Griffiths Intro to Quantum Mechanics, Self-Study

Selected Solutions for Griffiths' Intro to Quantum Mechanics (3rd)

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Preface

TODO blah blah

Chapter 1

The Wave Equation

1.1 Exercises

Exercise 1.3
Consider the gaussian distribution

$$\rho(x) = Ae^{-\lambda(x-a)^2}$$

where A, a, λ are all real constants.

- Find A from integrating the probability density over all reals.

$$1 = A \int_{\mathbb{R}} e^{-\lambda(x-a)^2} \, dx$$

$$= A\left[\int_{-\infty}^{0} e^{-\lambda(x-a)^2} \, dx + \int_{0}^{\infty} e^{-\lambda(x-a)^2} \, dx\right]$$

$$= A\left[-\int_{0}^{-\infty} e^{-\lambda(x-a)^2} \, dx + \int_{0}^{\infty} e^{-\lambda(x-a)^2} \, dx\right]$$

Make substitution of $u = \sqrt{\lambda}(x - a)$. Evaluate the error function accordingly, and note that the adjusted bounds can be reconstructed as the original's.

$$1 = \frac{1}{\sqrt{\lambda}}A\left[-\int_{0}^{-\infty} e^{-u^2} \, du + \int_{0}^{\infty} e^{-u^2} \, du\right]$$

$$= \frac{\sqrt{\pi}}{2}\frac{1}{\sqrt{\lambda}}A\left[-\mathrm{erf}(-\infty)^{-1} + \mathrm{erf}(0)^{0}\right] \implies A = \sqrt{\frac{\lambda}{\pi}}$$

$$\therefore \rho(x) = \sqrt{\frac{\lambda}{\pi}}e^{-\lambda(x-a)^2}$$

- Find the first two moments of position and the relevant standard deviation.

$$\langle x \rangle = \sqrt{\frac{\lambda}{\pi}} \int_{\mathbb{R}} xe^{-\lambda(x-a)^2} \, dx = a$$

$$\langle x^2 \rangle = \sqrt{\frac{\lambda}{\pi}} \int_{\mathbb{R}} x^2 e^{-\lambda(x-a)^2} \, dx = a^2 + \frac{1}{2\lambda}$$

$$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \frac{1}{2\lambda}$$

Where we used the fact that odd integrands over a symmetric interval sum to 0 and that the gamma function can be defined via a convergent improper integral.

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Exercise 1.4
Given positive constants A, a, and b:

$$\Psi(x,0) = \begin{cases} A(x/a), & \text{if } 0 \leq x \leq a, \\ A(b-x)/(b-a), & \text{if } a \leq x \leq b \\ 0 & \text{otherwise} \end{cases}$$

- Normalize Ψ.

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

$$A^2 \left(\int_0^a \frac{x^2}{a^2} \, dx + \int_a^b \frac{(b-x)^2}{(b-a)^2} \, dx \right) = 1$$

$$A^2 \left(\frac{a}{3} + \frac{b-a}{3} \right) = 1 \implies A = \sqrt[2]{\frac{3}{b}}$$

$$\Psi(x,0) = \begin{cases} \sqrt[2]{\frac{3}{b}}(x/a), & \text{if } 0 \leq x \leq a, \\ \sqrt[2]{\frac{3}{b}}(b-x)/(b-a), & \text{if } a \leq x \leq b \\ 0 & \text{otherwise} \end{cases}$$

- Where is particle most likely to be found at $t = 0$? Based on plots, you will see it is most likely at position a.

- Probablility of finding particle to the left of a? Check with b = a and b = 2a.

$$\int_0^a \left| \sqrt[2]{\frac{3}{b}}(x/a) \right|^2 \, dx$$

$$\int_0^a \frac{3}{b}(x^2/a^2) \, dx = \frac{a}{b}$$

- What is the first moment (expected value) of x?

$$\langle x \rangle = \int_0^b x\Psi(x,t)dx = \int_0^a \sqrt[2]{\frac{3}{b}}(x/a) \, dx + \int_a^b \sqrt[2]{\frac{3}{b}}(b-x)/(b-a) \, dx$$

$$= \frac{b+2a}{4}$$

Exercise 1.5MOD

Given positive, real constants A, λ, ω:

$$\Psi(x,t) = Ae^{-\lambda|x|-i\omega t}$$

- Normalize Ψ.

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

$$\int_{-\infty}^{\infty} A^2 e^{-2\lambda|x|} e^{-i\omega t} e^{i\omega t} \, dx = 1$$

$$A^2 \int_{-\infty}^{\infty} e^{-2\lambda|x|} \, dx = 1$$

$$A^2 \left(\int_{-\infty}^{0} e^{-2\lambda\cdot(-x)} \, dx + \int_{0}^{\infty} e^{-2\lambda\cdot(x)} \right) = 1$$

$$A^2 \left(\frac{1}{2\lambda} e^{2\lambda x} \right)\Big|_{-\infty}^{0} - A^2 \left(\frac{1}{2\lambda} e^{-2\lambda x} \right)\Big|_{0}^{\infty} = 1$$

$$\frac{A^2}{\lambda} = 1 \implies A = \sqrt[2]{\lambda}$$

$$\Psi(x,t) = \sqrt{\lambda}e^{-\lambda|x|-i\omega t}$$

$$|\Psi(x,t)|^2 = \Psi^*\Psi = \lambda e^{-\lambda|x|-i\omega t} e^{-\lambda|x|+i\omega t} = \lambda e^{-2\lambda|x|}$$

- Find the nth moment.

$$\langle x^n \rangle = \int_{\mathbb{R}} x^n \lambda e^{-2\lambda|x|} \, dx$$

$$= \lambda \left(\int_{-\infty}^{0} x^n e^{2\lambda x} + \int_{0}^{\infty} x^n e^{-2\lambda x} \right) \, dx$$

Now note the following is smells like the gamma function, and make substitution of $u = -x$ to change limits (also note that n is positive to extract the alternating negative one):

$$I_{n_-} = \int_{-\infty}^{0} x^n e^{2\lambda x} \, dx = \int_{\infty}^{0} (-u)^n e^{2\lambda(-u)} \, (-du) = -\int_{\infty}^{0} (-1)^n u^n e^{-2\lambda u} \, du = (-1)^n \int_{0}^{\infty} x^n e^{-2\lambda x} \, dx$$

By using substitution of the type $u = 2\lambda x$ we get,

$$I_{n_-} = \frac{(-1)^n}{2\lambda(2\lambda)^n} \int_{0}^{\infty} e^{-u} u^n du = \frac{(-1)^n}{(2\lambda)^{n+1}} \Gamma(n+1), \;\; \text{Re}(n) > -1$$

where the last equation can be used to show the required base case of $I_0 = \frac{1}{2\lambda}$. A similar analysis for the second integrand gives us the combined relation

$$\langle x^n \rangle = \lambda I_n = \lambda(I_{n_-} + I_{n_+})$$

$$= \lambda \left(\frac{(-1)^n + 1}{(2\lambda)^{n+1}} \right) \Gamma(n+1)$$

For practical purposes, we see that the first few moments give

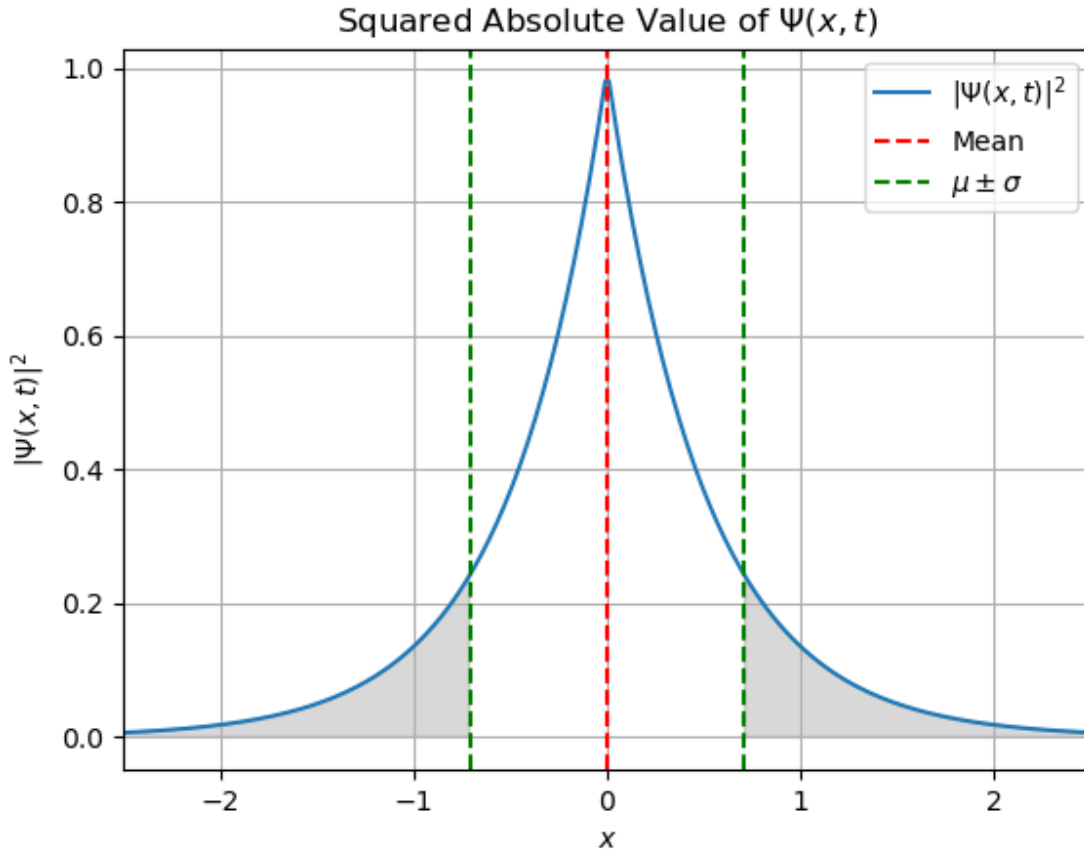$$\langle x \rangle = 0$$

$$\langle x^2 \rangle = \frac{2\lambda}{8\lambda^3} \Gamma(3) = \frac{1}{2\lambda^2}$$

$$\langle x^3 \rangle = 0$$

$$\langle x^4 \rangle = \frac{2\lambda}{32\lambda^5} \Gamma(4) = \frac{3}{8\lambda^4}$$

- Find standard deviation. Compute probability particle is outside one standard deviation from the mean.

$$\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 \implies \sigma = \frac{1}{\lambda\sqrt{2}}$$

$$|\Psi(0 \pm \sigma, t)|^2 = |A|^2 e^{-2\lambda\sigma} = \lambda e^{-\sqrt{2}}$$

$$P_{outside} = 1 - P_{inside} = 1 - \int_{-\sigma}^{\sigma} |\Psi|^2 \, dx = 1 - |A|^2 \int_{-\sigma}^{\sigma} e^{-2\lambda|x|} \, dx = 2\lambda \int_{\sigma}^{\infty} e^{-2\lambda x} \, dx = e^{-\sqrt{2}}$$

Squared Absolute Value of $\Psi(x, t)$

Exercise 1.6
Why can't you do integration-by-parts (IBP) directly in the middle expression of Equation 1.29 – pull the time derivative over into x, note that $\frac{\partial x}{\partial t} = 0$, and conclude that $\frac{\langle x \rangle}{dx} = 0$?

Well, you could but this would not allow us to do IBP over some domain D:

$$\frac{\partial x |\Psi|^2}{\partial t} = \frac{\partial x}{\partial t}|\Psi|^2 + x\frac{\partial |\Psi|^2}{\partial t} = x\frac{\partial |\Psi|^2}{\partial t}$$

$$\int_{\partial D} x\frac{\partial |\Psi|^2}{\partial t} dx = \int_{\partial D} \frac{\partial (x|\Psi|^2)}{\partial t} dx \neq (x|\Psi|^2)|_{\partial D}$$

Exercise 1.7
Calculate $\frac{d\langle p \rangle}{dt}$.

By Ehrenfest's theorem, expectation values are goverened by classical laws: $\langle p \rangle = m \langle v \rangle = m \frac{d \langle x \rangle}{dt}$. Recall the time derivatives for the conjugate pairs or derive it yourself. Also note that interchange of differentiaiton to integration (Leibnitz integral rule) implicitly assumes the (wave) function and its first partial derivative are continuous in time and space (both) in the open neighborhood of $\{x\} \times [a,b]$ for any continuous and differentiable functions a, b. Text assumes all partials continuous, and by extent differentiable (converse not necessarily true). Second order partials assumed continuous for Clairaut's Theorem, C^2, throughout text.

$$\frac{d\langle p \rangle}{dt} = -i\hbar \int \frac{\partial \Psi^* \frac{\partial \Psi}{\partial x}}{\partial t} \, dx$$

$$\frac{\partial \Psi^* \frac{\partial \Psi}{\partial x}}{\partial t}$$

$$= \frac{\partial \Psi^*}{\partial t} \frac{\partial \Psi}{\partial x} + \Psi^* \frac{\partial^2 \Psi}{\partial x \partial t}$$

$$= \left(\frac{-i\hbar}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} + \frac{iV(x,t)\Psi^*}{\hbar} \right) \frac{\partial \Psi}{\partial x} + \Psi^* \partial \frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \frac{iV(x,t)\Psi}{\hbar} \Big/ \partial x$$

$$= \frac{i\hbar}{2m} \left(\frac{\partial^3 \Psi}{\partial x^3} \Psi^* - \frac{\partial^2 \Psi^*}{\partial x^2} \frac{\partial \Psi}{\partial x} \right) + \frac{i}{\hbar} \left(V(x,t) \frac{\partial \Psi}{\partial x} - \Psi^* \frac{\partial V(x,t)\Psi}{\partial x} \right)$$

$$= \frac{i\hbar}{2m} \left(\frac{\partial^3 \Psi}{\partial x^3} \Psi^* - \frac{\partial^2 \Psi^*}{\partial x^2} \frac{\partial \Psi}{\partial x} \right) + \frac{i}{\hbar} \left(V(x,t) \frac{\partial \Psi}{\partial x} - \Psi^* V(x,t) \frac{\partial \Psi}{\partial x} - \Psi^* \frac{\partial V(x,t)}{\partial x} \Psi \right)$$

$$= \frac{i}{\hbar} \left(|\Psi|^2 \frac{\partial V(x,t)}{\partial x} \right)$$

Whereby we used IBP twice to drop the first term. Accordingly,

$$\frac{\partial \langle p \rangle}{\partial t} = -i\hbar \frac{i}{\hbar} \int_{\mathbb{R}} -|\Psi|^2 \frac{\partial V}{\partial x} \, dx = \langle -\frac{\partial V}{\partial x} \rangle$$

Thus, the time derivative of the expectation value of momentum is equal to the position derivative of the expectation value of potential well V.

