An up scale restaurant with a messenger dressing in concrete hues to match his granite disposition and a mansion that Gatsby couldn't imagine complete with provocative servants. Now a posh men's store with attendants whose names were "Pierre" and "Armin." He found himself looking at a rack of \$2200 suits. When "Armin" asks if he can assist my selection, maybe I'll suggest that my wardrobe requires a replacement rubberized overcoat... Before Armin could intervene, a gentleman wearing a white jacket with a red carnation in the lapel approached. He offered the greeting "How 'bout dem Bums?" to parry the gentleman's fixed attention. The gentleman responded by handing him a ticket to a Mets, Dodgers game and added the even but unexpected comment "Fourier found a need to dress warmly and should have been more cautious of stairs ..."

The Mathematics of Quantum Mechanics, Part 3

In the last two parts, calculations using small dimensional, discrete systems are featured. We will continue to illustrate calculations in small dimensional systems to provide a picture of the mathematical mechanics. These calculations are useful when working in a small dimensional subspace. They are also useful in generalizing to larger dimensional and even infinite dimensional systems. The generalization is essential because infinite dimensional systems model physical realism. Part 3 emphasizes the generalization to infinite dimensions.

Projection operators and the **completeness relation** depend upon an understanding of the **outer product**. You should have the a grasp on the rudiments of the notation quantum mechanics routinely uses to describe infinite dimensional systems in **position space**, **momentum space**, and **energy space**. The **Dirac delta function** and its derivative are used to express the second postulate of quantum mechanics. You need to understand its use within integrals and some of its properties. The **theta function** is the integral of the Dirac delta function. An infinite dimensional vector is equivalent to a continuous function. Calculations concerning infinite dimensional vectors expressed as functions are calculus problems. Any continuous function can be expressed as a **Fourier series**. Fourier series are precursors to **Fourier integrals** and **Fourier transforms** A Fourier transform is used to change the domain or the basis of a continuous function. For instance, a quantum mechanical Fourier transform is used change a state function from the position basis to the momentum basis or vice versa.

1. Given that
$$|v\rangle = \begin{pmatrix} 1\\ 2 \end{pmatrix}$$
 and $\langle w| = (3, 4)$, find $|v\rangle \langle w|$.

The object $|v\rangle < w|$ is an **outer product**. If $|v\rangle = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \end{pmatrix}$ and $< w| = (w_1, w_2, w_3, \cdots),$

then
$$|v\rangle < w| = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \end{pmatrix} (w_1, w_2, w_3, \cdots) = \begin{pmatrix} v_1 w_1 & v_1 w_2 & v_1 w_3 & \cdots \\ v_2 w_1 & v_2 w_2 & v_2 w_3 & \cdots \\ v_3 w_1 & v_3 w_2 & v_3 w_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

is the outer product. The outer product of two vectors is an operator.

$$|v\rangle < w| = \begin{pmatrix} 1\\2 \end{pmatrix} \begin{pmatrix} 3, 4 \end{pmatrix} = \begin{pmatrix} 1 \cdot 3 & 1 \cdot 4\\2 \cdot 3 & 2 \cdot 4 \end{pmatrix} = \begin{pmatrix} 3 & 4\\6 & 8 \end{pmatrix}$$

2. (a) Find the projection operator for the ket $|2\rangle$ in the basis of unit vectors where $|1\rangle$ is the first unit vector.

- (b) Apply this projection operator to an arbitrary ket.
- (c) Apply this projection operator to an arbitrary bra.

The projection operator is defined $\mathcal{P}_i = |i\rangle \langle i|$ for the ket $|i\rangle$, where $|i\rangle$ and $\langle i|$ are corresponding unit vectors. Here, $|2\rangle = \begin{pmatrix} 0\\1\\0\\\vdots \end{pmatrix}$. Use $|v\rangle = \begin{pmatrix} v_1\\v_2\\v_3\\\vdots \end{pmatrix}$ as the arbitrary ket.

(a)
$$|2><2| = \begin{pmatrix} 0\\1\\0\\\vdots \end{pmatrix} (0, 1, 0, \cdots) = \begin{pmatrix} 0 & 0 & 0 & \cdots\\0 & 1 & 0 & \cdots\\0 & 0 & 0 & \cdots\\\vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

(b)
$$|2><2|v> = \begin{pmatrix} 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} 0 \\ v_2 \\ 0 \\ \vdots \end{pmatrix}.$$

(c)
$$\langle v | 2 \rangle \langle 2 | = (v_1, v_2, v_3, \cdots) \begin{pmatrix} 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} = (0, v_2, 0, \cdots).$$

Postscript: The projection operator $|2\rangle \langle 2|$ selects the second component from any ket or bra. It "projects" the second component from the original vector. The result of operation with the projection operator $|2\rangle \langle 2|$ is a vector of the original type with the original second component and all other components zero. Similarly, \mathcal{P}_4 will project the fourth component from any vector, and \mathcal{P}_i will project the *i*th component from any vector.

3. What is the meaning of the consecutive projection operators $\mathcal{P}_i \mathcal{P}_j$?

Assume that the operator $\mathcal{P}_i \mathcal{P}_j$ acts on a ket to the right, for instance, $\mathcal{P}_i \mathcal{P}_j | v > .$ Then \mathcal{P}_j selects the j^{th} component, and all other components are zero. So \mathcal{P}_i operates on a vector with one non-zero component. If the non-zero component is in the i^{th} place in the vector, the operation

with \mathcal{P}_i will return the same ket with one non-zero component. If the non-zero component is in other than the i^{th} place in the vector, the operation with \mathcal{P}_i will return the zero vector. See if you can express these ideas symbolically using Dirac notation and the Kronecker delta.

 $\mathcal{P}_i \mathcal{P}_j = |i > < i |j > < j| = |i > \delta_{ij} < j| = |i > < j | \delta_{ij} = |i > < i| = \mathcal{P}_i.$

Postscript: Notice that $\langle j | \delta_{ij} = \langle i |$. It says that the only condition under which this product is non-zero is when i = j. A state vector that is zero indicates the absence of a system. Quantum mechanics is not interested in the absence of systems so cases that are zero are usually ignored.

You could finish the problem $|i > \delta_{ij} < j| = |j > < j| = \mathcal{P}_j$ if that suits your purpose.

4. Express the completeness relation in three dimensions.

In any given space, there are as many projection operators as the dimension of the space. Add them all to attain an identity operator, that is

$$\sum_{i} \mathcal{P}_{i} = \sum_{i} |i\rangle \langle i| = \mathcal{I}.$$

This is known as the **completeness relation**. It is a **resolution of the identity**, or another way to express an identity operator. It may be the most useful form of the identity for quantum mechanical calculations. This problem should illustrate the concept. Of course, the completeness relation can be expressed in arbitrary or infinite dimensions.

$$\sum_{i=1}^{3} \mathcal{P}_{i} = \sum_{i=1}^{3} |i\rangle \langle i| = \begin{pmatrix} 1\\0\\0 \end{pmatrix} (1, 0, 0) + \begin{pmatrix} 0\\1\\0 \end{pmatrix} (0, 1, 0) + \begin{pmatrix} 0\\0\\1 \end{pmatrix} (0, 0, 1)$$
$$= \begin{pmatrix} 1&0&0\\0&0&0\\0&0&0 \end{pmatrix} + \begin{pmatrix} 0&0&0\\0&1&0\\0&0&0 \end{pmatrix} + \begin{pmatrix} 0&0&0\\0&0&0\\0&0&1 \end{pmatrix} = \begin{pmatrix} 1&0&0\\0&1&0\\0&0&1 \end{pmatrix} = \mathcal{I}.$$

5. Show how the unitary transformation $\mathcal{U}^{\dagger}\mathcal{A}\mathcal{U}$ determines the transformation of vectors.

This problem is intended to amplify the concept of coordinate independence. It should also amplify some of the notation. In particular, one of the characteristics of Dirac notation is that it is independent of basis. Said another way, Dirac notation is coordinate independent.

An inner product is a scalar. An operator acting on a vector, such as $\mathcal{A} | v >$ is a vector, $\mathcal{A} | v > = | v' >$ for instance. Since $\langle w | \mathcal{A} | v > = \langle w | v' \rangle$, it follow that $\langle w | \mathcal{A} | v >$ is a

scalar because $\langle w | v' \rangle$ is a scalar. We will encounter numerous brakets where a bra and a ket sandwich an operator. This type of braket is a scalar, just as an inner product is a scalar.

When conducting a unitary transformation on an operator, any associated bras and kets also require transformation. Insert the identity in the braket $\langle w | \mathcal{A} | v \rangle$ to the immediate left and right of \mathcal{A} , use the fact that the identity can be expressed $\mathcal{UU}^{\dagger} = \mathcal{I}$, and examine pieces.

$$\langle w | \mathcal{A} | v \rangle = \langle w | \mathcal{I} \mathcal{A} \mathcal{I} | v \rangle$$

$$= \langle w | \mathcal{U} \mathcal{U}^{\dagger} \mathcal{A} \mathcal{U} \mathcal{U}^{\dagger} | v \rangle$$

$$= \underbrace{\left(\langle w | \mathcal{U} \right)}_{\text{transform bras}} \underbrace{\left(\mathcal{U}^{\dagger} \mathcal{A} \mathcal{U} \right)}_{\text{transform kets}} \underbrace{\left(\mathcal{U}^{\dagger} | v \rangle \right)}_{\text{transform kets}}.$$

The object in the center set of parenthesis is our unitary transformation. For general $\langle w |$ and $|v \rangle$, the last equation says we must transform a bra as $\langle w | \mathcal{U}$ and a ket as $\mathcal{U}^{\dagger} | v \rangle$ to be consistent with the form of the unitary transformation we have chosen.

