}^2 + (m\omega x)^2\right)}_{=\hat{H}}\psi = E\psi \tag{2.50}$$

There are two methods to solve the DE in this form; the method we're using will begin by attempting to factor $\hat{H}$ into the form $u^2 + v^2 = (iu + v)(-iu + v)$. Let our version of the first and second factors be[1]:

$$\begin{aligned}
\hat{a}_- &= \frac{1}{\sqrt{2\hbar m\omega}}(i\hat{p} + m\omega x) \\
\hat{a}_+ &= \frac{1}{\sqrt{2\hbar m\omega}}(-i\hat{p} + m\omega x) \\
\text{multiplying} \qquad \hat{a}_-\hat{a}_+ &= \frac{1}{2\hbar m\omega}(i\hat{p} + m\omega x)(-i\hat{p} + m\omega x) \\
&= \frac{1}{2\hbar m\omega}\left(\hat{p}^2 + (m\omega x)^2 - im\omega(x\hat{p} - \hat{p}x)\right)
\end{aligned}$$

Note that since $\hat{p}$ doesn't commute with x, we get a leftover term, and our Hamiltonian doesn't factor perfectly. This term is called the *commutator* and measures how much two operators don't commute. It is often written as $\left[\hat{A}, \hat{B}\right]$.

[1] Don't get confused! $\hat{a}$ having a plus or minus in the subscript has no correspondence with the signs of the terms

With this, we can rewrite the previous equation as:

$$\hat{a}_-\hat{a}_+ = \underbrace{\frac{1}{2\hbar m\omega}(\hat{p}^2 + (m\omega x)^2)}_{=\frac{1}{\hbar\omega}\hat{H}} - \frac{i}{2\hbar}\,[x,\hat{p}]$$

$$\frac{1}{\hbar\omega}\hat{H} = \hat{a}_-\hat{a}_+ + \frac{i}{2\hbar}\,[x,\hat{p}] \tag{2.51}$$

Now that we have the Hamiltonian in this form, we might want to investigate what the commutator of position and momentum actually does to a function on its own.

$$\begin{aligned}
[x,\hat{p}]f(x) &= \Big(x\big(\hat{p}f(x)\big) - \hat{p}\big(xf(x)\big)\Big) \\
&= \Big(x\big(-i\hbar\frac{\mathrm{d}f}{\mathrm{d}x}\big) + i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\big(xf(x)\big)\Big) \\
&= i\hbar\left(f(x) + x\frac{\mathrm{d}f}{\mathrm{d}x} - x\frac{\mathrm{d}f}{\mathrm{d}x}\right) \\
[x,\hat{p}]f(x) &= i\hbar f(x)
\end{aligned}$$

Now, clearly, the only thing the operator does is multiply by $i\hbar$. This fact is deep, and is called the *canonical commutation relation*, written as so:

$$[x,\hat{p}] = i\hbar \tag{2.52}$$

allowing us to rewrite (2.51) elegantly:

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

$$\hat{H} = \hbar\omega(\hat{a}_-\hat{a}_+ + \frac{1}{2}) \tag{2.53}$$