15. Find the sets of quantum numbers for a two-dimensional infinite square well that yield the lowest 12 eigenenergies. Identify the eigenenergies from this list that demonstrate degeneracy.

This problem demonstrates degeneracy in a pseudo-physical system. It is generally convenient to express eigenenergies in terms of ground state energy, however, the ground state energy of the onedimensional infinite square well which we denote E_0 is most convenient for this two-dimensional system since component eigenenergies are integral multiples of E_0 . Ground state energy is the lowest possible energy where zero energy is disallowed because a physical system cannot exist at zero energy. Zero is disallowed as a component quantum number for a multi-dimensional infinite square well because a zero component quantum number results in zero component wavefunction meaning that the system does not exist.

n_x	n_y	E		n_x	n_y	E	
1	1	$2E_0$	1	3	3	$18E_{0}$	7
2	1	$5E_0$	2	4	2	$20E_0$	8
1	2	$5E_0$	2	2	4	$20E_0$	8
2	2	$8E_0$	3	4	3	$25E_0$	9
3	1	$10E_{0}$	4	3	4	$25E_0$	9
1	3	$10E_{0}$	4	5	1	$26E_0$	10
3	2	$13E_0$	5	1	5	$26E_{0}$	10
2	3	$13E_0$	5	5	2	$29E_{0}$	11
4	1	$17E_{0}$	6	2	5	$29E_q$	11
1	4	$17E_{0}$	6	4	4	$32 E_0$	12

Degeneracy is seen at $5E_0$, $10E_0$, $13E_0$, $17E_0$, $20E_0$, $25E_0$, $26E_0$, and $29E_0$ in this list.

Postscript: Notice that component quantum number 4 is encountered in the energy sequence before component quantum number 3 is exhausted, and component quantum number 5 is encountered before component quantum number 4 is exhausted. This is a feature seen in realistic systems.

If a component quantum number of zero was allowed, for instance if $n_y = 0$, then

$$\psi_{n_x=1, n_y=0} = \frac{1}{\sqrt{a}} \cos\left(\frac{\pi x}{2a}\right) \frac{1}{\sqrt{a}} \sin(0) = 0.$$

A zero wavefunction is a system that does not exist so zero is disallowed as a component quantum number for a multi-dimensional infinite square well.

Practice Problems

16. Calculate the energies of the first five energy levels of an electron trapped in an infinite square well of width 2 Angstroms.

Using 0.511 MeV/c^2 for the mass of the electron and the value $hc = 1.24 \times 10^4 \text{ eV} \cdot \text{\AA}$ will make this calculation simpler than using MKS or CGS units. See problems 1 and 3.

17. (a) Write down the fifth and sixth position space eigenfunctions for an electron in an infinite square well of width 2 Angstroms.

(b) Sketch these eigenfunctions indicating what happens outside of the well.

(c) Sketch the probability densities corresponding to these eigenfunctions.

Sketch means show qualitatively the features of each $\psi_n(x)$. Since the walls are impermeable, the wave function must be zero outside the well. See problems 2 and 4.

18. Compare the probability of locating a particle in its first excited state in an infinite square well of width 2a between $\pm a/10$ at the center of the well and an interval of equal length at the right edge.

The first excited state means n = 2 for the infinite square well. Use the appropriate eigenfunction from problem 2 and the techniques from problem 5.

19. Compare the probability of locating a particle in an infinite square well of width 2a between $\pm a/10$ at the center of the well and an interval of equal length at the right edge given the state function

$$\Psi(x) = \frac{1}{4a^2} \sqrt{\frac{15}{a}} \left(a^2 - x^2\right).$$

The given state function is the normalized result of problem 11. Use the techniques of problem 5.

20. Does the product of the uncertainties of position and momentum in an infinite square well of width 2a obey the Heisenberg uncertainty relation?