Postscript: Notice that if we had chosen \mathcal{UAU}^{\dagger} as our unitary transformation, $\langle w | \mathcal{U}^{\dagger}$ would be the correct method to transform a bra and $\mathcal{U} | v \rangle$ would be the manner to transform a ket.

6. Given that
$$|f\rangle = \begin{pmatrix} 1\\2\\3 \end{pmatrix}$$
 and $|g\rangle = \begin{pmatrix} 4\\5\\6 \end{pmatrix}$, show that $\langle f | g \rangle$ is invariant under a unitary transformation where $\mathcal{U} = \begin{pmatrix} 1/2 & 1/\sqrt{2} & 1/2\\-1/\sqrt{2} & 0 & 1/\sqrt{2}\\1/2 & -1/\sqrt{2} & 1/2 \end{pmatrix}$.

This numerical example is intended to illustrate the procedures and a portion of the meaning of the coordinate independence addressed in the last problem. First find $\langle f | g \rangle$. Then find $\langle f | \mathcal{U} = \langle f' |$ and $\mathcal{U}^{\dagger} | g \rangle = | g' \rangle$. You will find that $\langle f | g \rangle = \langle f' | g' \rangle$. The unitary operator given is from problem 24 in part 2. Of course, the inner product must be the same for any unitary transformation.

$$< f \mid g > = (1, 2, 3) \begin{pmatrix} 4\\5\\6 \end{pmatrix} = 4 + 10 + 18 = 32.$$
$$\mathcal{U} = \begin{pmatrix} 1/2 & 1/\sqrt{2} & 1/2\\-1/\sqrt{2} & 0 & 1/\sqrt{2}\\1/2 & -1/\sqrt{2} & 1/2 \end{pmatrix} \Rightarrow \mathcal{U}^{\dagger} = \begin{pmatrix} 1/2 & -1/\sqrt{2} & 1/2\\1/\sqrt{2} & 0 & -1/\sqrt{2}\\1/2 & 1/\sqrt{2} & 1/2 \end{pmatrix}$$

$$< f \mid \mathcal{U} = (1, 2, 3) \begin{pmatrix} 1/2 & 1/\sqrt{2} & 1/2 \\ -1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 1/2 & -1/\sqrt{2} & 1/2 \end{pmatrix}$$
$$= \left(\frac{1}{2} - \frac{2}{\sqrt{2}} + \frac{3}{2}, \frac{1}{\sqrt{2}} - \frac{3}{\sqrt{2}}, \frac{1}{2} + \frac{2}{\sqrt{2}} + \frac{3}{2}\right) = (2 - \sqrt{2}, -\sqrt{2}, 2 + \sqrt{2}) = < f' \mid$$

$$\begin{aligned} \mathcal{U}^{\dagger} | g \rangle &= \begin{pmatrix} 1/2 & -1/\sqrt{2} & 1/2 \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 1/2 & 1/\sqrt{2} & 1/2 \end{pmatrix} \begin{pmatrix} 4 \\ 5 \\ 6 \end{pmatrix} = \begin{pmatrix} 2-5/\sqrt{2}+3 \\ 4/\sqrt{2}-6/\sqrt{2} \\ 2+5/\sqrt{2}+3 \end{pmatrix} = \begin{pmatrix} 5-5/\sqrt{2} \\ -\sqrt{2} \\ 5+5/\sqrt{2} \end{pmatrix} \\ &\leq f' | g' \rangle = \left(2-\sqrt{2}, \ -\sqrt{2}, \ 2+\sqrt{2}\right) \begin{pmatrix} 5-5/\sqrt{2} \\ -\sqrt{2} \\ 5+5/\sqrt{2} \end{pmatrix} \\ &= 10 - \frac{10}{\sqrt{2}} - 5\sqrt{2} + 5 + 2 + 10 + \frac{10}{\sqrt{2}} + 5\sqrt{2} + 5 = 32 \,. \end{aligned}$$

Postscript: The focal concept is basis independence. A vector expressed in Cartesian coordinates has different components than the same vector expressed in spherical coordinates. Similarly, the vectors $\langle f |$ and $\langle f' |$, and $|g \rangle$ and $|g' \rangle$, are the same vectors represented in different bases. The basis of $\langle f |$ and $|g \rangle$ is Cartesian. The basis for $\langle f' |$ and $|g' \rangle$ is the basis of eigenvectors of the operator \mathcal{B} of problem 24 in part 2.

7. Provide an informal argument that a vector of infinite dimension can contain the same information as a continuous function.

The concept in this problem is essential to understanding the physics that follows. A proof is beyond the scope of this book. We explain the primary difficulty in the postscript. You may never have the formal math background to fully comprehend the proof, but you can and must comprehend the concept.

You should carefully read the following comments now and try to recreate the critical steps after you have absorbed the content.

Consider a curve segment with boundaries 0 and a. A function f(x) could be used to describe this curve segment. If 20 points are thought to adequately describe this curve segment, then

$$f(x) = f(x_1) \begin{pmatrix} 1\\0\\0\\\vdots\\0 \end{pmatrix} + f(x_2) \begin{pmatrix} 0\\1\\0\\\vdots\\0 \end{pmatrix} + f(x_3) \begin{pmatrix} 0\\0\\1\\\vdots\\0 \end{pmatrix} + \dots + f(x_{19}) \begin{pmatrix} 0\\\vdots\\0\\1\\0 \end{pmatrix} + f(x_{20}) \begin{pmatrix} 0\\\vdots\\0\\0\\1 \end{pmatrix}$$

$$= \begin{pmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \\ \vdots \\ f(x_{20}) \end{pmatrix} = \sum_{i=1}^{20} f(x_i) |i\rangle,$$

Figure 1-3-1.

where $|i\rangle$ are unit vectors having 20 components with 1 as the i^{th} component, and the x_i are the positions of the i^{th} unit vectors on the *x*-axis. Though it is likely a better representation than a description using just 5 points or 10 points, 20 points cannot adequately describe a continuous function. If an arbitrarily large number, say n, is thought to adequately describe the given curve segment,

where $|i\rangle$ are unit vectors having *n* components and the 1 is the *i*th component, and the x_i are the positions of the *i*th unit vectors on the *x*-axis. This is an adequate representation of a curve segment for most macroscopic purposes for adequately large *n*. Of course, for mathematical or quantum mechanical purposes, any finite number of $f(x_i)$ cannot describe a continuous function. Given two successive points on the *x*-axis, say x_j and x_k , the point midway between them is excluded so the curve segment cannot be continuous. But in the limit of $n \to \infty$, or equivalently, as the interval between successive points on the *x*-axis $\Delta x \to 0$,

$$f(x) = f(x_1) \begin{pmatrix} 1\\0\\0\\\vdots \end{pmatrix} + f(x_2) \begin{pmatrix} 0\\1\\0\\\vdots \end{pmatrix} + f(x_3) \begin{pmatrix} 0\\0\\1\\\vdots \end{pmatrix} + \dots = \begin{pmatrix} f(x_1)\\f(x_2)\\f(x_3)\\\vdots \end{pmatrix} = \sum_{i=1}^{\infty} f(x_i) |i>, \quad (1)$$

where $|i\rangle$ are unit vectors having infinite components where the 1 is the i^{th} component, and the x_i are the positions of the i^{th} unit vectors on the x-axis.

Postscript: This procedure is related to numerous applications. A beginning student of algebra will choose a finite number of points to manually graph a function. Make Δx adequately small and the eye cannot distinguish the space between the points on a curve segment. This fact is used by computer monitors, printers, digital cameras, and scanners to name just a few applications. The difference is that neither a student doing paper and pencil graphing nor a computer graphing

application place the functional values in a column vector. An infinity of functional values <u>can</u> be placed into a column vector and that is the key point in the argument that a continuous function and a vector of infinite dimension are equivalent.

The difficult question is when do the function and the vector of infinite dimension converge? This question is addressed by the field of functional analysis. We do not address the question of convergence. However, the concept of the equivalence of continuous functions and vectors of infinite dimension introduced here informally is essential to many of the developments that are encountered in the study of quantum mechanics.

The unit vectors in this problem correspond to infinitesimally small increments in position. We are, therefore, using the **position basis** in **position space**. If the unit vectors represent infinitesimally small increments in momentum, *i.e.*, if the independent variable is momentum, the same paradigm applies except that it is using the **momentum basis** in **momentum space**. If this paradigm is used when energy is the independent variable, the unit vectors represent infinitesimally small increments in energy and the description is using the **energy basis** in **energy space**.

8. Write an infinite dimensional vector that is equivalent to a continuous function f(p) in momentum space.

This is the same as the last problem with the exception that momentum is the independent variable. Parallel equation (1) from problem 7 using the momentum basis.

$$f(p) = f(p_1) \begin{pmatrix} 1\\0\\0\\\vdots \end{pmatrix} + f(p_2) \begin{pmatrix} 0\\1\\0\\\vdots \end{pmatrix} + f(p_3) \begin{pmatrix} 0\\0\\1\\\vdots \end{pmatrix} + \dots = \begin{pmatrix} f(p_1)\\f(p_2)\\f(p_3)\\\vdots \end{pmatrix} = \sum_{i=1}^{\infty} f(p_i) |i > 1$$

9. Provide an informal explanation of the relations

$$<\mathbf{x} \mid g> = g(x), \quad <\mathbf{p} \mid g> = g(p), \text{ and } <\mathbf{E} \mid g> = g(E).$$

The relations introduced in this problem are fundamental. Your ability to use these relations will likely be significantly enhanced if they have meaning beyond rote memorization.

Like problem 7, study the following comments and then try to recreate the critical steps. You will encounter two new objects. Also, realize that the following argument depends directly on the fact that an infinite dimensional vector can contain the same information as a continuous function.