Exercise 1.8
Suppose we add a constant V_0 to the potential energy. In classical mechanics, this won't change a thing, but what about in quantum mechanics? Show that the function picks up a time-dependent phase factor. What effect does this have on the expectation value of a dynamic variable?

$$\frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar} V(x,t)\Psi(x,t)$$

Set $\zeta(x,t)$ to the wave function holding potential energy $V(x,t)+V_0$ and rewrite to notice a familiar separable PDE,

$$\frac{\partial \zeta}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \zeta}{\partial x^2} - \frac{i}{\hbar} \left(V(x,t) + V_0 \right) \zeta$$

$$\implies \frac{i\hbar}{2m} \frac{\partial^2 \zeta}{\partial x^2} - \frac{iV\zeta}{\hbar} = \frac{\partial \zeta}{\partial t} + \frac{iV_0\zeta}{\hbar}$$

We consider the following boundary conditions (BC): $\zeta(\infty, t) = \zeta(-\infty, t) = 0$. We then proceed with letting $\zeta = X(x)T(t)$. Also, for this course, we are dealing mostly with the time-independent wave equation, such

that the potential well is independent of time, $V(x,t) = V(x)$.

$$\zeta(x,t) = X(x)T(t)$$
$$\zeta(\infty,t) = X(\infty)T(t) \quad \forall t \implies c_1 = X(\infty) = 0$$
$$\zeta(-\infty,t) = X(-\infty)T(t) \quad \forall t \implies c_2 = X(-\infty) = 0$$
$$\frac{i\hbar}{2m}\frac{\partial^2 XT}{\partial x^2} - \frac{iV(x)XT}{\hbar} = \frac{\partial XT}{\partial t} + \frac{iV_0 XT}{\hbar}$$
$$\frac{i\hbar}{2m}X''T - \frac{iV(x)XT}{\hbar} = XT' + \frac{iV_0 XT}{\hbar}$$
$$-\frac{\hbar^2}{2m}\frac{X''}{X} + V(x) = \frac{T'}{T}i\hbar - V_0$$
$$k\frac{X''}{X} + V(x) = \frac{T'}{T}i\hbar - V_0 = E, \text{ up to constant E, now decompose to ODEs}$$
$$kX'' = X(E - V(x)), \text{ stop here as we need potential energy specified, else BC gives trivial solutions}$$
$$\frac{T'}{T} = -i\frac{E + V_0}{\hbar}$$

For arbitrary constant C (and thus also ζ_0),

$$\zeta(x,t) = e^{-\frac{i(E+V_0)t}{\hbar}+C} = \zeta_0 e^{-\frac{i(V_0+E)}{\hbar}t}$$

Thus, when plugging this back in to the wave equation (and seeings results from the next chapter!) we note the implication: $\Psi(x,t) = \zeta(x,t)e^{\frac{iV_0}{\hbar}t}$. If we substitute into Equation 1.36, then we see that it remains unchanged. We conclude that this has no effect on the expectation value of a dynamical variable, since the extra phase factor cancels out and is independent of position.

Exercise 1.9MOD
A particle of mass m has the wave function (for positive constants A, a) of

$$\Psi(x,t) = Ae^{-a\frac{mx^2}{\hbar}-ait}$$

- Normalize to find A. Watch video on Gaussian integral if stuck on how to derive it.

$$\int_{\mathbb{R}} |\Psi(x,t)|^2 \ dx = \int_{\mathbb{R}} \Psi^* \Psi \ dx = 1$$
$$= A^2 \int_{\mathbb{R}} e^{-\frac{2amx^2}{\hbar}} \ dx$$
$$= A^2 \sqrt{\frac{\pi\hbar}{2am}} \implies A = \sqrt[4]{\frac{2am}{\pi\hbar}}$$
$$\Psi(x,t) = \sqrt[4]{\frac{2am}{\pi\hbar}} e^{-a\frac{mx^2}{\hbar}-ait}$$

- For which potential energy function, $V(x)$, is this a solution to Schro's wave equation?

$$\frac{\partial \Psi}{\partial t} = -ia\Psi$$

$$\frac{\partial \Psi}{\partial x} = -\frac{2amx}{\hbar}\Psi$$

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{-2am}{\hbar}\left(\Psi + x\frac{\partial \Psi}{\partial x}\right)$$

$$= \frac{-2am}{\hbar}\left(1 - \frac{2amx^2}{\hbar}\right)$$

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

$$V(x) = i\hbar(-ia\Psi) + \frac{\hbar^2}{2m}\left(1 - \frac{2amx^2}{\hbar}\right)\left(\frac{-2am}{\hbar}\right)\Psi$$

$$= 2a^2mx^2$$

- Find the nth moment.

Recall details in problem 1.5 and note n is a positive constant. Here, we split up the integral as was performed then, for negative infinity to 0 then 0 to positive infinity. This simplifies calculation. We set $C = \frac{2am}{\hbar}$ and use A for constant above.

$$\int_{\mathbb{R}} x^n |\Psi(x,t)|^2 \, dx = \int_{\mathbb{R}} \Psi^*[x^n]\Psi \, dx$$

$$= A^2 \int_{\mathbb{R}} x^n e^{-Cx^2} \, dx$$

$$I_{left} = \int_{-\infty}^{0} x^n e^{-Cx^2} \, dx = (-1)^n \int_{0}^{\infty} (x^n) e^{-Cx^2} \, dx$$

From here, you may use substitution of $u = x^2$, then $z = Cu$, to arrive at:

$$\frac{(-1)^n}{2C^{\frac{n+1}{2}}} \int_{0}^{\infty} e^{-z} z^{\frac{n-1}{2}} \, dz = \frac{(-1)^n}{2C^{\frac{n+1}{2}}}\Gamma\left(\frac{n+1}{2}\right)$$

A similar analysis for the positive side results in a similar answer. Combining for the intended integral and substitute back into our original expression:

$$\langle x^n \rangle = \frac{A^2((-1)^n + 1)}{2C^{\frac{n+1}{2}}}\Gamma\left(\frac{n+1}{2}\right)$$

$$\langle x \rangle = 0$$

$$\langle x^2 \rangle = \frac{1}{2}(2)\sqrt[2]{\frac{2am}{\pi\hbar}}\left(\frac{2am}{\hbar}\right)^{-3/2}\Gamma\left(\frac{3}{2}\right)^{\frac{\sqrt{\pi}}{2}}$$

$$= \frac{\hbar}{4am}$$

- Find the expression for the pth momentum. Note it gives non-trivial position partials for the first five

degrees.

$$\langle p^n \rangle = \int_{\mathbb{R}} \Psi^* \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right)^n \Psi \, dx = \left(\frac{\hbar}{i} \right)^n \int_{\mathbb{R}} \Psi^* \frac{\partial^n \Psi}{\partial x^n}$$

$$\langle p \rangle = 0$$

$$\langle p^2 \rangle = am\hbar$$

- Find σ_x and σ_p. Is their product consistent with the uncertainty principle?

$$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle} = \frac{\hbar}{4am}$$

$$\sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle} = \sqrt{am\hbar}$$

$$\sigma_p \sigma_x = \frac{\hbar}{2} \geq \frac{\hbar}{2}$$

This implies we have a wave function that barely satisifes the uncertainty principle.

Exercise 1.11

Imagine a mass particle m and energy E in a potential well $V(x)$ sliding back and forth on a frictionless surface between a and b given in Figure 1.10. Classically, the probability of finding particle in range dx is equal to the fraction of time T it takes to get from a to b that it spends on the interval dx, and for speed $v(x)$:

$$\rho(x)dx = \frac{dt}{T} = \frac{\frac{dt}{dx}dx}{T} = \frac{1}{v(x)T}dx$$

$$T = \int_0^T dt = \int_a^b \frac{1}{v(x)}dx$$

$$\implies \rho(x) = \frac{1}{v(x)T}$$

- Use conservation of energy to express speed in terms of potential well and energy.

$$E = U + K = V(x) + \frac{mv(x)^2}{2}$$

- Find the probability density for simple harmonic oscillator, $V(x) = \frac{kx^2}{2}$. Check normalization.

$$v(x) = \pm\sqrt{\frac{2(E - V(x))}{m}} = \pm\sqrt{\frac{2E - kx^2}{m}}$$

$$\rho(x) = \frac{1}{\sqrt{\frac{2E-kx^2}{m}} \int_{-A}^{A} \frac{1}{\sqrt{\frac{2E-kx^2}{m}}} \, dx}$$

$$= \frac{1}{\sqrt{\frac{2E-kx^2}{m}} \sqrt{\frac{m}{2E}} \int_{-A}^{A} \frac{1}{\sqrt{1-\frac{kx^2}{2E}}} \, dx}$$

$$= \frac{1}{2\sqrt{1 - \frac{kx^2}{2E}} \int_0^A \frac{1}{\sqrt{1-\frac{kx^2}{2E}}} \, dx}$$

Now apply a trig substitution to simplify computation; see Paul's online math notes.

$$x = \frac{1}{\sqrt{\frac{k}{2E}}} \sin\theta = \sqrt{\frac{2E}{k}} \sin\theta, \ \theta \in \left[\frac{-\pi}{2}, \frac{\pi}{2}\right]$$

$$\cos^2\theta = 1 - \sin^2\theta = 1 - \frac{k}{2E}x^2 \implies \cos\theta = \sqrt{1 - \frac{kx^2}{2E}}$$

$$dx = \sqrt{\frac{2E}{k}} \cos\theta d\theta$$

Where we note that for a SHO, the turning points are at the amplitudes $\pm A$ of the oscillation and apply the familiar trigonometric substitution. We drop $\pm$ to focus on the magnitude of dx.

$$\frac{1}{2\sqrt{1 - \frac{kx^2}{2E}} \sqrt{\frac{2E}{k}} \int_{\theta=0}^{\theta=\sin^{-1} A\sqrt{\frac{k}{2E}}} d\theta} = \frac{1}{2\sqrt{1 - \frac{kx^2}{2E}} \sqrt{\frac{2E}{k}} \int_{\theta=0}^{\theta=\sin^{-1} 1} d\theta}$$

$$= \frac{1}{\pi\sqrt{A^2 - x^2}}$$

$$\rho(x) = \begin{cases} \frac{1}{\pi\sqrt{A^2 - x^2}}, & \text{if } -A < x < A, \\ 0 & \text{otherwise} \end{cases}$$

$$\int_{-A}^{A} \rho(x)\ dx = \frac{2}{\pi} \int_0^A \frac{1}{\sqrt{A^2 - x^2}}\ dx = \frac{2}{\pi} \sin^{-1}\frac{x}{A}\Big|_0^A = 1$$

- Find the first and second expected value of position. Find σ_x. Note that knowing the odd integrand for an even interval yields 0, but can verify with substitution, $u = A^2 - x^2$. It is also helpful to use $x = A\sin\theta$ for the second moment substitution.

$$\langle x \rangle = \int_{-A}^{A} \frac{x}{\pi\sqrt{A^2 - x^2}}\ dx\ /\ 1 = 0$$

$$\langle x^2 \rangle = \int_{-A}^{A} \frac{x^2}{\pi\sqrt{A^2 - x^2}}\ dx\ /\ 1 = \frac{2}{\pi} \left(\frac{-x\sqrt{A^2 - x^2}}{2} + \frac{A^2}{2} \sin^{-1}\frac{x}{A}\right)\Big|_{-A}^{A} = \frac{A^2}{2}$$

$$\sigma_x = \langle x^2 \rangle - \langle x \rangle^2 \implies \sigma_x = \frac{A}{\sqrt{2}}$$
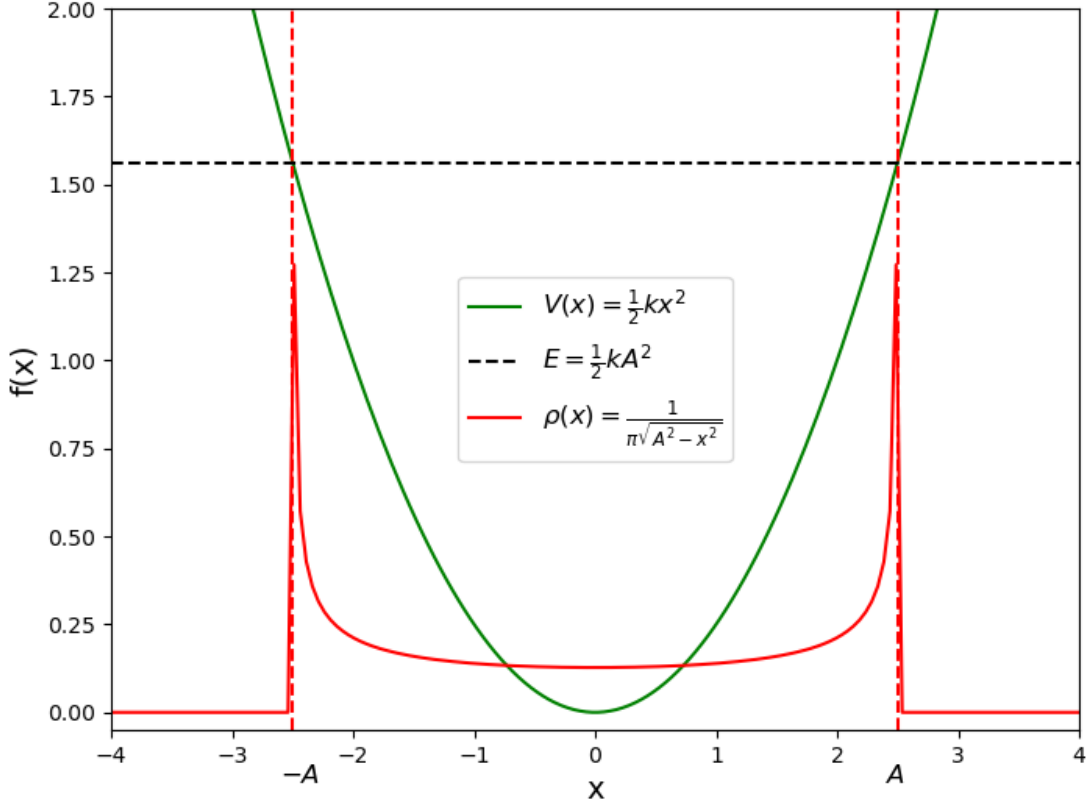
Exercise 1.12

What if we are interested in finding the momenta $(p = mv)$ distribution for the classical harmonic oscillator?