Problems 9 and 10 provide the uncertainties of position and momentum for an infinite square well of width 2a. Calculate the product in general, then calculate the product numerically for n = 1, 2, 3, and 4 as multiples of \hbar . Then show that the multiple of \hbar grows as n gets larger and that the limiting case of $n \to \infty$ is infinity. All products for all n are greater than $\hbar/2$.

21. Calculate the uncertainty in energy for a particle in an infinite square well of width 2a. Explain the result.

Use E_{op} in position space and procedures closely resembling problem 10. Calculate (a) $\langle E \rangle$, (b) $\langle E^2 \rangle$, and (c) ΔE for all n in one spatial dimension.

$$E_{op} = \frac{P_{op}^2}{2m} = \frac{1}{2m} \left(-i\hbar\nabla\right) \left(-i\hbar\nabla\right) \to -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$$

in one spatial dimension. The *n* odd and *n* even integrals for $\langle E \rangle$ are the same as those used to calculate $\langle p^2 \rangle$ in problem 10 divided by 2m. For $\langle E^2 \rangle$,

$$E_{op}^{2} = E_{op} E_{op} = \left(-\frac{\hbar^{2}}{2m}\frac{d^{2}}{dx^{2}}\right)\left(-\frac{\hbar^{2}}{2m}\frac{d^{2}}{dx^{2}}\right) = \frac{\hbar^{4}}{4m^{2}}\frac{d^{4}}{dx^{4}}$$

Since and cosines duplicate themselves when they are differentiated four times so this is not arduous. The uncertainties may be interesting. The E_n are eigenvalues of the Schrödinger equation. What do you anticipate for the uncertainty of an eigenvalue? Problem 1 may also be of interest.

Problems 22 through 31 all refer to an infinite square well of width 2a, where the wavefunction is in a superposition of eigenstates such that the state is a triangular wave centered in the well, i.e.

$$\Psi(x,0) = N\left(1 - \frac{|x|}{a}\right) \quad \text{for } |x| \le a$$
$$= 0 \qquad \text{for } |x| > a$$

22. Calculate the normalization constant N.

This problem is intended to reinforce the procedures of calculating a normalization constant for a continuous system. See problem 11 for procedures. The normalization condition for a continuous sytem in one variable for the given wavefunction is

$$1 = \int_{-a}^{a} \left[N\left(1 - \frac{|x|}{a}\right) \right]^{*} \left[N\left(1 - \frac{|x|}{a}\right) \right] dx = |N|^{2} \int_{-a}^{a} \left(1 - \frac{|x|}{a}\right)^{2} dx$$

where the limits of integration indicate the wavefunction is zero outside the well. Express this without the absolute value to clarify the integration. Treat it as a sum of two integrals describing regions on both sides of zero,

$$1 = |N|^{2} \int_{-a}^{0} \left(1 + \frac{x}{a}\right)^{2} dx + |N|^{2} \int_{0}^{a} \left(1 - \frac{x}{a}\right)^{2} dx.$$

These integrals are straightforward. You may recognize that the integrals have the same magnitude, so you can evaluate one integral and multiply it by 2 to get the same result.

23. Expand the initial state function $\Psi(x, 0)$ in terms of the position space eigenfunctions, $\psi_n(x)$, and use the time dependence of the $\psi_n(x)$'s, to write down the full time dependent $\Psi(x, t)$.

You have done time evolution calculations for discrete systems. The difference for continuous systems is that instead of two or three eigenstates there are an infinite number of eigenstates. Per

problem 8, determining which eigenstates contribute what amount is an exercise in calculating Fourier coefficients. Integration is the challenging part of this problem. Here

$$\psi(x,0) = \sum_{n \text{ odd}}^{\infty} b_n \sqrt{\frac{1}{a}} \cos\left(\frac{n\pi x}{2a}\right) + \sum_{n \text{ even}}^{\infty} d_n \sqrt{\frac{1}{a}} \sin\left(\frac{n\pi x}{2a}\right)$$