To this point, components of bras and kets have been scalars. Consider $\langle \mathbf{x} |$ which is not a typical bra, but a bra of unit ket vectors in position space, *i.e.*,

$$\langle \mathbf{x} | = \left(\begin{pmatrix} 1\\0\\0\\\vdots \end{pmatrix}, \begin{pmatrix} 0\\1\\0\\\vdots \end{pmatrix}, \begin{pmatrix} 0\\0\\1\\\vdots \end{pmatrix}, \cdots \right).$$

In words, $\langle \mathbf{x} |$ is a bra that represents the position basis. Also consider $|g\rangle$, an arbitrary vector,

$$|g\rangle = \begin{pmatrix} g_1 \\ g_2 \\ g_3 \\ \vdots \end{pmatrix}.$$

Notice that no independent variable is specified for the ket $|g\rangle$ or the components of $|g\rangle$. This is because $|g\rangle$ is completely abstract. This is another new object. It is an abstract vector with abstract components, and we know that the components exist, but we do not know what they are. We know only that the vector exists and it has a first component, a second component, and so on, ad infinitum. The abstract vector $|g\rangle$ is independent of basis. Independence from basis is one of the primary features of Dirac notation. Were we to form an inner product with $|g\rangle$, we attain

$$\langle \mathbf{x} | g \rangle = g_1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} + g_2 \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} + g_3 \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix} + \cdots$$

where we have fixed the location of the first component of $|g\rangle$ as that associated with $\begin{pmatrix} 1\\0\\0\\\vdots \end{pmatrix}$, so

this is the first x coordinate for $|g\rangle$, or equivalently, the first coordinate for $|g\rangle$ is at x_1 . The

location of the second component of $|g\rangle$ is that associated with $\begin{pmatrix} 0\\1\\0\\\vdots \end{pmatrix}$, so this is the second

x coordinate for $|g\rangle$, or the second coordinate for $|g\rangle$ is at x_2 , and so on, ad infinitum. We have fixed each component of $|g\rangle$ at a specific location in the position basis. In other words, it is the same as

$$<\mathbf{x} | g> = g(x_1) \begin{pmatrix} 1\\0\\0\\\vdots \end{pmatrix} + g(x_2) \begin{pmatrix} 0\\1\\0\\\vdots \end{pmatrix} + g(x_3) \begin{pmatrix} 0\\0\\1\\\vdots \end{pmatrix} + \dots = \begin{pmatrix} g(x_1)\\g(x_2)\\g(x_3)\\\vdots \end{pmatrix} = g(x).$$

In short $\langle \mathbf{x} | g \rangle = g(x)$, the inner product of an abstract ket with the bra that describes the position basis is equivalent to a function of position.

There exists a bra of unit ket vectors that describes the momentum basis, and another bra of unit kets that describes the energy basis. The arguments in momentum space and energy space are only cosmetically different than that for position space. The inner product of an abstract ket with the bra of unit ket vectors that describes the momentum basis is equivalent to a function of momentum, and the inner product of an abstract ket with the bra of unit ket vectors that describes the energy basis is equivalent to a function of energy. This means that $\langle \mathbf{p} | g \rangle = g(p)$ and $\langle \mathbf{E} | g \rangle = g(E)$.

Postscript: These three relations are known as **representations** of the abstract vector $|g\rangle$. The last two relations are refined $\langle \mathbf{p} | g \rangle = \hat{g}(p)$ and $\langle \mathbf{E} | g \rangle = \tilde{g}(E)$, using a hat for a quantity in momentum space and a tilde for a quantity in energy space to clearly denote the momentum or energy basis.

The first postulate of quantum mechanics indicates that a state vector $|\psi\rangle$ describes a system that we know to exist. Like $|g\rangle$ in this problem, the abstract ket $|\psi\rangle$ is a function without an argument. The functional argument is present in the basis chosen. The concept is that $|\psi\rangle$ exists and is expressible in <u>any</u> appropriate basis. A bra of unit kets is used to attain a functional form $\psi(x)$, or $\hat{\psi}(p)$, or $\tilde{\psi}(E)$, like $\langle \mathbf{x} | \psi \rangle = \psi(x)$ for instance. You cannot calculate abstract components of g_i or ψ_i without reference to a basis just the same as you cannot express the components of a two-dimensional vector without reference to Cartesian or polar or another coordinate system. You may want to calculate $g(x_i)$ or $\hat{\psi}(p_i)$ after the ket is represented. Representations are often used to transition from Dirac notation and the language of linear algebra to the language of calculus.

The symbol between the slashes and the angles for the bras are boldfaced in this problem to distinguish the new object. Most authors require the reader make the distinction between the bra of unit kets and a bra whose components are scalars. We will use the conventional notation $\langle x | g \rangle = g(x), \quad \langle p | g \rangle = g(p), \text{ and } \langle E | g \rangle = g(E), \text{ following the introduction presented}$ in this and the next problems.

10. Provide an informal explanation of the representation relations in the dual spaces, *i.e.*,

$$|\mathbf{x}| < g | \mathbf{x} > = g^*(x), \quad \langle g | \mathbf{p} \rangle = \widehat{g}^*(p), \text{ and } \langle g | \mathbf{E} \rangle = \widetilde{g}^*(E).$$

This problem extends the concept provided in problem 9 to the dual space. It also exposes pertinent notation and its meaning. Again, you are likely to have more utility with these relations if you have an idea of their meaning.

This problem parallels problem 9. The ket $|\mathbf{x}\rangle$ represents the entire basis in the dual space. It is a ket of unit bras. You need only to develop the argument in position space and state that the development of the momentum space and energy space cases are identical except that the different bases result in different functional arguments. Remember that the components of a ket that is the dual to a given bra has components that are conjugates of the given bra.

$$\begin{aligned} |\mathbf{x}\rangle &= \begin{pmatrix} (1, 0, 0, \cdots) \\ (0, 1, 0, \cdots) \\ (0, 0, 1, \cdots) \\ \vdots \end{pmatrix} \Rightarrow \langle g | \mathbf{x} \rangle = \begin{pmatrix} g_1, g_2, g_3, \cdots \end{pmatrix} \begin{pmatrix} (1, 0, 0, \cdots) \\ (0, 1, 0, \cdots) \\ (0, 0, 1, \cdots) \\ \vdots \end{pmatrix} \\ &= g_1 (1, 0, 0, \cdots) + g_2 (0, 1, 0, \cdots) + g_3 (0, 0, 1, \cdots) + \cdots \\ &= \begin{pmatrix} g (x_1), 0, 0, \cdots \end{pmatrix} + \begin{pmatrix} 0, g (x_2), 0, \cdots \end{pmatrix} + \begin{pmatrix} 0, 0, g (x_3), \cdots \end{pmatrix} + \cdots \\ &= \begin{pmatrix} g (x_1), g (x_2), g (x_3), \cdots \end{pmatrix} = \begin{pmatrix} g^* (x_1) \\ g^* (x_2) \\ g^* (x_3) \\ \vdots \end{pmatrix} = g^* (x) . \end{aligned}$$

The inner product of $\langle g |$ with the ket of unit bras that represents the momentum basis fixes the components of $\langle g |$ in momentum space so $\langle g | \mathbf{p} \rangle = \hat{g}^*(p)$. The inner product of $\langle g |$ with the ket of unit bras that represents the energy basis fixes the components of $\langle g |$ in energy space so $\langle g | \mathbf{E} \rangle = \tilde{g}^*(E)$.

11. Evaluate

(a)
$$2\int_{-\pi}^{\pi} \cos(2\theta) \,\delta(\theta) \,d\theta,$$

(b)
$$\int_{0}^{\infty} A \,\cos(x) \,e^{x^{2}} \,\delta(x+1) \,dx,$$

(c)
$$\int \cos\left(\frac{n\pi x}{l}\right) \,\sin\left(\frac{n\pi x}{l}\right) \,\delta(x-l) \,dx, \quad n = 1, 2, 3, \dots$$

(d)
$$\int_{0}^{1} dr \int_{-\infty}^{\infty} d\theta \,\frac{1}{r^{2}} \,\sin(\theta) \,\delta(r-a) \,\delta\left(\theta - \frac{\pi}{4}\right), \quad 0 < a < 1$$

This problem introduces the procedures to evaluate integrals that contain **Dirac delta functions**, often called just delta functions or δ functions. The Dirac delta function is defined

$$\int_{-\infty}^{\infty} \delta(x) \, dx = \begin{cases} 1 & \text{if } x = 0, \\ 0 & \text{if } x \neq 0 \end{cases}$$

To get a picture for a delta function, consider a normalized function of the real variable x that vanishes everywhere except inside a domain of length ϵ . The integral over this domain is unity because it is given to be normalized. If we diminish the domain, the function must become "taller" to remain normalized. In the limit of $\epsilon \to 0$, the functional value goes to ∞ . The delta function is an idealization of an infinitely high, infinitely thin spike that is normalized. We refer you to Boas¹, Arfken², or your favorite text on mathematical physics for greater depth.

Following Dirac, the most important property of $\delta(x)$ is

$$\int_{-\infty}^{\infty} f(x) \,\delta(x) \,dx = f(0) \,.$$

Informally, you can picture the value of $\delta(x)$ being zero everywhere except at the origin, so zero is the only location at which the product of the function f(x) and the delta function is non-zero. The value of the function at the origin is $f(x)|_{x=0} = f(0)$, which is a constant, so can be moved outside of the integral. The result is the constant f(0) times the defining integral which has a value of 1, or $f(0) \cdot 1 = f(0)$. The Dirac delta function in an integrand "picks out" the value of the function evaluated at the origin. If we "shift" the origin to x = a, the last equation becomes

$$\int_{-\infty}^{\infty} f(x) \,\delta(x-a) \, dx = f(a) \,.$$

¹Boas, Mathematical Methods in the Physical Sciences (John Wiley & Sons, New York, 1983), 2nd ed., pp. 665-670.