- Find the classical probability distribution $\rho(p)$; note that $p \in \left[-\sqrt{2mE}, \sqrt{2mE}\right]$. As before, we compute total energy and substitute.

$$E = U + K = \frac{kx^2}{2} + \frac{mv(x)^2}{2} = \frac{1}{2}kx^2 + \frac{p(x)^2}{2m}$$

$$\implies x(p) = \pm\sqrt{\frac{2mE - p^2}{mk}}$$

$$dx = \pm\frac{-p}{mk}\frac{1}{\sqrt{\frac{2mE-p^2}{mk}}}\ dp = \mp\frac{p}{mk}\frac{1}{\sqrt{\frac{2mE-p^2}{mk}}}\ dp = \mp\frac{p}{mk(2mE - p^2)}\ dp$$

$$\rho(x(p))dx = \frac{dt}{T} = \frac{\frac{dt}{dx}dx}{T} = \pm\frac{1}{v(x(p))T}dx = \frac{1}{v(x(p))T}\left(\mp\frac{p}{\sqrt{mk(2mE - p^2)}}\ dp\right)$$

$$= \mp\frac{1}{v(p)T}\left(\frac{p}{\sqrt{mk(2mE - p^2)}}\ dp\right) = \rho(p)\frac{p}{\sqrt{mk(2mE - p^2)}}\ dp$$

$$T = \int_{p(a)}^{p(b)} \mp\frac{1}{v(p)}\underbrace{\left(\frac{p}{\sqrt{mk(2mE - p^2)}}\ dp\right)}_{dx(p)}$$

$$\therefore \rho(p) = \frac{1}{v(p)\int_{-\sqrt{2mE}}^{\sqrt{2mE}} \mp\frac{1}{v(p)}\left(\frac{p}{\sqrt{mk(2mE-p^2)}}\ dp\right)}$$

Observe $\frac{1}{v(p)} = \frac{dt}{dx(p)}$, and so $\mp C(p) \; dp \implies \pm dx(p)$. Recall that the net external force equals the change in momentum of a system divided by the time over which it changes. As the particle moves leftward, the change in distance is negative but the change in momentum is positive, so $p(a) = \sqrt{2mE}$ (i.e., it starts to slow down while gaining momentum in the direction of the net restoring force, which pushes the particle in the opposite direction – namely, towards equilibrium where force is net zero.) Similarly, the particle reaches the equilibirum point but has gained momentum, moving past this location, with the restoring force growing to act in the opposite direction to slow the particle and return it to equilibirum; thus, the change in momentum is negative, and so $p(b) = -\sqrt{2mE}$. Energy is conserved if the process repeats ad nauseum without any frictional (damping) forces. To change the limits of integration to the form above, simply note that the inverse relationship holds as expressed in the $\mp$ indication of the integrand. We now drop this entirely to focus on the magnitude of change over the range, $dx(p)$.

$$\rho(p) = \frac{1}{v(p) \int_{-\sqrt{2mE}}^{\sqrt{2mE}} \frac{1}{v(p)} \left(\frac{p}{\sqrt{mk(2mE-p^2)}} \; dp \right)}$$

$$= \frac{1}{\frac{p}{m} \int_{-\sqrt{2mE}}^{\sqrt{2mE}} \frac{1}{\frac{p}{m}} \left(\frac{p}{\sqrt{mk(2mE-p^2)}} \; dp \right)}$$

$$= \frac{1}{\frac{p}{\sqrt{mk}} \int_{-\sqrt{2mE}}^{\sqrt{2mE}} \frac{dp}{\sqrt{2mE-p^2}}}$$

Make a trigonometric substitution,

$$p = \sqrt{2mE} \sin \theta, \; \theta \in \left[\frac{-\pi}{2}, \frac{\pi}{2} \right]$$

$$dp = \sqrt{2mE} \cos \theta$$

$$\theta = \sin^{-1} \frac{p(x)}{\sqrt{2mE}}$$

$$p^2 = 2mE \sin^2 \theta \implies 1 - \sin^2 \theta = \cos^2 \theta = 1 - \frac{p^2}{2mE}$$

$$\therefore 2mE \cos^2 \theta = 2mE - p^2$$

Making the substitutions and computing, we see that $\rho(p) = \frac{\sqrt{mk}}{\pi p}$. Also, by using trigonometric substitution, we can show

$$\int \rho(x(p)) \; dx = \int_{-\sqrt{2mE}}^{\sqrt{2mE}} \rho(p) \frac{p}{\sqrt{mk(2mE-p^2)}} \; dp = \int_{-\sqrt{2mE}}^{\sqrt{2mE}} \frac{\sqrt{mk}}{\pi p} \frac{p}{\sqrt{mk(2mE-p^2)}} \; dp = 1$$

- Calculate $\langle p \rangle$, $\langle p^2 \rangle$, and σ_p.

$$\langle p \rangle = \int_{-\sqrt{2mE}}^{\sqrt{2mE}} p\rho(x(p)) \; dp = \int_{-\sqrt{2mE}}^{\sqrt{2mE}} p \frac{\sqrt{mk}}{\pi p} \frac{p}{\sqrt{mk(2mE-p^2)}} \; dp = 0$$

$$\langle p^2 \rangle = \int_{-\sqrt{2mE}}^{\sqrt{2mE}} p^2 \rho(x(p)) \; dp = \int_{-\sqrt{2mE}}^{\sqrt{2mE}} p^2 \frac{\sqrt{mk}}{\pi p} \frac{p}{\sqrt{mk(2mE-p^2)}} \; dp = mE$$

$$\sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle} = \sqrt{mE}$$

- What is the classical undertainty product $\sigma_x \sigma_p$ for this system? Notice that this product can be as small as you like, classically, simply by sending $E \to 0$. But in quantum mechanics, the energy of a SHO cannot be less than $\hbar\omega/2$, where $\omega = \sqrt{k/m}$ is the classical frequency. In that case what can you say about the uncertainty product? Recall $\sigma_x = \frac{A}{\sqrt{2}}$ as found previously.

$$\sigma_p \sigma_x = A\sqrt{\frac{mE}{2}}$$

Now, for the quantum case, $E \geq \hbar\omega/2$. Therefore,

$$\sigma_p \sigma_x \geq A\sqrt{\frac{m\frac{\hbar\omega}{2}}{2}} = A\frac{\sqrt{\hbar\omega m}}{2}$$

With a more precisely determined amplitude of oscillation, the more precisely we can determine a particle's position and the less precisely we can determine its momentum. Conversely, with a more precisely determined particle frequency, the more precisely we can determine its momentum and the less precisely we can determine its position.

Aside: From the de Broglie relation, $\lambda = \frac{2\pi\hbar}{p}$. Also note $f = \frac{c}{\lambda}$. This shows that particles with higher momentum have a higher frequency.

Exercise 1.13
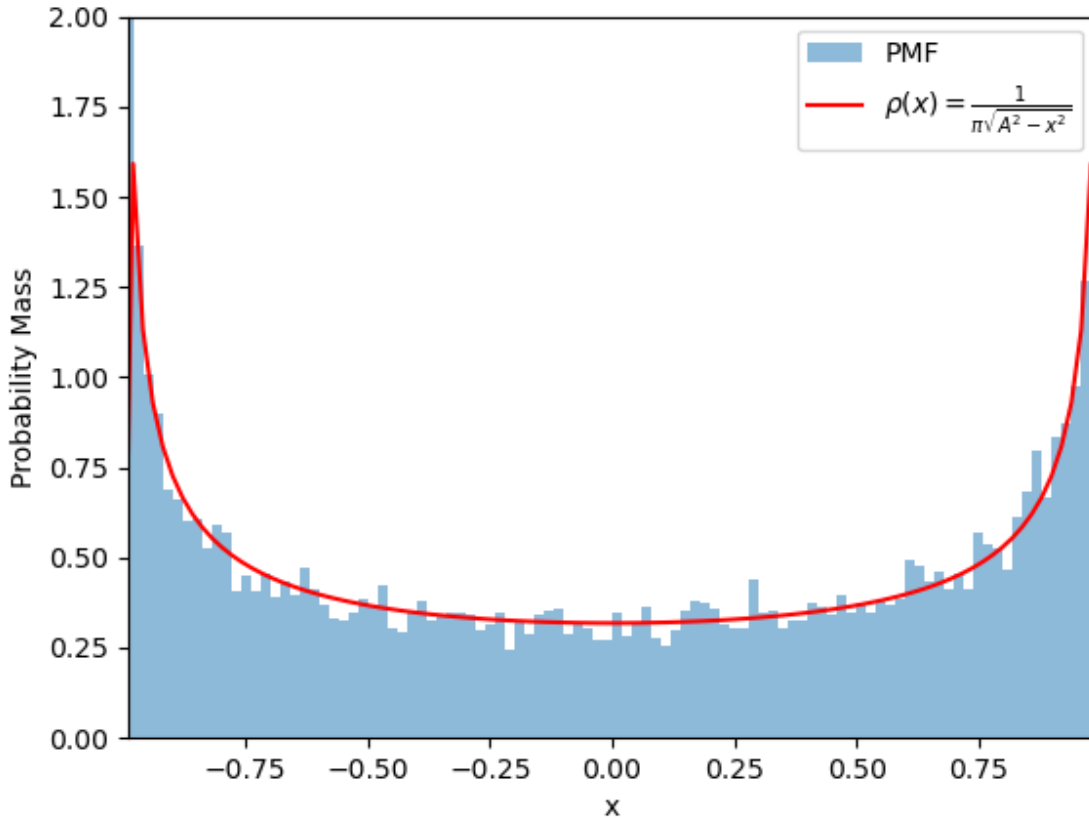
Experimental results agree with analytical expression.

Exercise 1.14
Let $P_{ab}(t)$ be the probability of finding the particle in the range $(a < x < b)$, at time t.

- Show that

$$\frac{\mathrm{d}P_{ab}}{\mathrm{d}t} = J(a,t) - J(b,t)$$

where

$$J(x,t) \equiv \frac{i\hbar}{2m}\left(\Psi\frac{\partial\Psi^*}{\partial x} - \Psi^*\frac{\partial\Psi}{\partial x}\right)$$

What are the units of $J(x,t)$? Comment: J is called the probability current, because it tells you the rate at which probability is "flowing" past point x. If $P_{ab}(t)$ is increasing, then the more probability is flowing into the region at one end than flows out the other.

$$\frac{\mathrm{d}P_{ab}}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\int_a^b |\Psi^2|\,dx = \int_a^b \frac{\partial\Psi^*\Psi}{\partial t}\,dx$$

$$= \int_a^b \frac{\partial\Psi}{\partial t}\Psi^* + \Psi\frac{\partial\Psi^*}{\partial t}\,dx$$

$$= \frac{i\hbar}{2m}\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2}\,dx$$

$$= \frac{i\hbar}{2m}\int_a^b \frac{\partial\Psi^*}{\partial x}\frac{\partial\Psi}{\partial x} + \Psi^*\frac{\partial^2\Psi}{\partial x^2} - \frac{\partial^2\Psi^*}{\partial x^2}\Psi - \frac{\partial\Psi}{\partial x}\frac{\partial\Psi^*}{\partial x}\,dx$$

$$= \frac{i\hbar}{2m}\int_a^b \frac{\partial\left(\Psi^*\frac{\partial\Psi}{\partial x} - \Psi^*\frac{\partial\Psi}{\partial x}\right)}{\partial x}\,dx$$

$$= \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial b} - \Psi\frac{\partial\Psi^*}{\partial b}\right) - \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial a} - \Psi\frac{\partial\Psi^*}{\partial a}\right)$$

$$= J(b,t) - J(a,t)$$

Probabilities don't have a dimension, so then J must have units of $1/\text{time}$, or s^{-1}, since this is a change in probability per change in time.

- Find the probability current for the wave function to 1.9.

$$\Psi(x,t) = \sqrt[4]{\frac{2am}{\pi\hbar}}e^{-a\frac{mx^2}{\hbar}-ait} = f(x)e^{-ait}$$

$$\Psi\frac{\partial\Psi^*}{\partial x} = f(x)e^{-ait}\frac{\partial f(x)}{\partial x}e^{ait} = f(x)\frac{\partial f(x)}{\partial x} = \Psi^*\frac{\partial\Psi}{\partial x}$$

$$\therefore J(x,t) = 0$$

Thus, we see a net zero probability flow in and out of this region: the probability of finding particle at position x is a constant over this region should we have probability current of 0.

Exercise 1.15
Show that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}}\Psi^*\Psi\,dx = 0$$

for any two (normalizable) solutions to Schro (with the same $V(x)$), Ψ_1, and Ψ_2.

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathbb{R}} \Psi^* \Psi \; dx &= \int_{\mathbb{R}} \frac{\partial \Psi^* \Psi}{\partial t} \; dx \\
&= \frac{i\hbar}{2m} \int_{\mathbb{R}} \left(\frac{\partial \Psi_1^*}{\partial t} \Psi_2 + \Psi_1^* \frac{\partial \Psi_2}{\partial x} \right) \; dx \\
&= \frac{i\hbar}{2m} \int_{\mathbb{R}} \left(-\frac{\partial^2 \Psi_1^*}{\partial x^2} \Psi_2 + \frac{iV \Psi_1^*}{\hbar} \Psi_2 + \frac{\partial^2 \Psi_2}{\partial x^2} \Psi_1^* - \frac{iV \Psi_2}{\hbar} \Psi_1^* \right) \; dx \\
&= -\frac{i\hbar}{2m} \int_{\mathbb{R}} \left(\frac{\partial^2 \Psi_1^*}{\partial x^2} \Psi_2 - \frac{\partial^2 \Psi_2}{\partial x^2} \Psi_1^* \right) \; dx \\
&= -\frac{i\hbar}{2m} \int_{\mathbb{R}} \left(\underbrace{\frac{\partial \Psi_1^*}{\partial x} \Psi_2 \Big|_{-\infty}^{\infty}}_{0} - \int_{\mathbb{R}} \frac{\partial \Psi_1^*}{\partial x} \frac{\partial \Psi_2}{\partial x} \; dx - \underbrace{\frac{\partial \Psi_2}{\partial x} \Psi_1^* \Big|_{-\infty}^{\infty}}_{0} + \int_{\mathbb{R}} \frac{\partial \Psi_1^*}{\partial x} \frac{\partial \Psi_2}{\partial x} \; dx \right) \; dx = 0
\end{aligned}
$$

QED

Exercise 1.16

A particle is represented (at time $t = 0$) by wave function

$$
\Psi(x,0) = \begin{cases} A(a^2 - x^2), & \text{if } -a \le x \le a, \\ \text{otherwise} \end{cases}
$$

- Determine normalization constant A.

$$
1 = |A|^2 \int_{-a}^{a} (a^2 - x^2) \; dx \implies A = \frac{1}{4a^2} \sqrt{\frac{15}{a}}
$$

- What is the expection value of x?

$$
\langle x \rangle = \int_{-a}^{a} x |\Psi|^2 \; dx = 0, \text{ odd integrand}
$$

- What is the expectation value of p? Note that you cannot get it from $\langle p \rangle = m \frac{\mathrm{d}\langle x \rangle}{\mathrm{d}t}$. Why? Since we only know $\langle x \rangle$ at $t = 0$, we cannot calculate this directly; we would need a Ψ valid for $\forall t$.

$$
\langle p \rangle = -i\hbar |A|^2 \int_{-a}^{a} (a^2 - x^2) \frac{\mathrm{d}(a^2 - x^2)}{\mathrm{d}x} \; dx = 0, \text{ odd integrand}
$$

- What is the expectation value of x^2?

$$
\langle x^2 \rangle = \int_{-a}^{a} x^2 |\Psi|^2 \; dx = \frac{a^2}{7}
$$

- What is the expectation value of p^2?

$$
\langle p^2 \rangle = -i\hbar |A|^2 \int_{-a}^{a} (a^2 - x^2) \frac{\mathrm{d}^2(a^2 - x^2)}{\mathrm{d}x^2} \; dx = \frac{5\hbar^2}{2a^2}
$$

- Find the uncertainty in x and the uncertainty in p. Check this is consistent with the uncertainty principle.

$$
\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \frac{a}{\sqrt{7}}
$$

$$
\sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\frac{5}{2}} \frac{\hbar}{a}
$$

$$
\sigma_x \sigma_p = \sqrt{\frac{10}{7}} \frac{\hbar}{2} \ge \frac{\hbar}{2}
$$

Exercise 1.17
Suppose you want to describe an unstable particle, that sponraneously disintegrates with a "lifetime of τ". In that case the total probability of findind the particle somehwhere should not be constant, but should decrease at (say) an exponential rate:

$$P(t) \equiv \int_{\mathbb{R}} |\Psi(x,t)|^2 \; dx = e^{-\frac{t}{\tau}}$$

A crude way of acheiveing this result is as follows. In Equation 1.24 we tacitly assumed to the conservation of probability enshrined in Equation 1.27. What if we assign to V an imaginary part:

$$V = V_0 - i\Gamma,$$

where V_0 is the true potential energy and Γ is a positive real constant?