This $\Psi(x,0)$ is an even function. Cosines are even functions and sines are odd functions. Odd functions, sine terms, will not contribute so all $d_n = 0$. You only have to find the b_n 's, and

$$b_n = \int_{-a}^{a} \psi_n^*(x) \,\Psi(x,0) \, dx = \int_{-a}^{a} \sqrt{\frac{1}{a}} \, \cos\left(\frac{n\pi x}{2a}\right) \sqrt{\frac{3}{2a}} \left[1 - \frac{|x|}{a}\right] \, dx$$

Remember that cosines correspond to the odd quantum numbers. To add time dependence

$$\Psi(x,t) = \sum_{n \text{ odd}}^{\infty} b_n \psi_n(x) \ e^{-iE_n t/\hbar}$$

where the E_n 's are those for an infinite square well of width 2a. See problem 1. You should find

$$\Psi(x,t) = 8\sqrt{\frac{3}{2}} \sum_{n \text{ odd}}^{\infty} \frac{1}{n^2 \pi^2} \cos\left(\frac{n\pi x}{2a}\right) \exp\left(-\frac{i\pi^2 \hbar n^2}{8ma^2}t\right)$$

for this system. Problem 12 may be illustrative.

24. Calculate the uncertainty in position for the particle in the state given as $\Psi(x, 0)$. Plot the probability density P(x) dx versus x at t = 0. Indicate your calculated values of $\langle x \rangle$ and Δx on the sketch.

 $\Psi(x,0)$ is a superposition of infinite eigenstates. All continuous wavefunctions are superpositions of infinite eigenstates. You do not need the eigenstates because the continuous wavefunction contains all the information about their "weighting."

Take advantage of the fact that $\Psi(x,0)$ is an even function, and use odd/even function arguments. For instance, the requested expectation value is

$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi^*(x) \ x \ \Psi(x) \ dx = \int_{-a}^{a} \sqrt{\frac{3}{2a}} \left(1 - \frac{|x|}{a}\right) \ x \ \sqrt{\frac{3}{2a}} \left(1 - \frac{|x|}{a}\right) \ dx.$$

The integrand is a product of an even function, $\Psi^*(x, 0)$, and an odd function, x, and another even function $\Psi(x, 0)$. This composite function is odd. An odd function integrated between symmetric limits is zero. Can you attain the required expectation value from this argument without making a calculation? Expect results for the second moment and the uncertainty that differ from the analogous calculations in problem 9. The second moment is likely easiest calculated

$$\langle x^{2} \rangle = \int_{-a}^{0} \sqrt{\frac{3}{2a}} \left(1 + \frac{x}{a}\right) x^{2} \sqrt{\frac{3}{2a}} \left(1 + \frac{x}{a}\right) dx + \int_{0}^{a} \sqrt{\frac{3}{2a}} \left(1 - \frac{x}{a}\right) x^{2} \sqrt{\frac{3}{2a}} \left(1 - \frac{x}{a}\right) dx.$$

The quantum number will not appear in any result in this problem.

25. Find the initial state momentum wavefunction $\widehat{\Psi}(p,0)$. Sketch $\widehat{\Psi}(p,0)$ versus p.

You need the "quantum mechanical" Fourier transform of part 3 of chapter 1,

$$\widehat{\psi}(p,0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{-ipx/\hbar} \psi(x,0) \, dx$$

The calculation is similar to problem 6, though the given $\Psi(x,0)$ is independent of quantum number. Break the integral into two parts from -a to zero, and from zero to a, clearing the absolute value in the process. Each of the parts is straight forward. You should get

$$\widehat{\Psi}(p,0) = \frac{\hbar^2}{ap^2} \sqrt{\frac{3}{\pi\hbar a}} \left[1 - \cos\left(\frac{p}{\hbar}a\right) \right], \text{ which is the function you want to sketch.}$$