²Arfken, Mathematical Methods for Physicists (Academic Press, New York, 1970), 2nd ed., pp. 413-415.

If the value that makes the argument of a delta function zero is not between the limits of integration, the integral of that delta function is zero on that interval, thus the product is zero everywhere, and therefore the original integral is zero. For example, if $f(x) = A e^{x^2}$, then

$$\int_{-\infty}^{\infty} A e^{x^2} \,\delta\left(x\right) dx = \left(A e^{x^2}\Big|_{x=0}\right) \int_{-\infty}^{\infty} \delta\left(x\right) dx = A e^0\left(1\right) = A.$$
$$\int_{-\infty}^{\infty} A e^{x^2} \,\delta\left(x-a\right) dx = \left(A e^{x^2}\Big|_{x=a}\right) \int_{-\infty}^{\infty} \delta\left(x-a\right) dx = A e^{a^2}\left(1\right) = A e^{a^2}.$$
$$\int_{-\infty}^{0} A e^{x^2} \,\delta\left(x-1\right) dx = 0 \quad \text{because 1 is not between the limits of integration}$$

One of the four integrals is zero because the value that makes the argument of the delta function zero is not between the limits of integration. The integral for part (c) has no limits. It is common to suppress the limits $-\infty$ and ∞ , particularly when these limits are encountered repetitively. Part (d) has two variables so you must address each coordinate independently.

(a) The argument of the delta function is zero at $\theta = 0$, so

$$2\int_{-\pi}^{\pi}\cos\left(2\theta\right)\delta\left(\theta\right)d\theta = 2\,\cos\left(2\theta\right)\bigg|_{\theta=0} = 2\,\cos\left(0\right) = 2\cdot 1 = 2$$

(b) The argument of the delta function is zero at $x + 1 = 0 \implies x = -1$, which is not within the limits of integration, therefore

$$\int_0^\infty A\,\cos\left(x\right)e^{x^2}\,\delta\left(x+1\right)dx=0\,.$$

(c) The argument of the delta function is zero at $x - l = 0 \Rightarrow x = l$, so

$$\int_{-\infty}^{\infty} \cos\left(\frac{n\pi x}{l}\right) \sin\left(\frac{n\pi x}{l}\right) \delta\left(x-l\right) dx = \cos\left(\frac{n\pi x}{l}\right) \sin\left(\frac{n\pi x}{l}\right) \bigg|_{x=l}$$
$$= \cos\left(n\pi\right) \sin\left(n\pi\right) = \cos\left(n\pi\right) (0) = 0 \quad \text{for all} \quad n.$$

(d) The argument of the angular delta function is zero at $x = \pi/4$ and the argument of the radial delta function is zero at r = a, so addressed in the order of integration,

$$\int_{0}^{1} dr \int_{-\infty}^{\infty} d\theta \, \frac{1}{r^{2}} \sin\left(\theta\right) \delta\left(r-a\right) \delta\left(\theta-\frac{\pi}{4}\right) = \int_{0}^{1} dr \, \frac{1}{r^{2}} \left(\left[\sin\left(\theta\right)\right]_{\theta=\pi/4}\right) \delta\left(r-a\right)$$
$$= \int_{0}^{1} dr \, \frac{1}{r^{2}} \frac{\sqrt{2}}{2} \, \delta\left(r-a\right) = \frac{\sqrt{2}}{2} \int_{0}^{1} dr \, \frac{1}{r^{2}} \, \delta\left(r-a\right) = \frac{\sqrt{2}}{2} \left.\frac{1}{r^{2}}\right|_{r=a} = \frac{\sqrt{2}}{2a^{2}} \text{ assuming } 0 < a < 1.$$

Postscript: The Dirac delta function is a generalization of the Kronecker delta. It is usually considered a generalized function³ or distribution, though Dirac, the originator, considered it an

³ Lighthill, An Introduction to Fourier Analysis and Generalised Functions (Cambridge University Press, Cambridge, England, 1958).

improper function. Some authors will use it only as a factor in an integrand. Even Dirac says "...it will be something which is to be used ultimately in an integrand." Nevertheless, delta functions commonly appear outside an integral in modern literature. The Dirac delta function is an idealization, much the same way as a mathematical point will model the location of a classical particle. Dirac indicates it is "...merely a convenient notation, enabling us to express in a concise form certain relations which we could, if necessary, rewrite in a form not involving improper functions, but only in a cumbersome way which would tend to obscure the argument."⁴ If the system is discrete, use of the Kronecker delta is appropriate to model an "all or none" quantity. If the system is continuous, use of the Dirac delta function is appropriate to model an "all or none" situation.

The Dirac delta function is an even function. A function is even if f(-x) = f(x), like a cosine, and a function is odd if f(-x) = -f(x), like a sine. The graph of an even function is symmetric about the vertical axis. If the graph of an even function is folded on the vertical axis, the two half curves overlap. Notice that figure 1–3–2 is symmetric about the vertical axis. The graph of an odd function is symmetric about the origin. If the graph of an odd function is rotated 180 degrees around the origin, the two half curves overlap. Most functions do not have any central symmetry so are neither even nor odd. For instance, f(x) = x + 1 is neither even nor odd. The fact that the Dirac delta function is even is often expressed

$$\delta(-x) = \delta(x)$$
 and $\delta(x - x') = \delta(x' - x)$.

This notation requires explanation because a delta function is "something which is to used ultimately in an integrand." A function and integral with the limits $-\infty$ and ∞ are implicit, *i.e.*,

$$\delta(x-x') = \delta(x'-x) \quad \Rightarrow \quad \int_{-\infty}^{\infty} f(x)\,\delta(x-x')\,dx = \int_{-\infty}^{\infty} f(x)\,\delta(x'-x)\,dx.$$

The function, integral, and limits often provide only clutter. These can be attached to complete the meaning of relationships involving "naked" delta functions, as seen in the next problem.

12. Show that $\delta(ax) = \frac{\delta(x)}{|a|}, a \neq 0.$

The second postulate of quantum mechanics is often stated using a delta function and its derivative. Some ability to use delta functions is necessary. Problems 12 to 17 are oriented toward building dexterity and exposing some of properties of the delta function, its integral, and its derivative.

Approach this problem by changing variables. Let

$$y = ax \Rightarrow x = \frac{y}{a} \Rightarrow dx = \frac{dy}{a}$$
. Change the variables in $\int_{-\infty}^{\infty} f(x) \,\delta(ax) \, dx$

for an arbitrary f(x). There are two cases, a > 0 and a < 0. Pay attention to the limits of integration to get the absolute value of a to emerge. You want to show that

$$\int_{-\infty}^{\infty} f(x) \,\delta(ax) \, dx = \int_{-\infty}^{\infty} f(x) \,\frac{\delta(x)}{|a|} \, dx$$

⁴ Dirac, *The Principles of Quantum Mechanics* (Clarendon Press, Oxford, England, 1958), 4th ed., pp. 58-59.

and that is the explicit meaning of the statement $\delta(ax) = \frac{\delta(x)}{|a|}$.

$$y = ax \Rightarrow x = \frac{y}{a} \Rightarrow dx = \frac{dy}{a}$$
. Consider $\int_{-\infty}^{\infty} f(x) \,\delta(ax) \, dx$

for an arbitrary f(x). There are two cases. Case I. $a > 0 \Rightarrow \infty \to \infty$ and $-\infty \to -\infty$, so

$$\int_{-\infty}^{\infty} f(x)\,\delta(ax)\,dx = \int_{-\infty}^{\infty} f\left(\frac{y}{a}\right)\,\delta(y)\,\frac{dy}{a} = \frac{1}{a}\int_{-\infty}^{\infty} f\left(\frac{y}{a}\right)\,\delta(y)\,dy = \frac{f(0)}{a} = \frac{f(0)}{|a|}$$

since a = |a|. Case II. $a < 0 \Rightarrow \infty \to -\infty$ and $-\infty \to \infty$, so

$$\int_{-\infty}^{\infty} f(x)\,\delta(ax)\,dx = \int_{\infty}^{-\infty} f\left(\frac{y}{a}\right)\,\delta(y)\,\frac{dy}{a} = -\frac{1}{a}\int_{-\infty}^{\infty} f\left(\frac{y}{a}\right)\,\delta(y)\,dy = -\frac{f(0)}{a} = \frac{f(0)}{|a|}$$

since a < 0. Combining cases I and II for a general constant a,

$$\int_{-\infty}^{\infty} f(x)\,\delta\left(ax\right)dx = \frac{f\left(0\right)}{\left|a\right|} = \int_{-\infty}^{\infty} f\left(x\right)\frac{\delta\left(x\right)}{\left|a\right|}dx\,, \quad \text{therefore,} \quad \delta\left(ax\right) = \frac{\delta\left(x\right)}{\left|a\right|}. \quad \text{Q.E.D.}$$

Postscript: The motivation to change variables is to attain a delta function with a single variable in the argument, like $\delta(x)$ or $\delta(r)$. The meaning as part of an integrand is then clear.