- Show that (in place of Equation 1.27) we now get

$$\frac{\mathrm{d}P}{\mathrm{d}t} = -\frac{2\Gamma}{\hbar}P$$

$$\frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar}(V_0 - i\Gamma)\Psi = \frac{i\hbar}{2m}\frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar}V_0\Psi - \frac{\Gamma}{\hbar}\Psi$$

$$\frac{\partial \Psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar}(V_0 + i\Gamma)\Psi^* = -\frac{i\hbar}{2m}\frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar}V_0\Psi^* - \frac{\Gamma}{\hbar}\Psi^*$$

$$\frac{\mathrm{d}P}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}}|\Psi|^2 \; dx = \int_{\mathbb{R}}\frac{\partial}{\partial t}\Psi\Psi^* \; dx = \int_{\mathbb{R}}\left(\Psi^*\frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t}\Psi\right) dx$$

$$= \frac{i\hbar}{2m}\int_{\mathbb{R}}\left(\Psi^*\frac{\partial^2 \Psi}{\partial x^2} - \Psi\frac{\partial^2 \Psi^*}{\partial x^2}\right) dx - \frac{2\Gamma}{\hbar}\int_{\mathbb{R}}\Psi^*\Psi \; dx$$

$$= \frac{i\hbar}{2m}\int_{\mathbb{R}}\left(\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \Psi\frac{\partial \Psi^*}{\partial x}\right)\right) dx - \frac{2\Gamma}{\hbar}\int_{\mathbb{R}}|\Psi|^2 \; dx$$

$$= \frac{i\hbar}{2m}\cancel{\left(\Psi^*\frac{\partial \Psi}{\partial x} - \Psi\frac{\partial \Psi^*}{\partial x}\right)\Big|_{\mathbb{R}}}^{\;0} - \frac{2\Gamma}{\hbar}P(t)$$

$$= -\frac{2\Gamma}{\hbar}P(t)$$

$$QED$$

- Solve for $P(t)$, and find the lifetime of the particle in terms of Γ.

$$\frac{dP(t)}{P(t)} = -\frac{2\Gamma}{\hbar} \; dt$$

$$\ln(P(t)) = -\frac{2\Gamma}{\hbar}t + C \implies P(t) = Ke^{-\frac{2\Gamma}{\hbar}t}$$

$$P(0) = 1 = K$$

$$\therefore P(t) = e^{-\frac{2\Gamma}{\hbar}t} \equiv e^{-\frac{t}{\tau}} \implies \tau = \frac{\hbar}{2\Gamma}$$

Exercise 1.18
Very roughly speaking, quantum mechanics is relevant when the de Broglie wavelength of the particle in question (h/p) is greater than the characteristic size of the system d. In thermal equilibirum at (Kelvin) temperature T, the average kinetic energy of a particle is

$$\frac{p^2}{2m} = \frac{3}{2}k_BT,$$

where k_B is the Boltzmann's constant, so the typical wavelength is

$$\lambda = \frac{h}{\sqrt{3mk_BT}}$$

The purpose of this problem is to determine which systems will have to be treated quantum mechanically, and which can be safely described classically.

- **Solids**. The lattice spacing in a typical solid is around $d = 0.3$ nm. Find the temperature below which the unbound electrons in a solid are quantum mechanical. Below what temperature are the nuclei in a solid quantum mechanical? (Use silicon as an example).

$$\lambda = \frac{h}{\sqrt{3mk_BT}} > d \implies T < \frac{h^2}{3mk_Bd^2}$$

$$T_e < 1.3 \times 10^5 K$$

$$T_{Si_{nuclei,\ solid}} < 2.5K$$

Where we have used $d = 0.3 \times 10^{-9}$ m, $m_{Si_{nuclei}} = 28.086m_p = 28.086 \times 1.7 \times 10^{-27}$ kg and $m_e = 9.8 \times 10^{-31}$ kg.

Moral: The free electrons in a solid are always quantum mechanical; the nuclei are generally not quantum mechanical. The same goes for liquids (for which the interatomic spacing is roughly the same), with the exception of helium below $4\ K$.

- **Gases**. For what temperatures are the atoms in an ideal gas at pressure P quantum mechanical? Obviously (for the gas to show quantum mechanical beahvior) we want the mass to be as small as possible, and pressure to be as large as possible. Put in the numbers for monoatomic hydrogen at atmospheric pressure. Is hydrogen in outer space (where the interatomic spacing is about one centimeter and the temperature around $3\ K$) quantum mechanical?

We assume volume ocuppied by one molecule ($N = 1$) as a cubic box, $V = d^3$.

$$PV = Nk_BT \implies d = \sqrt[3]{\frac{k_BT}{P}}$$

$$\lambda = \frac{h}{\sqrt{3mk_BT}} > d \implies T < \frac{1}{k_B}\left(\frac{h^2}{3m}\right)^{3/5} P^{2/5}$$

$$T_e < 2.8K$$

$$T_{H_{nuclei,\ gas}} < 6.3 \times 10^{-14}K$$

Where we have used $d = 1 \times 10^{-2}$ m, $m_{H_{nuclei}} = 4.003m_p = 4.003 \times 1.7 \times 10^{-27}$ kg, P $= 1\ atm =$ 101,325 Pa. We observe that at $3\ K$ (monoatomic) hydrogen will behave classically and the electrons will also operate in the classical regime.

Chapter 2

Time-Independent Schrodinger Equation

2.1 Exercises

Exercise 2.1MOD
Prove the following:

- For normalizable solutions, the separation constant E must be real. Hint: take $E = E_0 + i\Gamma$, for real constants Γ, E_0.

$$\int_{\mathbb{R}} |\Psi|^2 \ dx = 1$$

$$\Psi(x,t) = \psi(x) e^{-\frac{i(E_0 + i\Gamma)}{\hbar} t}$$

$$|\Psi(x,t)|^2 = \Psi^* \Psi = \psi^* e^{\frac{iE_0}{\hbar} t} e^{\frac{\Gamma}{\hbar} t} \psi e^{\frac{-iE_0}{\hbar} t} e^{\frac{\Gamma}{\hbar} t}$$

$$= \psi^* \psi e^{\frac{2\Gamma}{\hbar} t} = |\psi(x)|^2 e^{\frac{2\Gamma}{\hbar} t}$$

$$\int_{\mathbb{R}} |\Psi|^2 \ dx = e^{\frac{2\Gamma}{\hbar} t} \int_{\mathbb{R}} |\psi(x)|^2 \ dx = 1 \ \forall t \impliedby e^{\frac{2\Gamma}{\hbar} t} = C \implies \Gamma = 0$$

- The time-independent wave function $\psi(x)$ can always be taken to be real (unlike $\Psi(x,t)$). This doesn't mean that every solution to the time-ind. Schro equation is real; what it says is that if you've got one that is not, it can always be expressed as a linear combination of solutions (with the same energy) that are. So you might as well stick to ψs that are real.

$$f(x) = a + ib, \ a, b \in \mathbb{R}$$

$$f(x) + f^*(x) = 2a \implies a = \frac{f(x) + f^*(x)}{2}$$

$$f(x) - f^*(x) = 2ib \implies b = -i\frac{f(x) - f^*(x)}{2}$$

$$-\frac{\hbar^2}{2m} \frac{\mathrm{d}^2 \psi}{\mathrm{d}x^2} + (V(x) - E)\psi(x) = 0 = -\frac{\hbar^2}{2m} \frac{\mathrm{d}^2 \psi^*}{\mathrm{d}x^2} + (V(x) - E)\psi^*(x)$$

This last line shows the form for linear, homogeneous ODEs for which their weighted sum also serves as a solution to the original ODE. To get the values for the constants c, then we can use $c_1 = c_2 = 1/2$ values for real solutions implied by a, or $c_1 = -i/2$, $c_2 = i/2$ for real solutions implied by b as well:

$$f(x) = \psi(x) = c_1 \psi(x) + c_2 \psi^*(x)$$

If $\psi(x)$ did not have any imaginary term(s), then one would pick any real constants to produce a real solution. Hence, if the solutions for the complex conjugate and the conjugate satisfy the time-ind. Schro for real $E, V(x)$, any linear combination of these will also follow suit. Note that

$$\psi = \frac{1}{2}((\psi + \psi^*) + i(-i(\psi - \psi^*)))$$

which shows ψ can be written as a linear combination of two real solutions $\psi + \psi^*$ and $i(\psi - \psi^*)$. Recall that the complex number system extends the real numbers with the imaginary unit i satisfying $i^2 = -1$.

- If $V(x)$ is an even function (i.e., $V(-x) = V(x)$), then $\psi(x)$ can always be taken to be either even or odd.

$$x = -y \implies -\frac{\mathrm{d}y}{\mathrm{d}x} = 1$$

$$\frac{\mathrm{d}\psi(x)}{\mathrm{d}x} = \frac{\mathrm{d}\psi(-y)}{\mathrm{d}(-y)} \frac{\mathrm{d}(-y)}{\mathrm{d}x}^{\,1} = -\frac{\mathrm{d}\psi(-y)}{\mathrm{d}y}$$

$$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = \frac{\mathrm{d}}{\mathrm{d}x}\frac{\mathrm{d}\psi}{\mathrm{d}x} = -\frac{\mathrm{d}(-y)}{\mathrm{d}x}^{\,1}\frac{\mathrm{d}}{\mathrm{d}(-y)}\frac{\mathrm{d}\psi(-y)}{\mathrm{d}y} = \frac{\mathrm{d}^2\psi(-y)}{\mathrm{d}y^2}$$

Now substitute as needed,

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(-y)}{\mathrm{d}(-y)^2} + (V(-y) - E)\psi(-y) = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} + (V(x) - E)\psi(x) = 0$$

As before, we get a linear ODE for the even-odd pair whose weighted sum also produces a real solution as discussed prior

$$\psi(x) = c_1\psi(-x) + c_2\psi(x)$$

Thus, any (real) solution can be expressed as a linear combination of even or odd solutions given an even potential well function with $c_1 = c_2 = 1$ producing a possible even function or $c_1 = -1,\ c_2 = 1$ producing a possible odd function,

$$f_e = \frac{f(x) + f(-x)}{2}, \ \ f_o = \frac{f(x) - f(-x)}{2}$$

It's important to note that when dealing with a real physical system, the wave function is generally a complex-valued function. However, the even and odd classifications refer to the symmetry properties of the real part of the wave function. We add the "wiggle factor" when including time domain considerations that gets us into imaginary land.

- Does the prior statement hold for an odd potential function?

Here, the probability density of finding the particle is opposite on both sides of the origin. This occurs when the particle's state possesses spatial asymmetry. The statement does not hold for an odd potential well function, where we would strictly need an odd wave function $\psi(x) = -\psi(-x)$ to maintain the proper relation above; an even wave function would contradict the antisymmetric nature of the potential function in this case.

Exercise 2.2
Show that E must exceed the minimum value of $V(x)$, for every normalizable solution to the time-ind Schro. What is the classical analog to this statement?

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

Assume that there exists a normalizable solution $\psi(x)$ to the time-independent Schrödinger equation with energy E that satisfies $E < V(x)_{min}$, where $V(x)_{min}$ is the minimum value of the potential energy function $V(x)$. Then we can write:

$$E\psi = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x)\psi < V(x)_{min}\psi$$

Dividing both sides by ψ and rearranging, we get:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + (V(x) - V(x)_{min})\psi < 0$$

Since ψ is normalizable, it must approach zero as x approaches infinity or negative infinity; if we knew the function of $V(x)$ and set $D = V(x) - V(x)_{min}$ and solved for $\psi(x)$, we would get an expression in terms of x:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + D\psi = k, \; k \in \mathbb{R} \; (\textit{in Joules, } \psi \textit{ dimensionless!})$$

$$\psi(x) = \begin{cases} c_1 e^{-\frac{\sqrt{2Dm}}{\hbar}x} + c_2 e^{\frac{\sqrt{2Dm}}{\hbar}x} & \text{if } k = 0 \impliedby \psi = 0, \; E \nless 0 \text{ (see: ZPT, and exception QNEC)} \\ c_3 e^{-\frac{\sqrt{2Dm}}{\hbar}x} + c_4 e^{\frac{\sqrt{2Dm}}{\hbar}x} - \frac{|k|}{D} & \text{if } k < 0 \end{cases}$$

Both cases allow us to find constants for the normalization condition to hold. When $x \to \infty$ then $\psi(x) \to \infty$. When $x \to -\infty$ then $\psi(x) \to -\infty$. This implies that any further derivatives have the same sign in these regions. By indicating the negation, we are counteracting the growth of ψ to "head back" towards 0, therefore, the negated second derivative term must be zero (when we have non-normalizable $\psi = 0$, where the probability of finding the system in any particular state is not well-defined) or negative (substituting in $\pm\infty$ always yields a positive second derivative and we need a real solution – $D > 0$ as we shall soon see) for all values of x,

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} \leq 0$$

Combining this with the previous inequality, we get:

$$D = (V(x) - V(x)_{min}) < 0$$

But this contradicts the fact that $V(x)_{min}$ is the minimum value of $V(x)$, which means that $V(x) - V(x)_{min}$ is non-negative for all values of x. Also note this would otherwise produce complex-valued solutions to $\psi(x)$. Therefore, our initial assumption that $E < V(x)_{min}$ must be false, and we can conclude that E must meet or exceed the minimum value of $V(x)$ for every normalizable solution to the time-independent Schrödinger equation.

If the energy is equal to or less than the potential energy at a certain point, the particle would be confined to that region (held by an "infinite force") and unable to escape. This situation would violate the classical principle of conservation of energy, which states that the total energy of a system is conserved and cannot be created or destroyed. In this case, the particle would have less energy than the potential energy barrier, and therefore, energy conservation would be violated. A more sophisticated analysis can be done by showing this violates the principle of least action: the particle would be in a region where its kinetic energy is negative or zero, leading to an imaginary or zero action. However, the principle of least action requires that the action be minimized, which corresponds to a real, non-zero value (proof beyond scope of intro course).

Exercise 2.3
Show that there is no acceptable solution to the (time-ind.) Schro for the infinite square well with $E = 0$ or

$E < 0.$

Case where $E = 0$:

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi = 0 \implies \psi(x) = Ax + B$$

$$\psi(0) = \psi(a) = 0 \implies B = 0 \implies \psi(x) = Ax = 0$$

We get a non-normalizable result $\psi(x) = 0$ whereby any constant of integration becomes a normalization factor, whose simultaneity is nonsensical.