26. Calculate the uncertainty in momentum for the particle in the state given as $\Psi(x,0)$.

Use the P_{op} sandwich in position space to find $\langle p \rangle$ like problem 10. The calculation for $\langle p^2 \rangle$ is done below because it introduces the use of the theta function initially discussed in part 3 of chapter 1. Attempt to understand the use of the theta function and the fact that the theta function can be useful at discontinuities. If we attempt a P_{op}^2 sandwich,

$$\langle p^{2} \rangle = \int_{-\infty}^{\infty} \psi^{*}(x) \left(-i\hbar \frac{d}{dx}\right) \left(-i\hbar \frac{d}{dx}\right) \psi(x) dx$$

$$= -\hbar^{2} \int_{-a}^{a} \left(\sqrt{\frac{3}{2a}}\right)^{*} \left(1 - \frac{|x|}{a}\right)^{*} \frac{d^{2}}{dx^{2}} \sqrt{\frac{3}{2a}} \left(1 - \frac{|x|}{a}\right) dx$$

$$= -\hbar^{2} \frac{3}{2a} \int_{-a}^{0} \left(1 + \frac{x}{a}\right) \frac{d^{2}}{dx^{2}} \left(1 + \frac{x}{a}\right) dx - \hbar^{2} \frac{3}{2a} \int_{0}^{a} \left(1 - \frac{x}{a}\right) \frac{d^{2}}{dx^{2}} \left(1 - \frac{x}{a}\right) dx$$

$$= -\frac{3\hbar^{2}}{2a} \left\{ \int_{-a}^{0} \left(1 + \frac{x}{a}\right) \frac{d}{dx} \left(\frac{1}{a}\right) dx + \int_{0}^{a} \left(1 - \frac{x}{a}\right) \frac{d}{dx} \left(-\frac{1}{a}\right) dx \right\}$$

$$= -\frac{3\hbar^{2}}{2a} \left\{ \int_{-a}^{0} \left(1 + \frac{x}{a}\right) (0) dx + \int_{0}^{a} \left(1 - \frac{x}{a}\right) (0) dx \right\} = -\frac{3\hbar^{2}}{2a} \left\{ \int_{-a}^{0} (0) dx + \int_{0}^{a} (0) dx \right\}$$

which is not very satisfying. This allows us to ascertain only that $\langle p^2 \rangle = \text{constant}$. We expect $\langle p^2 \rangle \neq 0$ unless the particle is stationary in our reference frame. Other procedures are in order.

Consider the theta function, discussed in part 3 of chapter 1 as the integral of a delta function. The delta function is the derivative of the theta function. The theta function is

$$\Theta\left(x-x'\right) = \begin{cases} 1, & x-x'>0\\ 0, & x-x'<0 \end{cases} \quad \text{Now} \quad \int_{-\infty}^{\infty} \delta\left(x-x'\right) dx = 1. \text{ The integral} \\ \int_{-\infty}^{x} \delta\left(x-x'\right) dx = \begin{cases} 1, & -\infty < x' < x\\ 0, & x'>x \end{cases} \quad \Rightarrow \quad \int_{-\infty}^{x} \delta\left(x-x'\right) dx = \begin{cases} 1, & x-x'>0\\ 0, & x-x'<0 \end{cases} \quad \text{so} \\ \int_{-\infty}^{x} \delta\left(x-x'\right) dx = \Theta\left(x-x'\right) \Rightarrow \quad \delta\left(x-x'\right) = \frac{d}{dx} \Theta\left(x-x'\right) \end{cases}$$

We will use the form

$$\int_{-\infty}^{x} \delta(x) \, dx = \Theta(x) \quad \Rightarrow \quad \delta(x) = \frac{d}{dx} \Theta(x)$$

Our integral is
$$\langle p^2 \rangle = -\hbar^2 \int_{-a}^{a} \left(\sqrt{\frac{3}{2a}}\right)^* \left(1 - \frac{|x|}{a}\right)^* \frac{d^2}{dx^2} \sqrt{\frac{3}{2a}} \left(1 - \frac{|x|}{a}\right) dx$$

$$= -\frac{3\hbar^2}{2a} \int_{-a}^{a} \left(1 - \frac{|x|}{a}\right) \frac{d}{dx} \left[\frac{d}{dx} \left(1 - \frac{|x|}{a}\right)\right] dx$$