13. Show that $\delta(f(x)) = \sum_{i}^{n} \frac{\delta(x_{i} - x)}{|f'(x_{i})|}$ where the x_{i} are the zeros of f(x).

The integral $\int \delta(f(x)) g(x) dx$ will have a non-zero value where the argument of the delta function is zero, *i.e.*, where f(x) = 0. To find the zeros, expand f(x) in a Taylor series. Near each zero,

$$f(x) \simeq (x - x_i) f'(x_i), \quad \text{where} \quad f(x_i) = 0$$

and quadratic and higher order terms are negligible, so only terms with first derivatives remain. Substitute each $(x - x_i) f'(x_i)$, into the argument of the delta function. You then have a series of integrals containing delta functions. Each delta function has an argument that is a product of a difference and a first derivative evaluated at a point. The first derivative evaluated at a point is a scalar so you can use the result of problem 12. You need to use the fact that the delta function is even to attain the order of the argument that is specified in the problem. Express the result as a summation. The meaning of the premise is

$$\int_{-\infty}^{\infty} \delta\left(f(x)\right) g(x) \, dx = \int_{-\infty}^{\infty} \sum_{i}^{n} \frac{\delta\left(x_{i}-x\right)}{\left|f'(x_{i})\right|} g(x) \, dx.$$

Consider f(x) which is a continuous, analytic function on the interval $-\infty < x < \infty$. Then f(x) may be expanded in a Taylor series

$$f(x) = f(x_i) + (x - x_i) f'(x_i) + \frac{(x - x_i)^2}{2!} f''(x_i) + \frac{(x - x_i)^3}{3!} f'''(x_i) + \cdots$$

Each x_i is a zero of $f(x) \Rightarrow f(x) \simeq (x - x_i) f'(x_i)$ at points near x_i , where $f(x_i) = 0$, and quadratic and higher order terms are negligible near zeros. Under these conditions the integral is

$$\int_{-\infty}^{\infty} \delta\left(f(x)\right) g(x) \, dx \simeq \int_{-\infty}^{\infty} \delta\left((x-x_1) \, f'(x_1)\right) g(x) \, dx \\ + \int_{-\infty}^{\infty} \delta\left((x-x_2) \, f'(x_2)\right) g(x) \, dx + \int_{-\infty}^{\infty} \delta\left((x-x_3) \, f'(x_3)\right) g(x) \, dx + \cdots \\ = \int_{-\infty}^{\infty} \frac{\delta\left(x-x_1\right)}{|f'(x_1)|} g(x) \, dx + \int_{-\infty}^{\infty} \frac{\delta\left(x-x_2\right)}{|f'(x_2)|} g(x) \, dx + \int_{-\infty}^{\infty} \frac{\delta\left(x-x_3\right)}{|f'(x_3)|} g(x) \, dx + \cdots$$

using the result of the problem 12. Expressing the series in terms of a summation and using the fact that the Dirac delta function is even,

$$\int_{-\infty}^{\infty} \delta\left(f\left(x\right)\right) g\left(x\right) dx = \sum_{i}^{n} \int_{-\infty}^{\infty} \frac{\delta\left(x-x_{i}\right)}{\left|f'\left(x_{i}\right)\right|} g\left(x\right) dx = \sum_{i}^{n} \int_{-\infty}^{\infty} \frac{\delta\left(x_{i}-x\right)}{\left|f'\left(x_{i}\right)\right|} g\left(x\right) dx.$$

The last expression is the same as the integral of the sum, essentially reversing the direction of $\int (h(x) + j(x)) dx = \int h(x) dx + \int j(x) dx$, so can be written

$$\int_{-\infty}^{\infty} \delta\left(f\left(x\right)\right) g\left(x\right) dx = \int_{-\infty}^{\infty} \sum_{i} \frac{\delta\left(x_{i} - x\right)}{\left|f'\left(x_{i}\right)\right|} g\left(x\right) dx, \quad \Rightarrow \quad \delta\left(f\left(x\right)\right) = \sum_{i} \frac{\delta\left(x_{i} - x\right)}{\left|f'\left(x_{i}\right)\right|}. \quad \text{Q.E.D}$$

14. Show that
$$\int \delta(x) dx = \Theta(x)$$
.

This problem introduces the **theta function**. The delta function is the derivative of the theta function, as this problem demonstrates in integral form. The theta function is useful in establishing some of the properties of the delta function and in problems involving discontinuities.

The theta function, also known as the step function or the Heaviside step function, is defined

$$\Theta(x) = \begin{cases} 1, & \text{if } x > 0, \\ 0, & \text{if } x < 0. \end{cases}$$

If we "shift" the origin to x = x',

$$\Theta(x - x') = \begin{cases} 1, & \text{if } x > x', \\ 0, & \text{if } x < x'. \end{cases}$$

The last equation is illustrated in the figure. Notice that it is not defined at x = 0, and it is not continuous at x = 0. Like the delta function, the theta function is another "improper" or "pathological" function. It does not possess the properties of continuity and differentiability at the location where the argument is equal to zero.

As usual, assume the limits of integration are $-\infty$ and ∞ when a proper integral is anticipated and limits are not stated. Limits are the key to the meaning of the premise. Break the integral into two integrals at an arbitrarily small $\epsilon < 0$. This means the limits on the first integral are $-\infty$ to $-\epsilon$ and the limits on the second integral are $-\epsilon$ to ∞ . Examine the behavior of both integrals in the limit $\epsilon \to 0$.

$$\int_{-\infty}^{\infty} \delta(x) \, dx = \int_{-\infty}^{-\epsilon} \delta(x) \, dx + \int_{-\epsilon}^{\infty} \delta(x) \, dx,$$

where ϵ is an arbitrarily small number. There are two cases, either x > 0 or x < 0. If x > 0,

$$\int_{-\infty}^{-\epsilon} \delta(x) \, dx + \int_{-\epsilon}^{\infty} \delta(x) \, dx = 0 + 1 = 1 \,,$$

where the first integral is zero because values of x > 0 are not within the limits of the integral, and the second integral is 1 per the definition of the Dirac delta function. If x < 0, then

$$\int_{-\infty}^{-\epsilon} \delta(x) \, dx + \int_{-\epsilon}^{\infty} \delta(x) \, dx = 0 + 0 = 0 \,,$$

where the first integral is zero because the argument of the delta function cannot assume the value of x = 0 within limits that are both less than zero. The second integral is zero because the values x < 0 are not within the limits of the integral. If the circumstance $-\epsilon < x < 0$ were to occur, the second integral would be 1, but picking another ϵ such that $x < -\epsilon$ restores the situation in which both integrals vanish. Therefore, in the limit that $\epsilon \to 0$,

$$\int \delta(x) \, dx = \begin{cases} 1, & \text{if } x > 0, \\ 0, & \text{if } x < 0. \end{cases} = \Theta(x) \, .$$

Postscript: The differential form of this relationship is $\frac{d\Theta(x)}{dx} = \delta(x)$. The integral form is often more useful for calculation because of sensitivity to limits.

properties of delta parts, I know of no book that actually has an problem 17 may be unique in modern literature. By the way, since I confirm this procedure through any of the research that I have done, I hope that both

15. Use integration by parts to show that
$$\int_{a}^{c} f(x) \delta(x-b) dx = f(b), \quad a < b < c$$

As Dirac indicates, the fact that $\int f(x) \,\delta(x) \, dx = f(0)$, is a property. Establishing properties and understanding the methods by which they are established is more useful than rote memorization. Many of the properties of delta functions are established using integration by parts. For a definite integral, integration by parts means

$$\int_a^c u \, dv = uv \Big|_a^c - \int_a^c v \, du \, .$$

You need the result of the last problem to apply this formula. You also need to use the technique of breaking the resulting $\int_{a}^{c} v \, du$ into two integrals as demonstrated in the last problem. Use ϵ slightly less than b. You need the definition of the theta function to evaluate every term following the integration by parts. Finally, taking the limit $\epsilon \to 0$ establishes the premise.

Given
$$\int_{a}^{c} f(x) \,\delta(x-b) \,dx, \quad \text{and using} \quad \begin{array}{l} u &=& f(x) \Rightarrow du = f'(x) \,dx \\ dv &=& \delta(x-b) \,dx \Rightarrow v = \Theta(x-b) \end{array}$$
$$\Rightarrow \quad \int_{a}^{c} f(x) \,\delta(x-b) \,dx = f(x) \,\Theta(x-b) \left|_{a}^{c} - \int_{a}^{c} \Theta(x-b) \,f'(x) \,dx \right.$$
$$= f(c) \,\Theta(c-b) - f(a) \,\Theta(a-b) - \int_{a}^{b-\epsilon} \Theta(x-b) \,f'(x) \,dx - \int_{b-\epsilon}^{c} \Theta(x-b) \,f'(x) \,dx \quad (1)$$

where ϵ is arbitrarily close to zero. The condition a < b < c determines the first two Θ functions in equation (1) as $\Theta(c-b) = 1$, since c > b and $\Theta(a-b) = 0$ since a < b. Further,

$$\int_{a}^{b-\epsilon} \Theta(x-b) f'(x) dx = 0$$

since $\Theta(x-b) = 0$ because x < b for all possible values of x within the range of integration. Similarly,

$$\int_{b-\epsilon}^{c} \Theta(x-b) f'(x) dx = \int_{b-\epsilon}^{c} f'(x) dx$$

since $\Theta(x-b) = 1$ for all possible values of x within that range of integration because x > b. Using all these in equation (1),

$$\int_{a}^{c} f(x) \delta(x-b) dx = f(c) \cdot 1 - f(a) \cdot 0 - 0 - \int_{b-\epsilon}^{c} f'(x) dx$$
$$= f(c) - f(x) \Big|_{b-\epsilon}^{c}$$
$$= f(c) - f(c) + f(b-\epsilon) = f(b-\epsilon).$$

In the limit of $\epsilon \to 0$, $f(b-\epsilon) \to f(b)$, and the integral is

$$\int_{a}^{c} f(x) \,\delta\left(x-b\right) dx = f\left(b\right).$$

Postscript: The argument for infinite limits is the same except $a = -\infty$ and $c = \infty$.