Case where $E < 0$:

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{2mE}{\hbar^2}\psi \implies \psi(x) = Ae^{-\frac{\sqrt{2mE}}{\hbar}x} + Be^{\frac{\sqrt{2mE}}{\hbar}x}$$

$$\psi(0) = 0 \implies B = 0 \implies A = -B$$

$$\psi(a) = 0, \ A = -B \implies B = 0 \mid \frac{\sqrt{2mE}}{\hbar}x = -\frac{\sqrt{2mE}}{\hbar}x \implies \frac{\sqrt{2mE}}{\hbar} = 0$$

In this case all roads lead to having $\psi(x) = 0$ again, which is a non-normalizable solution.

Exercise 2.4
Calculate $\langle x \rangle$, $\langle x^2 \rangle$, $\langle p \rangle$, $\langle p^2 \rangle$, σ_x, σ_p for the nth stationary state for the infinite square well. Check that

the uncertainty principle is satisfied. Which state comes closest to the uncertainty limit?

$$\langle x \rangle = \int x |\psi^2| \, dx = \frac{2}{a} \int_0^a x \sin^2\left(\frac{n\pi x}{a}\right) \, dx = \frac{1}{a} \int_0^a x\left(1 - \cos\left(\frac{2n\pi x}{a}\right)\right) \, dx$$

$$= \frac{1}{a} \int_0^a x - x \cos\left(\frac{2n\pi x}{a}\right) \, dx$$

$$= \frac{a}{2} - \frac{1}{a} \int_0^a x \cos\left(\frac{2n\pi x}{a}\right) \, dx$$

$$= \frac{a}{2} + \left.\frac{x \sin\left(\frac{2n\pi x}{a}\right)}{2\pi n}\right|_0^a{}^{\nearrow 0} - \frac{1}{2\pi n} \int_0^a \sin\left(\frac{2\pi n x}{a}\right) \, dx$$

$$= \frac{a}{2} + \frac{a}{4\pi^2 n^2} \int_0^{2\pi n} \sin(u) \, du = \frac{a}{2} + \left.\frac{a}{4\pi^2 n^2} \cos(u)\right|_0^{2\pi n}{}^{\nearrow 0}$$

$$= \frac{a}{2}$$

$$\langle x^2 \rangle = \int x^2 |\psi^2| \, dx = \frac{2}{a} \int_0^a x^2 \sin^2\left(\frac{n\pi x}{a}\right) \, dx = \frac{1}{a} \int_0^a x^2 \left(1 - \cos\left(\frac{2n\pi x}{a}\right)\right) \, dx$$

$$= \frac{1}{a} \int_0^a x^2 - x^2 \cos\left(\frac{2n\pi x}{a}\right) \, dx$$

$$= \frac{1}{a}\left[\left.\frac{x^3}{3}\right|_0^a - \int_0^a x^2 \cos\frac{2n\pi x}{a} \, dx\right] = \frac{1}{a}\left[\frac{a^3}{3} - \frac{a^3}{8n^3\pi^3} \int_0^{2n\pi} y^2 \cos y \, dy\right]$$

$$= \frac{1}{a}\left[\frac{a^3}{3} - \frac{a^3}{8n^3\pi^3}\left(\left.y^2 \sin y\right|_0^{2n\pi}{}^{\nearrow 0} - 2 \int_0^{2n\pi} y \sin y \, dy\right)\right]$$

$$= \frac{1}{a}\left[\frac{a^3}{3} - \frac{a^3}{8n^3\pi^3}\left(\left.2y \cos y\right|_0^{2n\pi} - \left.2 \sin y\right|_0^{2n\pi}{}^{\nearrow 0}\right)\right]$$

$$= \frac{a^2}{3} - \frac{a^2}{2n^2\pi^2} = a^2\left(\frac{1}{3} - \frac{1}{2n^2\pi^2}\right)$$

$$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \frac{a}{2}\sqrt{\frac{1}{3} - \frac{2}{n^2\pi^2}}$$

$$\langle p \rangle = -i\hbar \int_0^a \psi_n^* \frac{\partial \psi_n}{\partial x} \, dx = m\frac{\mathrm{d}\langle x \rangle}{\mathrm{d}t} = 0$$

$$\langle p^2 \rangle = \int_0^a \psi_n^* \left[-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\right]^2 \psi_n \, dx = -\hbar^2 \int_0^a \psi_n^* \frac{\mathrm{d}^2 \psi_n}{\mathrm{d}x^2} \, dx$$

$$= \hbar^2 \int_0^a \psi_n^* k^2 \psi_n \, dx \quad \text{(by 2.24)}$$

$$= \frac{2mE_n\hbar^2}{\hbar^2} \int_0^a \psi_n^* \psi_n \, dx = 2mE_n = \left(\frac{n\pi\hbar}{a}\right)^2 \quad (\psi s \text{ orthonormal})$$

$$\sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \frac{n\pi\hbar}{a}$$

$$\sigma_p \sigma_x = \frac{\hbar}{2}\sqrt{\frac{n^2\pi^2}{3} - 2} \geq \frac{\hbar}{2}$$

Note that the complex-valued time dependence was "dropped" as those terms cancel out. The product is smallest for state $n = 1$, $1.136\hbar/2$. **Exercise 2.5**

A particle in the infinite square well has its initital wave function an even mixture of the first two stationary states:

$$\Psi(x,0) = A\left[\psi_1(x) + \psi_2(x)\right]$$

- Normalize $\Psi(x,0)$. Recall that, having normalized Ψ at $t = 0$, you can rest assured that it stays normalized – you can check this explicity after the next item.

$$1 = \int \Psi\Psi^* \, dx = |A|^2 \int (\psi_1^* + \psi_2^*)(\psi_1 + \psi_2) \, dx = |A|^2 \int |\psi_1|^2 + |\psi_2|^2 + \psi_1^*\psi_2 + \psi_2^*\psi_1 \, dx$$

$$= |A|^2(1 + 1 + 0 + 0) \quad (orthonormality)$$

$$A = \frac{1}{\sqrt{2}}$$

$$\Psi(x,0) = \underbrace{\frac{1}{\sqrt{2}}}_{c_n}\left[\psi_1(x) + \psi_2(x)\right]$$

- Find $\Psi(x,t)$, $|\Psi(x,t)|^2$. Express the latter as a sinusoidal function of time. To simplify, let $\omega = \frac{\pi^2\hbar}{2ma^2}$.

$$\Psi(x,t) = \sum_{n=1}^{2} c_n\psi_n e^{-\frac{iE_n}{\hbar}t} = \sum_{n=1}^{2} c_n\Psi(x,t) \impliedby \hbar n^2\omega = E_n$$

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\left[\psi_1(x)e^{-\frac{i\hbar\pi^2}{2ma^2}t} + \psi_2(x)e^{-\frac{4i\hbar\pi^2}{2ma^2}t}\right] = \frac{1}{\sqrt{2}}\left[\psi_1(x)e^{-i\hbar\omega t} + \psi_2(x)e^{-4i\omega t}\right]$$

$$= \frac{1}{\sqrt{2}}\sqrt{\frac{2}{a}}\left(\sin\frac{\pi x}{a}e^{-i\omega t} + \sin\frac{2\pi x}{a}e^{-4i\omega t}\right) = \frac{e^{-i\omega t}}{\sqrt{a}}\left(\sin\frac{\pi x}{a} + \sin\frac{2\pi x}{a}e^{-3i\omega t}\right)$$

$$|\Psi(x,t)|^2 = \frac{1}{a}\left(\sin^2\frac{\pi x}{a} + \sin\frac{2\pi x}{a}\sin\frac{\pi x}{a}(e^{-3i\omega t} + e^{3i\omega t}) + \sin^2\frac{2\pi x}{a}\right)$$

$$= \frac{1}{a}\left(\sin^2\frac{\pi x}{a} + \sin^2\frac{2\pi x}{a} + 2\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}\cos 3\omega t\right)$$

- Compute $\langle x\rangle$. Notice it oscillates in time. What is the angular frequency of this oscillation? What is the amplitude of oscillation? (If your amplitude is greater than $a/2$, go directly to jail)

$$\langle x\rangle = \int x|\Psi|^2 \, dx = \frac{1}{a}\int_0^a x\left(\sin^2\frac{\pi x}{a} + \sin^2\frac{2\pi x}{a} + 2\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}\cos 3\omega t\right) dx$$

$$= \frac{a}{2}\left(1 - \frac{32}{9\pi^2}\cos(3\omega t)\right) \quad (use \ trig. \ sum \ identities \ and \ IBP)$$

$$Amplitude: \ \frac{a}{2}\frac{32}{9\pi^2}$$

$$Angular \ Frequency: \ 3\omega = 3\frac{E_n}{\hbar n^2} = 3\frac{\pi^2\hbar}{2ma^2}$$

- Compute $\langle p\rangle$.

$$\langle p\rangle = m\frac{d\langle x\rangle}{dt} = \frac{8\hbar}{3a}\sin(3\omega t)$$

- If you measured the energy of this particle, what values might you get, and what is the probability of getting each of them? Find $\langle H \rangle$. How does it compare with E_1 and E_2?

$$\langle H \rangle = \sum_{n=1}^{2} |c_n|^2 E_n = |c_1|^2 E_1 + |c_2|^2 E_2 = P_1 E_1 + P_2 E_2 = |1/\sqrt{2}|^2 \frac{\pi^2 \hbar^2}{2ma^2} + |1/\sqrt{2}|^2 \frac{4\pi^2 \hbar^2}{2ma^2} = \frac{1}{2}(E_1 + E_2) = \frac{5\pi^2 \hbar^2}{4ma^2}$$

We see that the expectation value of the definite total energy (Hamiltonian) is the average of both excited states in this case.

Exercise 2.6
Although the overall phase constant of the wave function is of no physical significance (it cancels out whenever you calculate a measurable quantity), the relative phase of the coefficients of Eqn. 2.17 does matter. For example, suppose we change the relative phase from before:

$$\Psi(x,0) = A\left[\psi_1(x) + e^{i\phi}\psi_2(x)\right],$$

where ϕ is some constant. Find $\Psi(x,t)$, $|\Psi(x,t)|^2$, and $\langle x \rangle$. Study the special case $\phi = \pi/2$ and $\phi = \pi$. Compare with results prior.

$$A = \frac{1}{\sqrt{2}}$$

$$\Psi(x,t) = \frac{e^{-i\omega t}}{\sqrt{a}}\left[\sin\frac{\pi x}{a} + \sin\frac{2\pi x}{a} e^{i(\phi - 3\omega t)}\right]$$

$$|\Psi(x,t)|^2 = \frac{1}{a}\left[\sin^2\frac{\pi x}{a} + \sin^2\frac{2\pi x}{a} + 2\sin\frac{2\pi x}{a}\sin\frac{\pi x}{a}\cos(3\omega t - \phi)\right]$$

$$\langle x \rangle = \frac{a}{2}\left[1 - \frac{32}{9\pi^2}\cos(3\omega t - \phi)\right]$$

$$\phi = \frac{\pi}{2} \implies \Psi(x,0) = \frac{1}{\sqrt{2}}\left[\psi_1(x) + i\psi_2(x)\right]$$

$$\implies \langle x \rangle = \frac{a}{2}\left[1 - \frac{32}{9\pi^2}\sin(3\omega t)\right]$$

$$\implies \langle x \rangle = \frac{a}{2}, \; t = 0 \; (start\;time)$$

$$\phi = \pi \implies \Psi(x,0) = \frac{1}{\sqrt{2}}\left[\psi_1(x) - \psi_2(x)\right]$$

$$\implies \langle x \rangle = \frac{a}{2}\left[1 + \frac{32}{9\pi^2}\cos(3\omega t)\right]$$

$$\implies \langle x \rangle = \frac{a}{2}\left[1 + \frac{32}{9\pi^2}\right], \; t = 0 \; (start\;time)$$

The relative phase of the coefficients $\{c_n\}$ allow us to shift the starting point when measuring the expectation value of position.
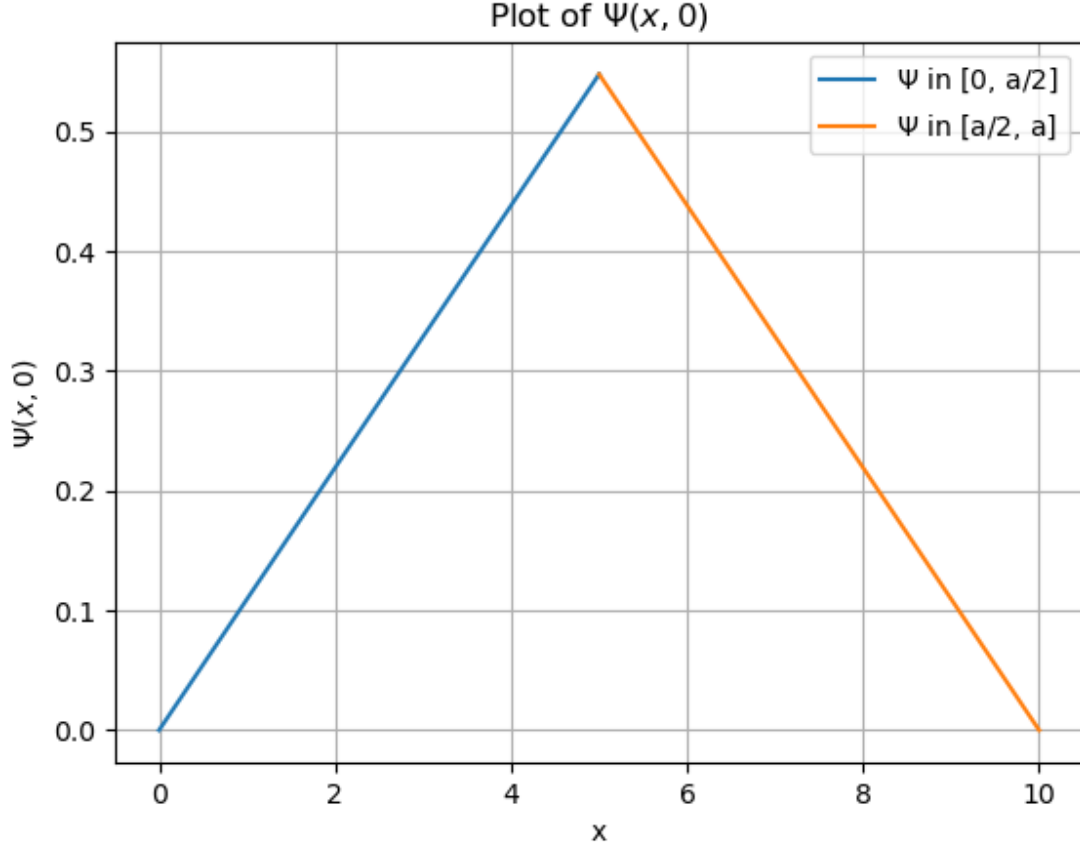
Exercise 2.7MOD
A particle in an infinite square well has the initial wave function

$$\Psi(x,0) = \begin{cases} Ax, & 0 \le x \le a \\ A(a-x), & a/2 \le x \le a \end{cases}$$

- Sketch this out and determine normalization constant.

$$1 = \int |\Psi|^2 \ dx = \int \Psi^* \Psi \ dx = |A|^2 \left[\int_0^{a/2} x^2 \ dx + \int_{a/2}^a (a-x)^2 \ dx \right] \implies A = \frac{2\sqrt{3}}{\sqrt{a^3}}$$

Plot of Ψ(x, 0)

- Find $\Psi(x,t)$.