Consider just the expression in the square brackets.

$$\frac{d}{dx}\left(1-\frac{|x|}{a}\right) = \frac{1}{a}\left(1-2\Theta(x)\right).$$

If you do not see this immediately, take the derivative on the left and apply the definition of the theta function for the cases x > 0 and x < 0 on the right. Replace the expression in square brackets by the right side of the last equation, or

$$= -\frac{3\hbar^{2}}{2a} \int_{-a}^{a} \left(1 - \frac{|x|}{a}\right) \frac{d}{dx} \left[\frac{1}{a} \left(1 - 2\Theta(x)\right)\right] dx$$

$$= -\frac{3\hbar^{2}}{2a^{2}} \int_{-a}^{a} \left(1 - \frac{|x|}{a}\right) \frac{d}{dx} \left[1 - 2\Theta(x)\right] dx$$

$$= \frac{3\hbar^{2}}{a^{2}} \int_{-a}^{a} \left(1 - \frac{|x|}{a}\right) \delta(x) dx = \frac{3\hbar^{2}}{a^{2}} \left[1 - \frac{|x|}{a}\right]_{x=0} = \frac{3\hbar^{2}}{a^{2}}$$

This calculation uses a theta function to caste an integral into a form containing a delta function so that the integral is then easily evaluated. Theta functions are useful at discontinuities. The "tent" wave function is continuous, but its first derivative is discontinuous by a constant amount which is why the second derivative is zero. Another approach not involving theta functions is to find $\langle E \rangle$, then $\langle p^2 \rangle = 2m \langle E \rangle$. To take this path, you need to work problem 29 first. It is straightforward to now find Δp .

27. Write a general time–dependent wavefunction in momentum space as a summation of the momentum space eigenfunctions.

The important point in this problem is that you can decompose a wavefunction into its component eigenstates in momentum space just as is done in position space. Similar to problem 8,

$$\begin{aligned} |\psi\rangle &= \mathcal{I} |\psi\rangle = \sum_{n} |E_{n}\rangle \langle E_{n} |\psi\rangle \\ \Rightarrow &$$

$$\Rightarrow \quad \widehat{\Psi}(p) \to \sum_{n} \widehat{\psi}_{n}(p) \int \left(\widehat{\psi}_{n}^{*}(p)\right) \left(\widehat{\Psi}(p)\right) dp$$
$$\Rightarrow \quad \widehat{\Psi}(p) = \sum_{n} \beta_{n} \widehat{\psi}_{n}(p) \quad \text{where} \quad \beta_{n} = \int \widehat{\psi}_{n}^{*}(p) \ \widehat{\Psi}(p) dp \quad \text{and}$$
$$\widehat{\Psi}(p,t) = \sum_{n} \beta_{n} \widehat{\psi}_{n}(p) \ e^{-iE_{n}t/\hbar}.$$

You have the momentum space state function from the previous problem and the momentum space eigenfunctions for an infinite square well of width 2a from problem 6. Simply substitute them appropriately into the last line. Do NOT attempt the integrations—using Mathematica, Maple, MatLab, or some other computer–based application is much more time efficient in this case if a closed form solution or numerical values are actually required.

28. Express the time-dependent wavefunction in energy space, $\widetilde{\Psi}(E,t)$, in terms of the energy space eigenfunctions, $\widetilde{\psi}_n(E)$'s, in general for the given $\Psi(x,0)$.

Can you use Dirac notation including insertion and resolution of the identity well enough to find

$$\widetilde{\Psi}(E,t) = \sum_{n \text{ odd}} b_n \, \widetilde{\psi}_n(E) \, e^{-iE_n t/\hbar} \, ?$$

Follow problems 8 and 27. Here $\langle E | E_n \rangle = \widetilde{\psi}_n(E)$.

29. Calculate the uncertainty in energy for the particle in the state given as $\Psi(x,0)$. Write an initial state wavefunction $\widetilde{\Psi}(E,0)$ and sketch $\widetilde{\Psi}(E,0)$ versus E.