16. Evaluate (a) $\int V_0 \left(\frac{a}{x} - \frac{x}{a}\right)^2 \delta'(x-a) dx$, and (b) $\int V_0 \left(\frac{a}{x} - \frac{x}{a}\right)^2 \delta'(x-b) dx$.

This problem introduces derivatives of delta functions. Like delta functions, derivatives of delta functions are always intended to be used as a portion of an integrand though they will frequently appear without an integral or companion function for reasons of notational economy. The derivative of the Dirac delta function is the negative of the derivative of the companion function evaluated at the point that makes the argument of δ' zero. Symbolically,

$$\int \delta' (x-a) f(x) dx = -f'(a).$$

For $f(x) = x^2$, f'(x) = 2x, so $\int \delta'(x-a) x^2 dx = -2a$, for instance. A second example is $f(x) = A e^{-x^2} \Rightarrow f'(x) = A e^{-x^2} (-2x) = -2A x e^{x^2}$, so $\int \delta'(x-b) A e^{x^2} dx = 2A b e^{b^2}$. We could attach the limits understood to be $-\infty$ and ∞ but they add only clutter here so have been suppressed. The potential given in this problem is realistic and is sometimes used to model an asymmetric potential well in radial coordinates (*i.e.*, $x \to r$ and r > 0).

(a) The derivative of the function is

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

$$\Rightarrow \int V_{0} \left(\frac{a}{x} - \frac{x}{a} \right)^{2} \delta' \left(x - a \right) dx = - \left[-2 V_{0} \left(\frac{a}{x} - \frac{x}{a} \right) \left(\frac{a}{x^{2}} + \frac{1}{a} \right) \right]_{x=a}$$

$$= 2 V_{0} \left(\frac{a}{a} - \frac{a}{a} \right) \left(\frac{a}{a^{2}} + \frac{1}{a} \right) = 2 V_{0} \left(0 \right) \left(\frac{2}{a} \right) = 0.$$

(b) Having calculated the derivative for part (a),

$$\int V_0 \left(\frac{a}{x} - \frac{x}{a}\right)^2 \delta'(x-b) \, dx = -\left[-2 \, V_0 \left(\frac{a}{x} - \frac{x}{a}\right) \left(\frac{a}{x^2} + \frac{1}{a}\right)\right]_{x=b}$$
$$= 2 \, V_0 \left(\frac{a}{b} - \frac{b}{a}\right) \left(\frac{a}{b^2} + \frac{1}{a}\right) = 2 \, V_0 \left(\frac{a^2}{b^3} + \frac{1}{b} - \frac{1}{b} - \frac{b}{a^2}\right)$$
$$= 2 \, V_0 \left(\frac{a^2}{b^3} - \frac{b}{a^2}\right).$$

17. Show that
$$\int \delta'(x-a) f(x) dx = -f'(a)$$
 using integration by parts.

This problem is meant to further develop your appreciation of the Dirac delta function and its derivative. It also further illustrates the process of integration by parts that is consistently referenced but rarely demonstrated in discussions of the Dirac delta function.

Consider $\int_{a}^{c} \delta'(x-b) f(x) dx$ for a < b < c. Integration by parts is reviewed in problem 15. You are left with two terms that have delta functions that are not part of an integrand following the integration by parts. Both terms vanish because the arguments of the delta functions cannot be zero. The rest is straightforward.

Given
$$\int_{a}^{c} f(x) \,\delta'(x-b) \,dx, \quad \text{let} \quad \begin{array}{l} u &=& f(x) \Rightarrow du = f'(x) \,dx \\ dv &=& \delta'(x-b) \,dx \Rightarrow v = \delta(x-b) \end{array}$$
$$\Rightarrow \quad \int_{a}^{c} \delta'(x-b) \,f(x) \,dx = f(x) \,\delta(x-b) \left|_{a}^{c} - \int_{a}^{c} \delta(x-b) \,f'(x) \,dx. \right|^{c}$$

The term $f(x) \delta(x-b) \Big|_{a}^{c} = f(c) \delta(c-b) - f(a) \delta(a-b) = 0$ because $c-b \neq 0$, and $a-b \neq 0$, so the argument of neither delta function can be zero, therefore, the integrals with respect to any

variable of integration is necessarily zero. More formally,

$$\int dc \left(\int_{a}^{c} \delta' \left(x - b \right) f \left(x \right) dx \right) = \int f \left(c \right) \delta \left(c - b \right) dc + \int dc \left(-f \left(a \right) \delta \left(a - b \right) - \int_{a}^{c} \delta \left(x - b \right) f' \left(x \right) dx \right) = 0 + \int dc \left(-f \left(a \right) \delta \left(a - b \right) - \int_{a}^{c} \delta \left(x - b \right) f' \left(x \right) dx \right) \Rightarrow \int_{a}^{c} \delta' \left(x - b \right) f \left(x \right) dx = -f \left(a \right) \delta \left(a - b \right) - \int_{a}^{c} \delta \left(x - b \right) f' \left(x \right) dx,$$

and then repeat the process with respect to a. In either event,

$$\int_{a}^{c} \delta'(x-b) f(x) \, dx = -\int_{a}^{c} \delta(x-b) \, f'(x) \, dx = -f'(b) \quad \text{since} \quad a < b < c \,.$$

to you, (it looks on the page.

18. Establish relations applicable to continuous systems in position space, momentum space, and energy space, for

- (a) the orthonormality condition and
- (b) the completeness relation.

Infinities are inherent in descriptions of systems that are continuous. The infinite dimensional vector that contains the same information as a continuous function is but one example. Though not mathematically rigorous, physicists frequently reason using finite dimensional analogs treating the infinite as a generalization⁵. This seems a practical if not a mathematical necessity.

There is enough new notation in this problem that we recommend that you simply read the discussion carefully. If you prefer to venture an effort, realize that in position space, for instance,

$$i \text{ or } x_i \longrightarrow x, \quad \delta_{ij} \longrightarrow \delta(x - x'), \quad \text{and} \quad \sum_i \longrightarrow \int dx,$$

when generalizing from the discrete to the continuous. Suppress the limits of $-\infty$ and ∞ to keep the notation clean.

(a) The orthonormality condition is denoted $\langle i | j \rangle = \delta_{ij}$ in general. If specifically in position space, it can be written $\langle x_i | x_j \rangle = \delta_{ij}$ where x_i and x_j denote unit vectors that corresponded to the i^{th} and j^{th} positions on the x-axis. If i = j, then $\langle x_i | x_j \rangle = 1$. Let the distance between unit vectors approaches zero, modelling a continuous system. The discrete x_i and x_j become indistinguishable as the distance between them approaches zero, so are superceded by x and x' for continuous systems. Symbology that describes coincidence or non-coincidence is then,

 $\langle x_i | x_j \rangle = \delta_{ij} \longrightarrow \langle x | x' \rangle = \delta(x - x')$ for a continuous system in position space.

If the argument is made in momentum space, $\langle p_i | p_j \rangle = \delta_{ij} \longrightarrow \langle p | p' \rangle = \delta(p - p')$.

If the argument is made in energy space, $\langle E_i | E_j \rangle = \delta_{ij} \longrightarrow \langle E | E' \rangle = \delta(E - E')$.

(b) The completeness relation is $\sum_{i=1}^{n} |i\rangle \langle i| = \mathcal{I}$ or $\sum_{i=1}^{n} |x_i\rangle \langle x_i| = \mathcal{I}$ for position space. In the limit as $n \to \infty$, $|x_i\rangle \to |x\rangle$ and $\sum_{i} \to \int dx$ in position space, so

$$\sum_{i=1}^{n} |x_i\rangle \langle x_i| = \mathcal{I} \quad \longrightarrow \quad \int |x\rangle \langle x| \, dx = \mathcal{I} \text{ for position space,}$$

$$\sum_{i=1}^{n} |p_i\rangle \langle p_i| = \mathcal{I} \quad \longrightarrow \quad \int |p\rangle \langle p| \, dp = \mathcal{I} \text{ for momentum space, and}$$

$$\sum_{i=1}^{n} |E_i\rangle \langle E_i| = \mathcal{I} \quad \longrightarrow \quad \int |E\rangle \langle E| \, dE = \mathcal{I} \text{ for energy space.}$$

Postscript: The relations established in this problem should be viewed as definitions because of the question of convergence. The extension $\sum_{i} \rightarrow \int dx$ is subject to the question of

⁵ Cohen-Tannoudji, Diu, & Laloe, Quantum Mechanics (John Wiley & Sons, New York, 1977), 4th ed., pp. 94.

convergence but is more fundamentally a redefinition. The development of a Riemann integral often concerns the area under a curve where the area is approximated by $\sum_{i=1}^{n} f(x_i) \Delta x$. Then as $n \to \infty$, $\Delta x \to 0$. The Δx in this development is the distance between the infinite dimensional unit vectors, so Δx is implicit in the index *i* for the extension $\sum_{i=1}^{n} \int dx$.

19. Use the technique of insertion of the identity to establish expressions applicable to continuous systems in position space, momentum space, and energy space, for an inner product.

This problem establishes a fundamental tenet while applying representations. It should start to convince you of the economy and convenience inherent in Dirac notation. Each of the three solutions require only about one line.

Start with an inner product of two abstract vectors, say $\langle f | g \rangle$. Insert the identity to get $\langle f | \mathcal{I} | g \rangle$. Use the completeness relation for a continuous system from problem 18 appropriate to each space, then find the representations of problems 9 and 10. You should find $\langle f | g \rangle = \int f^*(x) g(x) dx$ for position space, for instance.

$$< f | g > = < f | \mathcal{I} | g > = < f | \left(\int |x > < x | dx \right) | g > = \int < f | x > < x | g > dx = \int f^* (x) g (x) dx .$$

$$< f | g > = < f | \mathcal{I} | g > = < f | \left(\int |p > = \int < f | p > dp = \int \hat{f}^* (p) \hat{g} (p) dp .$$

$$< f | g > = < f | \mathcal{I} | g > = < f | \left(\int |E > < E | dE \right) | g >$$

$$= \int < f | E > < E | g > dE = \int \tilde{f}^* (E) \tilde{g} (E) dE .$$

Postscript: See problem 41 for a comment concerning the validity of moving the bra and ket inside the integrand.