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-\frac{iE_n t}{\hbar}} = \sum_{n=1}^{\infty} c_n \Psi_n(x,t)$$

$$c_n = \sqrt{\frac{2}{a}} \int_0^a \sin \frac{n\pi x}{a} \Psi(x,0) \ dx = \frac{2\sqrt{3}}{\sqrt{a^3}} \sqrt{\frac{2}{a}} \left[\int_0^{a/2} x \sin \frac{\pi n x}{a} \ dx + \int_{a/2}^a (a-x) \sin \frac{\pi n x}{a} \ dx \right]$$

$$= \frac{4\sqrt{6}}{n^2 \pi^2} \sin \frac{n\pi}{2} = \begin{cases} (-1)^{\frac{n-1}{2}} \frac{4\sqrt{6}}{n^2 \pi^2}, & n \text{ odd} \\ 0, & n \text{ even} \end{cases}$$

$$\therefore \Psi(x,t) = \frac{4\sqrt{6}}{\pi^2} \sqrt{\frac{2}{a}} \sum_{1,3,5,\dots} \frac{(-1)^{\frac{n-1}{2}}}{n^2} \sin \frac{n\pi x}{a} e^{-\frac{iE_n t}{\hbar}}$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

- What is the probability that the measurement of the energy would yield a value E_1?

$$|c_1|^2 = 0.9855$$

- Find the expectation value of the energy, using Eqn. 2.21.

$$\langle H \rangle = \sum_{n=1,3,5,\ldots}^{\infty} |c_n|^2 E_n = \frac{96\hbar^2}{2ma^2\pi^2}\left(\frac{1}{1^2} + \frac{1}{3^2} + \frac{1}{5^2} + \ldots\right) = \frac{96\hbar^2}{2ma^2\pi^2}\underbrace{(1-2^{-2})\zeta(2)}_{\frac{\pi^2}{8}} = \frac{6\hbar^2}{ma^2}$$

- Determine how the Fourier Transform, Riemann's Zeta Function, and Basel problem are related.

Consider the Basel problem. We can express a function using the Fourier Transform. Consider the function x^2 that is continuos and differentiable on $[-L, L] = [-\pi, \pi]$.

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty}\left(a_n \cos\frac{n\pi x}{L} + b_n \sin\frac{n\pi x}{L}\right)$$

$$\frac{a_0}{2} = \frac{1}{2L}\int_{-L}^{L} f(x)\,dx = \frac{2}{2\pi}\int_{0}^{\pi} x^2\,dx = \frac{\pi^2}{3}$$

$$a_n = \frac{1}{L}\int_{-L}^{L} f(x)\cos\frac{n\pi x}{L}\,dx = \frac{2}{\pi}\int_{0}^{\pi} x^2\cos(nx)\,dx = \frac{4}{n^2}(-1)^n$$

$$b_n = \frac{1}{L}\int_{-L}^{L} f(x)\sin\frac{n\pi x}{L}\,dx = \frac{1}{\pi}\int_{-\pi}^{\pi} x^2\sin(nx)\,dx = 0$$

$$f(\pi) = \pi^2 = \frac{\pi^2}{3} + \sum_{n=1}^{\infty}\frac{4(-1)^n}{n^2}\cancel{\cos(\pi n)}^{(-1)^n} \Longleftrightarrow 4\sum_{n=1}^{\infty}\frac{1}{n^2} = \frac{2\pi^2}{3} \implies \sum_{n=1}^{\infty}\frac{1}{n^2} = \frac{\pi^2}{6}$$

$$f(0) = 0 = \frac{\pi^2}{3} + \sum_{n=1}^{\infty}\frac{4(-1)^n}{n^2}\cancel{\cos(0)}^{1} \Longleftrightarrow -\sum_{n=1}^{\infty}\frac{(-1)^n}{n^2} = \sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n^2} = \frac{\pi^2}{12}$$

The last two last lines are two such "problems" and note how we can take different functions to determine coefficients which the below will also show. Euler did the above differently (see YouTube) but now we can turn to Riemann's Zeta Function.

$$\frac{\pi^2}{6} = \frac{1}{1^2} + \frac{1}{2^2} + \frac{1}{3^2} + \ldots$$

$$\frac{1}{2^2}\frac{\pi^2}{6} = \frac{1}{2^2} + \frac{1}{4^2} + \frac{1}{6^2} + \ldots$$

$$(1-\frac{1}{2^2})\frac{\pi^2}{6} = \frac{1}{1^2} + \frac{1}{3^2} + \frac{1}{5^2} + \ldots = \frac{\pi^2}{8}$$

$$(1-\frac{2}{2^2})\frac{\pi^2}{6} = \frac{1}{1^2} - \frac{1}{2^2} + \frac{1}{3^2} - \frac{1}{4^2} + \ldots = \frac{\pi^2}{12}$$

Now, generalize.

$$\zeta(z) = \frac{\pi^2}{6} = \frac{1}{1^z} + \frac{1}{2^z} + \frac{1}{3^z} + \ldots$$

$$(1-\frac{1}{2^z})\zeta(z) = \frac{1}{1^z} + \frac{1}{3^z} + \frac{1}{5^z} + \ldots$$

$$\frac{1}{2^z}\zeta(z) = \frac{1}{2^z} + \frac{1}{4^z} + \frac{1}{6^z} + \ldots$$

$$(1-\frac{2}{2^z})\frac{\pi^2}{6} = \frac{1}{1^z} - \frac{1}{2^z} + \frac{1}{3^z} - \frac{1}{4^z} + \ldots$$

Note for the harmonic series case, we may assume it converges. With this in mind, the second line below produces a greater sum, which we assume also converges. But, the sum of this line must be the sum of the last line, which is greater still. Thus, our initial assumption was wrong and all of them must diverge.

$$\zeta(1) = \frac{1}{1} + \frac{1}{2} + \frac{1}{3} + \ldots = \infty$$

$$(1 - 0.5)\zeta(1) = \frac{1}{1} + \frac{1}{3} + \frac{1}{5} + \ldots = 0.5\zeta(1) = \infty$$

$$0.5\zeta(1) = \frac{1}{2} + \frac{1}{4} + \frac{1}{6} + \ldots = \infty$$

- Discuss the general equation for the Riemann zeta function at even integers.

The equation for the Riemann zeta function at even integers can be stated as follows:

For any positive even integer s, where $s = 2k$ for some positive integer k, the Riemann zeta function $\zeta(s)$ is given by:

$$\zeta(2k) = \frac{(-1)^{k+1} \cdot (2\pi)^{2k} \cdot B_{2k}}{2 \cdot (2k)!},$$

where π is the mathematical constant pi, B_{2k} is the $2k$th Bernoulli number, and $(2k)!$ is the factorial of $2k$.

One common definition of the Bernoulli numbers is through their generating function:

$$\frac{t}{e^t - 1} = \sum_{n=0}^{\infty} \frac{B_n}{n!} t^n,$$

where B_n represents the nth Bernoulli number.

Another way to define the Bernoulli numbers is using the recursive formula:

$$B_0 = 1, \quad \text{and} \quad B_n = -\frac{1}{n+1} \sum_{k=0}^{n-1} \binom{n+1}{k} B_k,$$

where $\binom{n+1}{k}$ denotes the binomial coefficient, which is the number of ways to choose k objects from a set of $n+1$ objects.

These definitions allow us to compute the Bernoulli numbers for any given index n. However, it's worth noting that for odd indices n greater than 1, the Bernoulli numbers are always equal to zero. In summary, the Riemann zeta function at even integers is expressed in terms of the Bernoulli numbers and the constant π, providing a closed-form formula for these specific values of s. No closed-form expression yet exists for odd positive integers of the Ziemann function.

Exercise 2.8
A particle of mass m in the infinite square well (of width a) starts out in the state

$$\Psi(x, 0) = \begin{cases} A, & 0 \leq x \leq a/2 \\ 0, & a/2 \leq x \leq a \end{cases}$$

for some constant A, so it is (at $t = 0$) equally likely to be found at any point in the left half of the well. What is the probability that a measurement of the energy at some later time would yield the value of $\frac{\hbar^2 \pi^2}{2ma^2}$?

$$1 = \int \Psi \Psi^* \ dx = |A|^2 \int_0^{a/2} dx \implies A = \sqrt{\frac{2}{a}}$$

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2} \implies E_1 = \frac{\hbar^2 \pi^2}{2ma^2} \impliedby n = 1$$

$$c_n = \sqrt{\frac{2}{a}} \int_0^a \sin \frac{\pi x n}{a} \Psi(x,0) \ dx = \sqrt{\frac{2}{a}} \sqrt{\frac{2}{a}} \int_0^{a/2} \sin \frac{\pi n x}{a} \ dx = -\frac{2}{\pi} \left(\cos \frac{\pi n}{2} - 1 \right)$$

$$c_1 = \frac{2}{\pi} \implies P_1 = |c_1|^2 = 0.4053$$

Exercise 2.9

For the wave function in Example 2.2, find the expectation value of H, at time $t = 0$, the old-fashioned way:

$$\langle H \rangle = \int \Psi(x,0)^* \hat{H} \Psi(x,0) \ dx$$

Compare this result to that of Example 2.3. Because $\langle H \rangle$ is time-ind. then no loss of generality in using this time.

$$\langle H \rangle = \int \Psi(x,0)^* \hat{H} \Psi(x,0) \ dx$$

$$= \int_0^a \left[\sqrt{\frac{30}{a^5}} x(a-x) \right]^* \left[-\frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} + \cancel{V(x)}^{\,0} \right] \left[\sqrt{\frac{30}{a^5}} x(a-x) \right] \ dx$$

$$= \int_0^a \left[\sqrt{\frac{30}{a^5}} x(a-x) \right] \left[-\frac{\hbar}{2m} \frac{\partial^2 \sqrt{\frac{30}{a^5}} x(a-x)}{\partial x^2} \right] \ dx$$

$$= -\frac{\hbar^2}{m} \frac{30}{a^5} \int_0^a x^2 - ax \ dx$$

$$= -\frac{5\hbar^2}{ma^2}$$

We arrive at the same result using $\langle H \rangle = \sum_{n=1}^\infty |c_n|^2 E_n = \sum_{n=1}^\infty P_n E_n$.

Exercise 2.10

- Construct ψ_2. We will construct from $\sqrt{2}^{-1}(\hat{a}_+)^2 \psi_0$, but can also do (easier) $\sqrt{2}^{-1}(\hat{a}_+)\psi_1$ since ψ_1
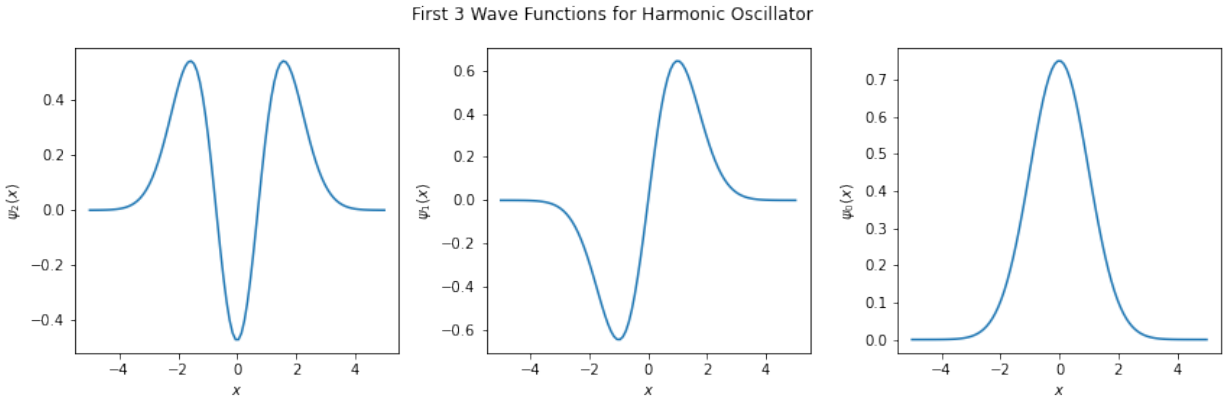
provided by text.

$$\psi_2 = \frac{1}{\sqrt{2}}(\hat{a}_+)^2\psi_0 = \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2\hbar m\omega}}(-i\hat{p} + m\omega x)\right)^2\psi_0$$

$$= \frac{1}{2\sqrt{2}\hbar m\omega}\left(\hbar^2\frac{\partial^2}{\partial x^2} + m^2\omega^2 x^2 - 2m\omega\hbar x\frac{\partial}{\partial x} - \hbar m\omega\right)\psi_0$$

$$= \frac{\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}}{2\sqrt{2}\hbar m\omega}\left(\hbar^2\frac{\partial^2}{\partial x^2} + m^2\omega^2 x^2 - 2m\omega\hbar x\frac{\partial}{\partial x} - \hbar m\omega\right)e^{-\frac{m\omega}{2\hbar}x^2}$$

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

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

Where we have used the fact that $-im\omega(x\hat{p} + \hat{p}x) = -m\omega(2\hbar x\frac{\partial}{\partial x} + \hbar)$.

- Check orthgonality of first three wave functions.

First observe that ψ_0, ψ_2 are even and ψ_1 is odd; a product of an even and odd function gives an odd integrand over a symmetric integral that is then evaluated to zero. Thus, only one computation needed.

$$\int_{\mathbb{R}}\psi_2^*\psi_0 \; dx = \sqrt{2}\left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\int_{\mathbb{R}}\left(\frac{m\omega x^2}{\hbar} - \frac{1}{2}\right)e^{-\frac{m\omega}{\hbar}x^2} \; dx = 0$$

First 3 Wave Functions for Harmonic Oscillator

Exercise 2.11MOD

- Compute a general form for $I_s = \int_{\mathbb{R}}e^{-sx^2} \; dx$ for $s > 0$. Give an expression for $-\frac{\mathrm{d}I_s}{\mathrm{d}s}$ and also show a general form for its integral over the real numbers.

$$I_s^2 = \iint_{\mathbb{R}} e^{-s(x^2+y^2)} \; dxdy$$

$$= \int_0^\infty e^{-sr^2} r \; dr \int_0^{2\pi} d\theta \quad (polar\ coord.\ transformation)$$

$$= \pi \int_0^\infty e^{-st} \; dt \quad (substitute\ t = r^2)$$

$$= \frac{\pi}{s} \implies I_s = \sqrt{\frac{\pi}{s}}$$

$$-\frac{dI_s}{ds} = \int_{\mathbb{R}} x^2 e^{-sx^2} \; dx$$

$$= -\frac{d\sqrt{\frac{\pi}{s}}}{ds} = \frac{\sqrt{\pi}}{2s^{3/2}}$$

- Compute $\langle x \rangle, \langle x^2 \rangle, \langle p \rangle, \langle p^2 \rangle$ for states ψ_0, ψ_1 using explicit integration.