Follow problem 21 by finding (a) $\langle E \rangle$, (b) $\langle E^2 \rangle$, and (c) ΔE . Remember that

$$\langle \psi | \Omega | \psi \rangle = \langle \Omega \rangle = \sum_{i=1}^{\infty} P(\omega_i) \omega_i$$

is another expression for expectation value. Applying this to E,

$$< E > = \sum_{n=1}^{\infty} P(E_n) E_n = \sum_{n=1}^{\infty} | < E_n | \Psi > |^2 E_n$$

using postulate 4. An intermediate result from problem 8 is

$$\Psi(x) = \sum_{i=1}^{\infty} \psi_n(x) \sum_{i=1}^{\infty} \left(\langle E_n | x \rangle \right) \left(\langle x | \psi \rangle \right) = \sum_{i=1}^{\infty} \psi_n(x) b_n$$
$$\Rightarrow \quad \Psi(x) = \sum_{i=1}^{\infty} \psi_n(x) \langle E_n | \sum_{i=1}^{\infty} \left(\langle x | x \rangle \right) | \psi \rangle = \sum_{i=1}^{\infty} \psi_n(x) \langle E_n | x \rangle$$

$$\Rightarrow \ <\! E\! > = \sum_{n=1}^{\infty} \|b_n\|^2 E_n \,. \quad \text{In problem 8 you calculated} \quad b_n = \frac{8}{n^2 \pi^2} \sqrt{\frac{3}{2}} \,.$$

and the E_n are calculated in problem 1. Again, consider only odd n. Of interest is form 1.3.1.5.11 in Handbook of Mathematical Formulas and Integrals by Jeffrey,

$$\sum_{k=1}^{\infty} \frac{1}{(2k-1)^2} = \frac{\pi^2}{8}$$

For part (b), realize

$$<\Omega>=\sum_{i=1}^{\infty}P(\omega_i)\omega_i \quad \Rightarrow \quad <\Omega^2>=\sum_{i=1}^{\infty}P(\omega_i)\omega_i^2.$$

The expectation value of the square of energy diverges for part (b), *i.e.* $\langle E^2 \rangle \to \infty$, which also fixes the value of the uncertainty at infinity in part (c). The initial state wavefunction $\widetilde{\Psi}(E,0)$ is a two or three line problem if you understand the delta function arguments of part 3 of chapter 1. You should find

$$\widetilde{\Psi}(E,t) = \sum_{n \text{ odd}}^{\infty} 8 \sqrt{\frac{3}{2}} \frac{1}{n^2 \pi^2} \delta(E - E_n).$$

The sketch will be a series of spikes; delta functions "finitized" by the coefficients of each eigenenergy. Try to get the right location of each "spike" and the size relative to the other spikes.

- 30. (a) If the energy of the system is measured at time t, what results can be found
- (b) and with what probabilities will these results be found?
- (c) Sketch the position space wavefunction, $\Psi(x,t)$, and the energy space wavefunction, $\Psi(E,t)$, before and after the energy measurement when you measure E_3 at t = 0.

This problem illustrates the meaning of some of the postulates in the realm of a continuous system. For part (a), the possible results of a measurement of energy are the energy eigenvalues per postulate 3. See problem 1. Examine the equations in the discussion of the last problem if it is not readily apparent how to do part (b). You will find a relationship involving the coefficients b_n that enables a one line solution to part (b). Probabilities are the realm of postulate 4. Immediately before you measure the energy, the wave function is $\Psi(x,0)$. Immediately after you measure the energy, the wavefunction is $\psi_n(x,t)$ per postulate 5. That is what you are asked to sketch in part (c). Remember that neither $\widetilde{\Psi}(E,t)$ nor $\widetilde{\psi}_n(E)$ is continuous.