20. (a) Use the result of problem 19 to establish an expression of the normalization condition in position space.

(b) Normalize $f(x) = A e^{-Bx^2}$.

This is a practical problem. First, you know the representation of $\langle f | g \rangle$ in position space, so the what is the representation of $\langle f | f \rangle$? Transition to a representation such as position space is often accompanied by a transition to calculus based arguments. You may find form 3.323.2 from Gradshteyn and Ryzhik useful. It is

$$\int_{-\infty}^{\infty} \exp\left(-p^2 x^2 \pm q x\right) dx = \exp\left(\frac{q^2}{4p^2}\right) \frac{\sqrt{\pi}}{p}, \quad p > 0.$$

(a) The normalization condition is $\langle f | f \rangle = 1 \implies \int f^*(x) f(x) dx = 1$ in position space.

(b)
$$\langle f | f \rangle = 1 \Rightarrow \int_{-\infty}^{\infty} \left(A e^{-Bx^2} \right)^* \left(A e^{-Bx^2} \right) dx = 1 \Rightarrow \left| A \right|^2 \int_{-\infty}^{\infty} e^{-2Bx^2} dx = 1.$$

Using form 3.323.2 from Gradshteyn and Ryzhik, our integral has $p^2 = 2B$, q = 0, therefore

$$\left|\mathbf{A}\right|^{2} e^{0} \sqrt{\frac{\pi}{2\mathrm{B}}} = 1 \quad \Rightarrow \quad \left|\mathbf{A}\right|^{2} \sqrt{\frac{\pi}{2\mathrm{B}}} = 1 \quad \Rightarrow \quad \mathbf{A} = \left(\frac{2\mathrm{B}}{\pi}\right)^{1/4} \quad \Rightarrow \quad f(x) = \left(\frac{2\mathrm{B}}{\pi}\right)^{1/4} e^{-\mathrm{B}x^{2}}$$

21. (a) Show that

$$\psi_n(x) = \cos\left(\frac{n\pi x}{l}\right)$$
 and $\psi_m(x) = \sin\left(\frac{m\pi x}{l}\right)$ are orthogonal on the interval $-l < x < l$.

(b) Orthonormalize $\psi_n(x)$ and $\psi_m(x)$.

There are many reasons for this problem at this point. Part (a) is an application of an inner product in position space. Cosines, sines, and orthogonality are intrinsic to the discussion of Fourier series that follows. Finally, we will see these wave functions again when discussing the infinite square well, meaning that they are realistic enough to be useful. A substantial portion of the reason that they are useful is the property of orthonormality addressed in part (b).

To show orthogonality for part (a), you must find that the inner product of each wavefunction with itself is non-zero, *i.e.*, $\langle \psi_n | \psi_n \rangle \neq 0$ and $\langle \psi_m | \psi_m \rangle \neq 0$. Then you must show that

$$<\psi_{n_i} | \psi_{n_j} > = <\psi_{m_i} | \psi_{m_j} > = <\psi_n | \psi_m > = 0.$$

Here are some indefinite integrals taken from the 30th edition of CRC Standard Mathematical Tables and Formulae that you should find useful.

$$\int \cos^2 ax \, dx = \frac{x}{2} + \frac{1}{4a} \sin 2ax \,, \qquad \int \sin^2 ax \, dx = \frac{x}{2} - \frac{1}{4a} \sin 2ax \,,$$
$$\int (\sin ax) (\cos ax) \, dx = \frac{1}{2a} \sin^2 ax \,,$$

and some others from Gradshteyn and Ryzhik,

$$\int (\cos ax) (\cos bx) dx = \frac{\sin (a-b)x}{2(a-b)} + \frac{\sin (a+b)x}{2(a+b)}, \quad a^2 \neq b^2,$$
$$\int (\sin ax) (\sin bx) dx = \frac{\sin (a-b)x}{2(a-b)} - \frac{\sin (a+b)x}{2(a+b)}, \quad a^2 \neq b^2,$$
$$\int (\sin ax) (\cos bx) dx = -\frac{\cos (a-b)x}{2(a-b)} - \frac{\cos (a+b)x}{2(a+b)}, \quad a^2 \neq b^2.$$

The appropriate limits on these integrals are -l and l. Indices are used only to enumerate eigenstates, thus, all n and m are positive integers. Also remember that cosine is an even function and sine is an odd function.

$$\langle \psi_n | \psi_n \rangle = \int_{-l}^{l} \left(\cos\left(\frac{n\pi x}{l}\right) \right)^* \left(\cos\left(\frac{n\pi x}{l}\right) \right) dx = \int_{-l}^{l} \cos^2\left(\frac{n\pi x}{l}\right) dx$$
$$= \left[\frac{x}{2} + \frac{l}{4n\pi} \sin\frac{2n\pi x}{l} \right]_{-l}^{l} = \frac{l}{2} - \frac{-l}{2} + \frac{l}{4n\pi} \sin\frac{2n\pi l}{l} - \frac{l}{4n\pi} \sin\frac{-2n\pi l}{l}$$
$$= l + \frac{l}{4n\pi} \left(\sin 2n\pi + \sin 2n\pi \right) = l + \frac{l}{2n\pi} \sin 2n\pi = l \neq 0 ,$$

where the sine is struck because the sine of any integral multiple of π is zero. Similarly

$$\langle \psi_m | \psi_m \rangle = \int_{-l}^{l} \left(\sin\left(\frac{m\pi x}{l}\right) \right)^* \left(\sin\left(\frac{m\pi x}{l}\right) \right) dx = \int_{-l}^{l} \sin^2\left(\frac{m\pi x}{l}\right) dx$$
$$= \left[\frac{x}{2} - \frac{l}{4m\pi} \sin\frac{2m\pi x}{l} \right]_{-l}^{l} = \frac{l}{2} - \frac{-l}{2} - \frac{l}{4m\pi} \sin\frac{2m\pi l}{l} + \frac{l}{4m\pi} \sin\frac{-2m\pi l}{l}$$
$$= l - \frac{l}{4m\pi} \left(\sin 2m\pi + \sin 2m\pi \right) = l - \frac{l}{2m\pi} \sin^2 2m\pi = l \neq 0 .$$

Conjugation is cosmetic when functions are real so is hereafter suppressed. Then

$$\langle \psi_{n_{i}} | \psi_{n_{j}} \rangle = \int_{-l}^{l} \left(\cos \frac{n_{i} \pi x}{l} \right) \left(\cos \frac{n_{j} \pi x}{l} \right) dx$$

$$= \left[\frac{\sin \left(\frac{n_{i} \pi x}{l} - \frac{n_{j} \pi x}{l} \right)}{2 \left(\frac{n_{i} \pi}{l} - \frac{n_{j} \pi}{l} \right)} + \frac{\sin \left(\frac{n_{i} \pi x}{l} + \frac{n_{j} \pi x}{l} \right)}{2 \left(\frac{n_{i} \pi}{l} + \frac{n_{j} \pi}{l} \right)} \right]_{-l}^{l}$$

$$= \frac{l}{2\pi} \frac{\sin (n_{i} - n_{j}) \pi}{(n_{i} - n_{j})} - \frac{l}{2\pi} \frac{\sin (-n_{i} + n_{j}) \pi}{(n_{i} - n_{j})} + \frac{l}{2\pi} \frac{\sin (n_{i} + n_{j}) \pi}{(n_{i} + n_{j})} - \frac{l}{2\pi} \frac{\sin (-n_{i} - n_{j}) \pi}{(n_{i} + n_{j})}.$$

Remember that $n_i \neq n_j$, because the case $n_i = n_j = n$ is covered by $\langle \psi_n | \psi_n \rangle$. The arguments of all the sine functions are sums and differences of integers times π , so are integral multiples of π . The numerators of all terms are therefore zero, so $\langle \psi_{n_i} | \psi_{n_j} \rangle = 0$. Next

$$<\psi_{m_{i}} |\psi_{m_{j}}> = \int_{-l}^{l} \left(\sin \frac{m_{i}\pi x}{l}\right) \left(\sin \frac{m_{j}\pi x}{l}\right) dx$$
$$= \left[\frac{\sin \left(\frac{m_{i}\pi x}{l} - \frac{m_{j}\pi x}{l}\right)}{2\left(\frac{m_{i}\pi}{l} - \frac{m_{j}\pi}{l}\right)} - \frac{\sin \left(\frac{m_{i}\pi x}{l} + \frac{m_{j}\pi x}{l}\right)}{2\left(\frac{m_{i}\pi}{l} + \frac{m_{j}\pi}{l}\right)}\right]_{-l}^{l}$$
$$\frac{l}{2\pi} \frac{\sin (m_{i} - m_{j})\pi}{(m_{i} - m_{j})} - \frac{l}{2\pi} \frac{\sin (-m_{i} + m_{j})\pi}{(m_{i} - m_{j})} - \frac{l}{2\pi} \frac{\sin (m_{i} + m_{j})\pi}{(m_{i} + m_{j})} + \frac{l}{2\pi} \frac{\sin (-m_{i} - m_{j})\pi}{(m_{i} + m_{j})}$$