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

$$\psi_1(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \sqrt{\frac{2m\omega}{\hbar}} x e^{-\frac{m\omega}{2\hbar}x^2}$$

$$\langle x_0 \rangle = \int_{\mathbb{R}} \psi_0^* x \psi_0 \, dx = \sqrt{\frac{m\omega}{\pi\hbar}} \int_{\mathbb{R}} x e^{-\frac{m\omega}{\hbar}x^2} \, dx = 0$$

$$\langle x_1 \rangle = \int_{\mathbb{R}} \psi_1^* x \psi_1 \, dx = \sqrt{\frac{4m^3\omega^3}{\pi\hbar^3}} \int_{\mathbb{R}} x^3 e^{-\frac{m\omega}{\hbar}x^2} \, dx = 0$$

$$\langle x_0^2 \rangle = \int_{\mathbb{R}} \psi_0^* x^2 \psi_0 \, dx = \sqrt{\frac{m\omega}{\pi\hbar}} \int_{\mathbb{R}} x^2 e^{-\frac{m\omega}{\hbar}x^2} \, dx$$

$$= \sqrt{\frac{m\omega}{\pi\hbar}} \sqrt{\pi} \frac{1}{2\frac{m\omega}{\hbar}\sqrt{\frac{m\omega}{\hbar}}}$$

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

$$\langle p_0 \rangle = \int_{\mathbb{R}} \psi_0^* -i\hbar \frac{\partial}{\partial x} \psi_0 \, dx = -i\hbar \int_{\mathbb{R}} \psi_0^* \frac{d\psi_0}{dx} \, dx$$

$$= im\omega \sqrt{\frac{m\omega}{\pi\hbar}} \int_{\mathbb{R}} x e^{-\frac{m\omega}{\hbar}x^2} \, dx = 0$$

$$\langle p_1 \rangle = \int_{\mathbb{R}} \psi_1^* -i\hbar \frac{\partial}{\partial x} \psi_1 \, dx = -i\hbar \int_{\mathbb{R}} x(1 - \frac{m\omega}{\hbar}x^2) e^{-\frac{m\omega}{\hbar}x^2} \, dx = 0$$

$$\zeta \equiv \sqrt{\frac{m\omega}{\hbar}} x$$

$$\langle x_1^2 \rangle = \frac{2}{\sqrt{\pi}} \frac{\hbar}{m\omega} \int_{\mathbb{R}} \zeta^4 e^{-\zeta^2} d\zeta$$

$$= \frac{4}{\sqrt{\pi}} \frac{\hbar}{m\omega} \int_0^\infty \zeta^4 e^{-\zeta^2} d\zeta$$

$$= \frac{2}{\sqrt{\pi}} \frac{\hbar}{m\omega} \int_0^\infty u^{3/2} e^{-u} du = \frac{2}{\sqrt{\pi}} \frac{\hbar}{m\omega} \Gamma(5/2)$$

$$= \frac{3\hbar}{2m\omega}$$

$$\langle p_0^2 \rangle = -\frac{2\hbar m\omega}{\sqrt{\pi}} \left(\int_0^\infty \zeta^2 e^{-\zeta^2} \, d\zeta - \int_0^\infty e^{-\zeta^2} \, d\zeta \right)$$

$$= -\frac{2\hbar m\omega}{\sqrt{\pi}} \left(\frac{1}{2} \Gamma(5/2) - \sqrt{\pi} \right) = \frac{\hbar m\omega}{2}$$

$$\langle p_1^2 \rangle = \frac{4\hbar m\omega}{\sqrt{\pi}} \left(3 \int_0^\infty \zeta^2 e^{-\zeta^2} \, d\zeta - \int_0^\infty \zeta^4 e^{-\zeta^2} \, d\zeta \right)$$

$$= \frac{4\hbar m\omega}{\sqrt{\pi}} \left(\frac{3}{2} \Gamma(3/2) - \frac{1}{2} \Gamma(5/2) \right) = \frac{3\hbar m\omega}{2}$$

$$\sigma_{x_0} = \sqrt{\frac{\hbar}{2m\omega}}$$

$$\sigma_{p_0} = \sqrt{\frac{\hbar m\omega}{2}}$$

$$\sigma_{x_0}\sigma_{p_0} = \frac{\hbar}{2}$$

$$\sigma_{x_1} = \sqrt{\frac{3\hbar}{2m\omega}}$$

$$\sigma_{p_1} = \sqrt{\frac{3\hbar m\omega}{2}}$$

$$\sigma_{x_1}\sigma_{p_1} = \frac{3\hbar}{2}$$

- Check the uncertainty principle in these cases.

$$\sigma_{x_0}\sigma_{p_0} = \frac{\hbar}{2} \geq \frac{\hbar}{2}$$

$$\sigma_{x_1}\sigma_{p_1} = \frac{3\hbar}{2} \geq \frac{\hbar}{2}$$

- Compute $\langle T \rangle, \langle V \rangle$ for the states. Is sum what you would expect?

$$\langle V_0 \rangle = \langle \frac{m\omega^2 x^2}{2} \rangle = \frac{m\omega^2 \langle x^2 \rangle}{2} = \frac{\hbar\omega}{4}$$

$$\langle T_0 \rangle = \langle \frac{p^2}{2m} \rangle = \frac{\langle p^2 \rangle}{2m} = \frac{\hbar\omega}{4}$$

$$\langle T_0 \rangle + \langle V_0 \rangle = \frac{\hbar}{2}$$

$$\langle V_1 \rangle = \langle \frac{m\omega^2 x^2}{2} \rangle = \frac{m\omega^2 \langle x^2 \rangle}{2} = \frac{3\hbar\omega}{4}$$

$$\langle T_1 \rangle = \langle \frac{p^2}{2m} \rangle = \frac{\langle p^2 \rangle}{2m} = \frac{3\hbar\omega}{4}$$

$$\langle T_1 \rangle + \langle V_1 \rangle = \frac{3\hbar}{2}$$

We see that the sums are the appropriate energy levels for the ground state and first excited state, respectively.

2.12 Compute $\langle x \rangle, \langle x^2 \rangle, \langle p \rangle, \langle p^2 \rangle, \langle T \rangle$ for n^{th} stationary state using ladder operators.

$$\langle x \rangle = \int_{\mathbb{R}} \psi_n^* \hat{x} \psi_n \, dx = \int_{\mathbb{R}} \psi_n^* \left[\sqrt{\frac{\hbar}{2m\omega}} (\hat{a}_+ + \hat{a}_-) \right] \psi_n \, dx = \sqrt{\frac{\hbar}{2m\omega}} \int_{\mathbb{R}} \psi_n^* (\hat{a}_+ \psi_n + \hat{a}_- \psi_n) \, dx$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \int_{\mathbb{R}} \psi_n^* (A_{n+1}\psi_{n+1} + A_{n-1}\psi_{n-1}) \, dx$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \left[A_{n+1} \int_{\mathbb{R}} \psi_n^* \psi_{n+1} \, dx \xrightarrow{\;0\;} + A_{n-1} \int_{\mathbb{R}} \psi_n^* \psi_{n-1} \, dx \xrightarrow{\;0\;} \right] = 0$$

$$\langle x^2 \rangle = \int_{\mathbb{R}} \psi_n^* \left[\sqrt{\frac{\hbar}{2m\omega}} (\hat{a}_+ + \hat{a}_-) \right]^2 \psi_n \, dx$$

$$= \frac{\hbar}{2m\omega} \int_{\mathbb{R}} \psi_n^* (\hat{a}_+^2 + \hat{a}_-\hat{a}_+ + \hat{a}_+\hat{a}_- + \hat{a}_-^2) \psi_n \, dx$$

$$= \frac{\hbar}{2m\omega} \int_{\mathbb{R}} \psi_n^* \left[A_{n+2}\psi_{n+2} + n\psi_n + (n+1)\psi_n + A_{n-2}\psi_{n-2} \right] dx$$

$$= \frac{\hbar}{2m\omega} \left[A_{n+2} \int_{\mathbb{R}} \psi_n^* \psi_{n+2} \, dx \xrightarrow{\;0\;} + n \int_{\mathbb{R}} \psi_n^* \psi_n \, dx \xrightarrow{\;1\;} + (n+1) \int_{\mathbb{R}} \psi_n^* \psi_n \, dx \xrightarrow{\;1\;} + A_{n-2} \int_{\mathbb{R}} \psi_n^* \psi_{n-2} \, dx \xrightarrow{\;0\;} \right]$$

$$= \frac{\hbar}{2m\omega} (2n+1)$$

$$\langle p \rangle = \int_{\mathbb{R}} \psi_n^* \hat{p} \psi_n \, dx = i\sqrt{\frac{\hbar m\omega}{2}} \int_{\mathbb{R}} \psi_n^* (\hat{a}_+ - \hat{a}_-) \psi_n \, dx$$

$$= i\sqrt{\frac{\hbar m\omega}{2}} \int_{\mathbb{R}} \psi_n^* (A_{n+1}\psi_{n+1} - A_{n-1}\psi_{n-1}) \, dx = 0$$

$$\langle p^2 \rangle = -\frac{\hbar m\omega}{2} \int_{\mathbb{R}} \psi_n^* (\hat{a}_+^2 - \hat{a}_-\hat{a}_+ - \hat{a}_+\hat{a}_- + \hat{a}_-^2) \psi_n \, dx$$

$$= -\frac{\hbar m\omega}{2} (-(n+1) - n)$$

$$= \frac{\hbar m\omega}{2} (2n+1)$$

$$\sigma_x \sigma_p = \frac{\hbar(2n+1)}{2}$$

$$\langle T \rangle = \frac{\langle p^2 \rangle}{2m} = \frac{\hbar\omega}{4} (2n+1)$$

Exercise 2.13

A particle in the harmonic oscillator potential starts out in state

$$\Psi(x,0) = A \left(3\psi_0(x) + 4\psi_1(x) \right)$$

- Find A.

$$1 = \int_{\mathbb{R}} \Psi^* \Psi \, dx = |A|^2 \int_{\mathbb{R}} 9\psi_0\psi_0^* + 12\psi_0\psi_1^* + 12\psi_1\psi_0^* + 16\psi_1\psi_1^* \, dx$$

$$= A^2 \left[9 \int_{\mathbb{R}} \psi_0\psi_0^* \, dx + 12 \int_{\mathbb{R}} \psi_0\psi_1^* \, dx + 12 \int_{\mathbb{R}} \psi_1\psi_0^* \, dx + 16 \int_{\mathbb{R}} \psi_1\psi_1^* \, dx \right]$$

$$= 25A^2 \implies A = \frac{1}{5}$$

$$\Psi(x,0) = \frac{3}{5}\psi_0 + \frac{4}{5}\psi_1$$

- Construct $\Psi(x,t), |\Psi(x,t)|^2$. What would have happened if we specified ψ_2 instead of ψ_1?

$$\Psi(x,t) = \frac{3}{5}\psi_0 e^{-i\frac{E_0}{\hbar}t} + \frac{4}{5}\psi_1 e^{-i\frac{E_1}{\hbar}t}$$

$$= \frac{3}{5}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} e^{i\frac{\omega t}{2}} + \frac{4}{5}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} xe^{-\frac{3m\omega}{2\hbar}x^2} e^{-i\frac{3\omega t}{2}}$$

$$|\Psi(x,t)|^2 = \Psi\Psi^* = \frac{1}{25}\sqrt{\frac{m\omega}{\pi\hbar}}\left(\frac{32m\omega x^2}{\hbar} + 24\sqrt{\frac{2m\omega}{\hbar}}x\cos(\omega t) + 9\right)e^{-\frac{m\omega}{\hbar}x^2}$$

The subsitution for the next higher energy state is left as an exercise.

- Find $\langle x \rangle, \langle p \rangle$. Check that Ehrenfest's Theorem (Eq. 1.38) holds for this wave function.

$$\zeta \equiv \sqrt{\frac{m\omega}{\hbar}}x$$

$$\langle x \rangle = \int_{\mathbb{R}} \Psi^* x \Psi \, dx = \int_{\mathbb{R}} x|\Psi|^2 \, dx = \frac{24}{25}\sqrt{\frac{2}{\pi}}\cos(\omega t)\int_{\mathbb{R}} \frac{m\omega}{\hbar}x^2 e^{-\frac{m\omega}{\hbar}x^2} \, dx$$

$$= \frac{48}{25}\sqrt{\frac{2\hbar}{\pi m\omega}}\cos(\omega t)\underbrace{\int_0^\infty \zeta^2 e^{-\zeta^2} \, d\zeta}_{\frac{1}{2}\Gamma(3/2)}$$

$$= \frac{12}{25}\sqrt{\frac{2\hbar}{m\omega}}\cos(\omega t)$$

$$\langle p \rangle = \int_{\mathbb{R}} \Psi^* - i\hbar\frac{\partial}{\partial x}\Psi \, dx = -i\hbar\int_{\mathbb{R}} \Psi^*\frac{\partial\Psi}{\partial x} \, dx$$

$$= -\frac{12}{25}\sqrt{2\hbar m\omega}\sin(\omega t)$$

Confirmation left as an exercise; i.e., $\langle p \rangle = m\langle v \rangle = m\frac{\mathrm{d}\langle x \rangle}{\mathrm{d}t}$; should also see that $\frac{\mathrm{d}\langle p \rangle}{\mathrm{d}t} = \langle -\frac{\mathrm{d}V}{\mathrm{d}x}\rangle$

- If you measured the energy of this particle, what values might you get? What are their probabilities?

$$P_0 = \left[\frac{3}{5}\right]^2 = 0.36$$

$$P_1 = \left[\frac{4}{5}\right]^2 = 0.64$$

$$E_0 = \frac{\hbar\omega}{2}$$

$$E_1 = \frac{3\hbar\omega}{2}$$

Exercise 2.14
In the ground state of the harmonic oscillator, what is the probability (correct to 3 sig figs) of finding the particle outside the classically allowed region? Hint: classically, the energy of the oscillator is $E = 0.5kA^2 =$

$0.5m\omega^2 A^2$ for amplitude A. Thus the region is for an energy E extending from $-\sqrt{2E/m\omega^2}$ to $\sqrt{2E/m\omega^2}$.

$$\zeta \equiv \sqrt{\frac{m\omega}{\hbar}}x$$

$$1 - \int_{-A}^{A} |\Psi_0(x,t)|^2 \, dx = 1 - \int_{-A}^{A} \psi_0^2 \, dx = 1 - \sqrt{\frac{m\omega}{\pi\hbar}} \int_{-A}^{A} e^{-\frac{m\omega}{\hbar}x^2} \, dx$$

$$= 1 - \frac{2}{\sqrt{\pi}} \int_0^{\sqrt{\frac{m\omega}{\hbar}}A} e^{-\zeta^2} \, d\zeta$$

$$= 1 - \mathrm{erf}\left(\sqrt{\frac{m\omega}{\hbar}}A\right)$$

$$E_0 = \frac{\hbar\omega}{2} = \frac{m\omega^2 A^2}{2} \implies A = \sqrt{\frac{\hbar}{m\omega}}$$

$$\therefore 1 - P = 1 - \mathrm{erf}(1) \approx 0.157$$

Exercise 2.15MOD
Use recusion formula (Eq. 2.85) to work out $H_5(\xi)$. Invoke the convention that the highest power of ξ is 2^n to fix the overall constant. Then, compute the normalization constant. As $n = 5$, we need to set $a_0 = 0$ to kill off even power terms and set $j = 5$ to stop at the proper odd term.