- 31. (a) Show that the probability of finding a system in its *j*th eigenstate is $P(j) = |c_j|^2$, where c_j is the expansion coefficient of the *j*th eigenstate.
- (b) What are the probabilities of finding the particle given to be in the state $\Psi(x,0)$ in its ground state and in each of its first four excited states?
- (c) What is the probability of finding the particle given to be in the state $\Psi(x, 0)$ in any excited state greater than the fourth excited state?

This problem should reinforce both probability calculations for a continuous system and some common terminology. For any continuous system, the probability of finding the particle in any eigenstate is the magnitude squared of the expansion coefficient of that eigenstate. Symbolically,

$$\Psi(x) = \sum c_n \psi_n(x) \quad \Rightarrow \quad P(n) = |c_n|^2.$$

The c_n 's are known as **probability amplitudes** or simply **amplitudes** because of this fact. You can prove part (a) by picking an arbitrary eigenstate, say n = j, then calculating probability using postulate 4. You must assume that the eigenstates are orthonormal. In fact, an expansion is not useful if the eigenstates are not orthonormal because it is not unique. Orthonormality is essential for a system to have probability amplitudes. The solution to part (a) can be completed in one line. You can attain numerical values for part (b) because you have the expansion coefficients that were denoted b_n in problem 29. Deciphering which coefficients to use requires that you know the ground state is the lowest possible energy state. It will correspond to the lowest possible quantum number, in this case, n = 1. The next lowest energy or next possible quantum number corresponds to the first excited state meaning n = 3 for the given "tent function" system. The second excited state has the n = 5 the third excited state has n = 7, and so on. Add the probabilities you attained for the first five possible states for part (c). The complement is the probability of finding a system in any excited state is usually very small, which your part (c) calculations will illustrate for this system.

- 32. Consider the problem of the infinite square well.
- (a) What operator is Hermitian?
- (b) What are the basis vectors in position space?
- (c) Do the basis vectors constitute a linear vector space?
- (d) Are the basis vectors linearly independent?
- (e) Are the basis vectors orthonormal?

It can appear that the chapter 1 mathematics is a different subject after the position space representation of the Schrodinger equation is introduced. This problem should help you correlate the chapter 1 mathematics with a continuous system. The eigenfunctions of the infinite square well are simply a more sophisticated version of the unit vectors that form a basis for a diagonal matrix. The sines and cosines form a convenient basis for the infinite square well. They are the basis vectors of this infinite dimensional space. This fact is camouflaged because these basis vectors are functions. Nevertheless, the sines and cosines of problem 2 have the same meaning for the infinite square well that unit vectors have for a diagonal operator.

There is a dominant operator that is used in the fourth postulate. It is the answer to part (a). The eigenfunctions of problem 2 holds the answer to parts (b) through (e). Do these functions satisfy the conditions of a linear vector space? Are they linearly independent and orthornormal? The answers, of course, are all affirmative.

33. Given a particle in an infinite square well where the wave function is

 $\Psi \left(x \right) = \begin{cases} x + a & -a < x < a \\ 0 & \text{elsewhere} \end{cases}$

- (a) normalize the wave function,
- (b) expand the wave function in terms of its eigenfunctions,
- (c) calculate the time dependent wave function,
- (d) calculate the probability of finding the particle in the ground state,
- (e) calculate the probability of finding the particle in the third excited state,
- (f) find the expectation value $\langle x \rangle$,
- (g) find the expectation value of $\langle x^2 \rangle$,
- (h) find the uncertainty in position, and
- (i) calculate the minimum uncertainty in momentum.

Though there is more that follows, this problem is essentially the culmination of this chapter. The normalization of part (a) is important because that makes the expansion of part (b) unique. The result of part (b) is the superposition of eigenfunctions implied by the first postulate. The expansion is unique because the eigenfunctions are orthonormal. The part (c) time-dependence of the stationary state wavefunction is not particularly significant because this time dependence does not affect probabilities. The probabilities of finding the particle in any given eigenstate are the conjugate squares of the expansion coefficients following from postulate four. Expectation values can be useful and are a first step to attaining the information contained in the Heisenberg uncertainty relation.