$$a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)}a_j$$

$$a_3 = \frac{-2(5-1)}{(1+1)(1+2)}a_1 = -\frac{4}{3}a_1$$

$$a_5 = \frac{-2(5-3)}{(3+1)(3+2)}a_3 = -\frac{a_3}{5} = \frac{4}{15}a_1 = 2^5 \implies a_1 = 120$$

$$h_5(\xi) = a_1(\xi - \frac{4}{3}\xi^3 + \frac{4}{15}\xi^5) = 32\xi^5 - 160\xi^3 + 120\xi$$

$$\psi_5(\xi) = h_5(\xi)e^{-\frac{\xi^2}{2}} = 120(\xi - \frac{4}{3}\xi^3 + \frac{4}{15}\xi^5)e^{-\frac{\xi^2}{2}}$$

Because of the association of the wavefunction with a probability density, it is necessary for the wavefunction

to include a normalization constant. We take the moment generating function for the Hermite polynomial and exploit its orthgonality.

$$\psi_n(\xi) = c_n H_n(\xi) e^{-\frac{\xi^2}{2}}$$

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

(*First by generating functions*)

$$I = \int_{\mathbb{R}} g(\xi, t) e^{-\xi^2/2} g(\xi, s)^* e^{-\xi^2/2} \, d\xi$$

$$= e^{st} \int_{\mathbb{R}} e^{-u^2} \, du$$

$$= \sqrt{\pi} e^{2st}$$

(*Now with Hermite polynomials*)

$$I = \int_{\mathbb{R}} g(\xi, t) e^{-\xi^2/2} g(\xi, s)^* e^{-\xi^2/2} \, d\xi$$

$$= \int_{\mathbb{R}} \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(\xi) \sum_{m=0}^{\infty} \frac{s^m}{m!} H_m(\xi)$$

$$= \sum_{n=0}^{\infty} \frac{t^n}{n!} \sum_{m=0}^{\infty} \frac{s^m}{m!} \underbrace{\int_{\mathbb{R}} H_n(\xi) H_m(\xi) e^{-\xi^2} \, d\xi}_{A_{nm}}$$

We know the expansion of the Euler constant is $x^n/n!$, so we equate both series as such

$$\sqrt{\pi} \sum_{n=0}^{\infty} \frac{(2st)^n}{n!} = \sum_{n=0}^{\infty} \frac{t^n}{n!} \sum_{m=0}^{\infty} \frac{s^m}{m!} A_{nm}$$

$$\sqrt{\pi}(2s)^n = \sum_{m=0}^{\infty} \frac{s^m}{m!} A_{nm} \implies n = m$$

$$\sqrt{\pi}(2)^n = \frac{1}{n!} A_{nn} \implies \int_{\mathbb{R}} H_n(\xi) H_m(\xi) e^{-\xi^2} \, d\xi = \delta_{nm} \sqrt{\pi} 2^n n!$$

$$1 = \int_{\mathbb{R}} |\Psi_n|^2 \, dx = \int_{\mathbb{R}} \psi_n^2 \, dx = c_n^2 \int_{\mathbb{R}} H_n(\xi)^2 e^{-\xi^2} \, d\xi = \sqrt{\pi} 2^n n!$$

$$c_n = \sqrt{\frac{1}{\sqrt{\pi} 2^n n!}}$$

$$\therefore \psi_n(\xi) = \frac{\pi^{-1/4}}{\sqrt{n! 2^n}} H_n(\xi) e^{-\frac{\xi^2}{2}}$$

We want a more explicit form in terms of position, so recall $\xi \equiv \sqrt{\frac{m\omega}{\hbar}} x$, which implies $dx = \sqrt{\frac{\hbar}{m\omega}} d\xi$. It

follows that

$$\int_{\mathbb{R}} H_n(\xi)H_m(\xi)e^{-\xi^2}\, d\xi = \sqrt{\frac{\hbar}{m\omega}}\int_{\mathbb{R}} H_n(\sqrt{\frac{m\omega}{\hbar}}x)H_m(\sqrt{\frac{m\omega}{\hbar}}x)e^{-\frac{m\omega x^2}{2\hbar}}\, dx = \delta_{nm}\sqrt{\pi}2^n n!$$

$$\implies c_n = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}$$

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

Exercise 2.16
In this problem we explore some of the more useful theorems (stated without proof) involving Hermite polynomials.

- The Rodrigues forula says that

$$h(\xi) = (-1)^n e^{\xi^2}\frac{d^n}{d\xi^n}e^{-\xi^2}$$

  Use it to derive H_3 and H_4.

$$H_3(\xi) = -e^{\xi^2}\frac{d^3 e^{-\xi^2}}{d\xi^3} = 8\xi^3 - 12\xi$$

$$H_4(\xi) = e^{\xi^2}\frac{d^4 e^{-\xi^2}}{d\xi^4} = 16\xi^4 - 48\xi^2 + 12$$

- The following relation gives you H_{n+1} in terms of the preceding Hermite polynomials:

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

  Use it, together with previous results, to obtain H_4 and H_5.

$$H_5 = 2\xi H_4 - 8H_3 = 32\xi^5 - 160\xi^3 + 120\xi$$
$$H_6 = 2\xi H_5 - 10H_5 = 64\xi^6 - 480\xi^4 + 720\xi^2 - 120$$

- If you differentiate a polynomial of order n, you get one of order $n-1$. For Hermite polynomials,

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

  Check this by differentiating H_5 and H_6.

$$\frac{dH_5}{d\xi} = \frac{d(32\xi^5 - 160\xi^3 + 120\xi)}{d\xi} = 10(16\xi^4 - 48\xi^2 + 12) = 10H_4$$

$$\frac{dH_6}{d\xi} = \frac{d(64\xi^6 - 480\xi^5 + 720\xi^3 - 120)}{d\xi} = 12(32\xi^5 - 160\xi^3 + 120\xi) = 12H_5$$

- $H_n(\xi)$ is the nth z-derivative, at $z=0$, of the generating function $e^{-z^2+2z\xi}$; or, to put it another way, it's the coefficient $z^n/n!$ in the Taylor series expansion for this function:

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

Use this to obtain H_1, H_2, and H_3.

$$f(z) = \sum_{n=0}^{\infty} \frac{f^{(n)}(z_0)}{n!}(z-z_0)^n, \ z_0 = 0$$

$$f^{(0)}(z) = e^{-z^2+2z\xi} \qquad\qquad\qquad \Longrightarrow \ f^{(0)}(0) = 1$$

$$f^{(1)}(z) = e^{-z^2+2z\xi}(2\xi - 2z) \qquad\qquad \Longrightarrow \ f^{(1)}(0) = 2\xi$$

$$f^{(2)}(z) = e^{-z^2+2z\xi}(2\xi - 2z)^2 - 2e^{-z^2+2z\xi} \qquad\qquad \Longrightarrow \ f^{(2)}(0) = 4\xi^2 - 2$$

$$f^{(3)}(z) = e^{-z^2+2z\xi}(2\xi - 2z)^3 - 4e^{-z^2+2z\xi}(2\xi - 2z) + 4e^{-z^2+2z\xi}(z - \xi) \quad \Longrightarrow \ f^{(3)}(0) = 8\xi^3 - 12\xi$$

$$\therefore e^{-z^2+2z\xi} = f^{(0)}(z) + f^{(1)}(z)z + f^{(2)}(z^2)/2! + f^{(3)}(z)/3! + \dots$$

$$= 1 + 2z\xi + (4\xi^2 - 2)z^2/2 + (8\xi^3 - 12\xi)z^3/6 + \dots$$

$$= \sum_{n=0}^{\infty} f^{(n)}(0)\frac{z^n}{n!} \ \Longrightarrow \ f^{(n)}(0) \equiv H_n(\xi)$$

Exercise 2.17
Show that $Ae^{ikx} + Be^{-ikx}$ and $C\cos(kx) + D\sin(kx)$ are equivalent ways of writing the same function of x, and determine the constants in terms of one another. In quantum mechanics, when $V = 0$, the exponentials represent traveling waves, and are most convenient in discussing free particles, whereas sines and cosines correspond to traveling waves, which arise naturally in the case of the infinite square well.

$$Ae^{ikx} + Be^{-ikx} = (A+B)\cos(kx) + i(A-B)\sin(kx)$$

$$C = A + B \iff A = \frac{1}{2}(C - iD)$$

$$D = i(A-B) \iff B = \frac{1}{2}(C + iD)$$

Exercise 2.18
Find the probability current J for the free particle wave function (using Eq 2.95). Which direction does the probability flow?

$$J(x,t) = \frac{i\hbar}{2m}\left(\Psi\frac{\partial\Psi^*}{\partial x} - \Psi^*\frac{\partial\Psi}{\partial x}\right)$$

$$= \frac{\hbar k|A|^2}{m}$$

As k is positive, probability is flowing past point x in the positive direction.

Exercise 2.19
This problem is designed to guide you through the "proof" of Plancherel's theorem, by starting with the theory of ordinary Fourier series on a finite interval, and allowing it to then expand to infinity.

- Dirichlet's theorem say that any suitable function $f(x)$ on the interval $[-a, a]$ can be expanded to a Fourier series:

$$f(x) = \sum_{n=0}^{\infty}\left[a_n\sin\left(\frac{n\pi x}{a}\right) + b_n\cos\left(\frac{n\pi x}{a}\right)\right]$$

Show this can be written as

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{-in\pi x/a}$$

What is c_n in terms of a_n and b_n?

$$f(x) = b_0 + \sum_{n=1}^{\infty}\left[a_n \sin\left(\frac{n\pi x}{a}\right) + b_n \cos\left(\frac{n\pi x}{a}\right)\right]$$

$$\int_{-a}^{a} f(x)\, dx = \int_{-a}^{a} b_0 + \sum_{n=1}^{\infty}\left[a_n \sin\left(\frac{n\pi x}{a}\right) + b_n \cos\left(\frac{n\pi x}{a}\right)\right] dx = 2ab_0 \implies b_0 = \frac{1}{2a}\int_{-a}^{a} f(x)\, dx$$

$$f(x)\cos\left(\frac{m\pi x}{a}\right) = b_0 \cos\left(\frac{m\pi x}{a}\right) + \sum_{n=1}^{\infty} a_n \sin\left(\frac{n\pi x}{a}\right)\cos\left(\frac{m\pi x}{a}\right) + \sum_{n=1}^{\infty} b_n \cos\left(\frac{n\pi x}{a}\right)\cos\left(\frac{m\pi x}{a}\right)$$

$$\implies \int_{-a}^{a} f(x)\cos\left(\frac{n\pi x}{a}\right) dx = ab_n \implies b_n = \frac{1}{a}\int_{-a}^{a} f(x)\cos\left(\frac{n\pi x}{a}\right) dx$$

$$f(x)\sin\left(\frac{m\pi x}{a}\right) = b_0 \sin\left(\frac{m\pi x}{a}\right) + \sum_{n=1}^{\infty} a_n \sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{m\pi x}{a}\right) + \sum_{n=1}^{\infty} b_n \cos\left(\frac{n\pi x}{a}\right)\sin\left(\frac{m\pi x}{a}\right)$$

$$\implies \int_{-a}^{a} f(x)\sin\left(\frac{n\pi x}{a}\right) dx = aa_n \implies a_n = \frac{1}{a}\int_{-a}^{a} f(x)\sin\left(\frac{n\pi x}{a}\right) dx$$

We now use Euler's forula to express sinusoidal terms in terms of exponentials. We skip to the good part:

$$f(x) = b_0 + \sum_{n=1}^{\infty} \frac{b_n - ia_n}{2} e^{in\pi x/a} + \sum_{n=1}^{\infty} \frac{b_n + ia_n}{2} e^{-in\pi x/a}$$

$$c_0 \equiv b_0$$

$$c_n = \frac{b_n - ia_n}{2}, \; n \in \mathbb{Z}_1^+$$

$$c_{-n} = \frac{b_{-n} + ia_{-n}}{2}, \; n \in \mathbb{Z}_1^-$$

$$\implies f(x) = \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/a}$$

- Show, by modification of Fourier's trick, that

$$c_n = \frac{1}{2a}\int_{-a}^{a} c_n e^{in\pi x/a}\, dx$$

$$f(x)e^{-im\pi x/a} = \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/a} e^{-im\pi x/a}$$

$$\int_{-a}^{a} f(x)e^{-im\pi x/a}\, dx = \int_{-a}^{a}\sum_{n=-\infty}^{\infty} c_n e^{in\pi x/a} e^{-im\pi x/a}\, dx = \sum_{n=-\infty}^{\infty} c_n \underbrace{\int_{-a}^{a} e^{i(n-m)x/a}\, dx}_{2a\delta_{nm}}$$

$$\therefore \int_{-a}^{a} f(x)e^{-in\pi x/a}\, dx = 2ac_n \implies c_n = \frac{1}{2a}\int_{-a}^{a} e^{-in\pi x/a}\, dx \; (n=m)$$

- Eliminate n and c_n in favor of new variables $k = n\pi/a$ and $F(k) = \sqrt{2/\pi}ac_n$. Show that

$$f(x) = \frac{1}{\sqrt{2\pi}}\sum_{n=-\infty}^{\infty} F(k)e^{ikx}\Delta k; \quad F(k) = \frac{1}{\sqrt{2\pi}}\int_{-a}^{a} f(x)e^{-ikx}\, dx,$$

where Δk is the increment in k from one n to the next.

$$c_n = \frac{1}{a}\sqrt{\frac{\pi}{2}}F(k) = \frac{1}{2a}\int_{-a}^{a} f(x)e^{-in\pi x/a}\ dx \implies F(k) = \frac{1}{\sqrt{2\pi}}\int_{-a}^{a} f(x)e^{-ikx}\ dx$$

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

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/a} = \sum_{n=-\infty}^{\infty}\left(\frac{1}{2a}\int_{-a}^{a} f(x)e^{-in\pi x/a}\ dx\right)e^{in\pi x/a}$$

$$= \sum_{k=-\infty}^{\infty}\left(\frac{1}{2a}\int_{-a}^{a} f(x)e^{-ikx}\ dx\right)e^{ikx}$$

$$= \frac{\pi}{a\sqrt{2\pi}}\sum_{k=-\infty}^{\infty}\left(\frac{1}{\sqrt{2\pi}}\int_{-a}^{a} f(x)e^{-ikx}\ dx\right)e^{ikx}$$

$$= \frac{1}{\sqrt{2\pi}}\sum_{n=-\infty}^{\infty} F(k)e^{ikx}\Delta k \quad (limits:\ n\ and\ k\ both\ directly\ proportional)$$

- Take the limit as $a \to \infty$ to obtain Plancherel's Theorem. In view of quite different origins, it is surprising that two formulas have such similar structure in this limit.

With this limit, k becomes a continuos variable.

$$\lim_{a\to\infty} f(x) = \frac{1}{\sqrt{2\pi}}\int_{k=-\infty}^{\infty} F(k)e^{ikx}\ dk$$

$$\lim_{a\to\infty} F(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{-ikx}\ dx$$