The normalization constant is
$$\frac{1}{2a}\sqrt{\frac{3}{2a}}$$
. The time-dependent wavefunction is

$$\Psi(x,t) = \frac{2}{\pi} \sqrt{\frac{3}{2a}} \left(\sum_{n \text{ odd}}^{\infty} \frac{(-1)^{\frac{n-1}{2}}}{n} \cos\left(\frac{n\pi x}{2a}\right) + \sum_{n \text{ even}}^{\infty} \frac{(-1)^{\frac{n-2}{2}}}{n} \sin\left(\frac{n\pi x}{2a}\right) \right) \exp\left(-i\frac{\pi^2 n^2 \hbar}{8ma^2} t\right) \,,$$

which includes the answers to both parts (b) and (c). Notice that the given wavefunction is neither even nor odd so both the b_n 's and d_n 's must be considered. $P(\text{ground state}) = 6/\pi^2$, and $P(3^{\text{rd}} \text{ excited state}) = 3/8\pi^2$. The minimum uncertainty in momentum is $\hbar\sqrt{5}/a\sqrt{3}$.

34. Write down the wavefunctions for a particle in a two dimensional infinite square well of width 2a on each side, and show that they are dimensionally consistent.

This problem addresses an important point in the variables separable solution to a partial differential equation. The solution in two dimensions is the product of the two one-dimensional solutions, or $\psi(x,y) = f(x)g(y) = \psi_{n_x}(x)\psi_{n_y}(y)$ in this case. Problem 2 provides the solutions in one dimension so form the four possible products and annotate them properly. A wavefunction in position space in two dimensions must have the dimensions of $(1/\sqrt{\text{length}})^2 = 1/\text{length}$.

35. Find the eigenenergies and eigenfunctions of a particle in a retangular two–dimensional infinite square well of length 2a and width 2b.

This is a minor variation on problem 14. The width of the well does not enter the derivation of problem 14 until component energies are added to attain total energies. What changes when there are different widths to consider? If you understand the question posed in this problem, and problems 1, 2, 14, and 34, there is no calculation to do—simply write the answers.

- 36. (a) Find the eigenenergies of a three-dimensional infinite square well of width 2a on each side.
- (b) Find the sets of quantum numbers that yield the lowest ten eigenenergies.
- (c) Identify the eigenenergies from part (b) that demonstrate degeneracy.
- (d) Write expressions for probability and probability density for a three-dimensional infinite square well. What are the units of probability and probability density in this case?

This problem is intended to provide practice in solving a PDE using a variables separable approach. You should find

$$E_{n_x,n_y,n_z} = E_x + E_y + E_z = \frac{\pi^2 \hbar^2}{8ma^2} \left(n_x^2 + n_y^2 + n_z^2 \right) \,.$$

This result can be generalized from problem 14. The intent, however, is to solve an easy PDE using a variables separable method with problem 14 as a guide. The PDE's that we will soon encounter are not nearly so straightforward—those will be more accessible if you practice the variables separable method on this accessible problem. Follow the procedures of problem 15 to attain eigenenergies and address degeneracy.

Degeneracy is the circumstance where different linear combinations of eigenstates have the same energy—the result is that we cannot uniquely identify which combination of eigenstates yield a degenerate energy. Degeneracy cannot occur in a one–dimensional system. It is a requirement in realistic systems to uniquely identify the eigenstates for all energies including degenerate energies. This is done using a **Complete Set of Commuting Observables** (CSCO). We will address how a CSCO is built and used to establish uniqueness. For the moment, realize that a continuous system that can be addressed in a two-dimensional subspace, a two-dimensional system, has two quantum numbers; and a continuous system that can be addressed in a three endimensional system, has three quantum numbers; and a continuous system that can be addressed in a three quantum numbers; and a continuous system that can be addressed in a n-dimensional subspace, an n-dimensional system, has n quantum numbers; and any system higher than one dimensional may be degenerate.