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Again, $m_i \neq m_j$, because the case $m_i = m_j = m$ is addressed by $\langle \psi_m | \psi_m \rangle$. Again, the arguments of all the sine functions are sums and differences of integers times π , so are integral multiples of π . The numerators of all terms are again zero, so $\langle \psi_{m_i} | \psi_{m_j} \rangle = 0$. Then

$$<\psi_{m} | \psi_{n} > = \int_{-l}^{l} \left(\sin \frac{m\pi x}{l} \right) \left(\cos \frac{n\pi x}{l} \right) dx$$
$$= \left[-\frac{\cos \left(\frac{m\pi x}{l} - \frac{n\pi x}{l} \right)}{2 \left(\frac{m\pi}{l} - \frac{n\pi}{l} \right)} - \frac{\cos \left(\frac{m\pi x}{l} + \frac{n\pi x}{l} \right)}{2 \left(\frac{m\pi}{l} + \frac{n\pi}{l} \right)} \right]_{-l}^{l}$$
$$= -\frac{l}{2\pi} \frac{\cos (m-n)\pi}{(m-n)} + \frac{l}{2\pi} \frac{\cos (-m+n)\pi}{(m-n)} - \frac{l}{2\pi} \frac{\cos (m+n)\pi}{(m+n)} + \frac{l}{2\pi} \frac{\cos (-m-n)\pi}{(m+n)}.$$

The cosine is an even function, so $\cos(-m+n)\pi = \cos(m-n)\pi$ and $\cos(-m-n)\pi = \cos(m+n)\pi$. Substituting in the last line,

$$\langle \psi_m \, | \, \psi_n \rangle = -\frac{l}{2\pi} \frac{\cos\left(m-n\right)\pi}{(m-n)} + \frac{l}{2\pi} \frac{\cos\left(m-n\right)\pi}{(m-n)} - \frac{l}{2\pi} \frac{\cos\left(m+n\right)\pi}{(m+n)} + \frac{l}{2\pi} \frac{\cos\left(m+n\right)\pi}{(m+n)} \, ,$$

and the first and second terms are identical except they have opposite signs so sum to zero, similarly, the third and fourth terms sum to zero, so we conclude $\langle \psi_m | \psi_n \rangle = 0$, $m \neq n$. The qualification $m \neq n$ applies to the last calculation because m = n is not covered by any previous case. Since both indices are equal for this calculation, let m = n = k

$$\langle \psi_{k} | \psi_{k} \rangle = \int_{-l}^{l} \left(\sin \frac{k\pi x}{l} \right) \left(\cos \frac{k\pi x}{l} \right) \, dx = \frac{l}{2k\pi} \, \sin^{2} \left. \frac{k\pi x}{l} \right|_{-l}^{l}$$
$$= \frac{l}{2k\pi} \left(\sin^{2} k\pi - \sin^{2} (-k\pi) \right) = \frac{l}{2k\pi} \left(\sin^{2} k\pi - \sin^{2} k\pi \right) = 0$$

since \sin^2 is an even function. Also, the sine of an integral multiple of π is zero so the squares of integral multiples of π are zero. This exhausts all possibilities for indices that are positive integers. Therefore,

$$\psi_n(x) = \cos\left(\frac{n\pi x}{l}\right)$$
 and $\psi_m(x) = \sin\left(\frac{m\pi x}{l}\right)$ are orthogonal on the interval $-l < x < l$.

(b) In the first two calculations we found $\langle \psi_n | \psi_n \rangle = \langle \psi_m | \psi_m \rangle = l$, so

$$\langle \psi_n | \mathbf{A}^* \mathbf{A} | \psi_n \rangle = | \mathbf{A} |^2 \langle \psi_n | \psi_n \rangle = | \mathbf{A} |^2 l = 1 \quad \Rightarrow \quad \mathbf{A} = \frac{1}{\sqrt{l}}$$
$$\Rightarrow \quad \psi_n(x) = \frac{1}{\sqrt{l}} \cos\left(\frac{n\pi x}{l}\right) \quad \text{and} \quad \psi_m(x) = \frac{1}{\sqrt{l}} \sin\left(\frac{n\pi x}{l}\right)$$

are orthonormal on the interval -l < x < l.

22. (a) Show that if indices of n < 0 where to apply, $a_{-n} = a_n$, and that $a_0 = \frac{1}{l} \int_{-l}^{l} f(x) dx$ for a basic Fourier series.

(b) Show that if indices of n < 0 where to apply, $b_{-n} = -b_n$, and that $b_0 = 0$ for a basic Fourier series.

(c) Express the c_n that are the coefficients of the exponential format of the Fourier series in terms of the basic Fourier coefficients a_n and b_n , and show that $c_0 = a_0/2$.

(d) Demonstrate the equivalence of the basic Fourier series and the exponential format of the Fourier series.

the same period? A Fourier series is a representation of a periodic function as a linear combination of all cosine and sine functions that have the same period. The periodic function f(x) = f(x+2l), has a period of 2l, or repeats itself every 2l. In a basic Fourier series,

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

where the coefficients are

$$a_n = \frac{1}{l} \int_{-l}^{l} f(x) \cos\left(\frac{n\pi x}{l}\right) dx$$
, and $b_n = \frac{1}{l} \int_{-l}^{l} f(x) \sin\left(\frac{n\pi x}{l}\right) dx$,

given that the period is 2l. The Fourier series in a exponential format for a function that is periodic over the length 2l is

$$f(x) = \sum_{-\infty}^{\infty} c_n e^{in\pi x/l}, \quad \text{where} \quad c_n = \frac{1}{2l} \int_{-l}^{l} f(x) e^{-in\pi x/l} dx.$$

Use the defining integrals for a_n , b_n , and c_n , for parts (a), (b), and (c). Cosines are even functions and sines are odd functions. Substituting these results into the summation that defines the exponential form yields the basic Fourier series required for part (d). It is wise to divide the summation into three parts that coincide with the three cases, namely: n < 0 implies a summation from $-\infty$ to -1, n = 0 is one term of the summation, and n > 0 implies a summation from 1 to ∞ . The tricky part is switching the indices on the summation from $-\infty$ to -1. It may require some reflection, but realize that

$$\sum_{-\infty}^{-1} \frac{1}{2} (a_n - ib_n) e^{in\pi x/l} = \sum_{1}^{\infty} \frac{1}{2} (a_n + ib_n) e^{-in\pi x/l}.$$

(a)
$$a_{-n} = \frac{1}{l} \int_{-l}^{l} f(x) \cos\left(\frac{-n\pi x}{l}\right) dx = \frac{1}{l} \int_{-l}^{l} f(x) \cos\left(\frac{n\pi x}{l}\right) dx = a_{n},$$

and $a_{0} = \frac{1}{l} \int_{-l}^{l} f(x) \cos(0) dx = \frac{1}{l} \int_{-l}^{l} f(x) dx.$
(b) $b_{-n} = \frac{1}{l} \int_{-l}^{l} f(x) \sin\left(\frac{-n\pi x}{l}\right) dx = -\frac{1}{l} \int_{-l}^{l} f(x) \sin\left(\frac{n\pi x}{l}\right) dx = -b_{n},$

(c)
$$c_{n} = \frac{1}{2l} \int_{-l}^{l} f(x) e^{-in\pi x/l} dx = \frac{1}{2l} \int_{-l}^{l} f(x) \sin(0) dx = 0.$$

$$= \frac{1}{2l} \int_{-l}^{l} f(x) e^{-in\pi x/l} dx = \frac{1}{2l} \int_{-l}^{l} f(x) \left[\cos\left(\frac{n\pi x}{l}\right) - i\sin\left(\frac{n\pi x}{l}\right) \right] dx$$

$$= \frac{1}{2l} \int_{-l}^{l} f(x) \cos\left(\frac{n\pi x}{l}\right) dx - \frac{i}{2l} \int_{-l}^{l} f(x) \sin\left(\frac{n\pi x}{l}\right) dx = \frac{1}{2} (a_{n} - ib_{n})$$
Where $n = 0$, the component of the componential is zero.

When n = 0, the argument of the exponential is zero, so

$$c_0 = \frac{1}{2l} \int_{-l}^{l} f(x) e^0 dx = \frac{1}{2l} \int_{-l}^{l} f(x) dx = \frac{1}{2} a_0$$

(d) For convenience, let $\theta = \pi x/l$. The summation is

$$f(x) = \sum_{-\infty}^{\infty} c_n e^{in\theta} = \sum_{-\infty}^{-1} \frac{1}{2} (a_n - ib_n) e^{in\theta} + \frac{1}{2} a_0 + \sum_{1}^{\infty} \frac{1}{2} (a_n - ib_n) e^{in\theta}$$

$$= \frac{1}{2} a_0 + \sum_{1}^{\infty} \left(\frac{a_n}{2} + \frac{ib_n}{2}\right) e^{-in\theta} + \sum_{1}^{\infty} \left(\frac{a_n}{2} - \frac{ib_n}{2}\right) e^{in\theta}$$
(1)
$$= \frac{1}{2} a_0 + \sum_{1}^{\infty} \left(\frac{a_n}{2} e^{-in\theta} + \frac{ib_n}{2} e^{-in\theta} + \frac{a_n}{2} e^{in\theta} - \frac{ib_n}{2} e^{in\theta}\right)$$

$$= \frac{1}{2} a_0 + \sum_{1}^{\infty} \left(\frac{a_n}{2} \cos n\theta - \frac{a_n}{2} i \sin/n\theta + \frac{ib_n}{2} \cos/n\theta + \frac{b_n}{2} \sin n\theta + \frac{a_n}{2} \cos n\theta + \frac{a_n}{2} i \sin/n\theta - \frac{ib_n}{2} \cos/n\theta + \frac{b_n}{2} \sin n\theta\right)$$
(2)
$$= \frac{1}{2} a_0 + \sum_{1}^{\infty} \left(a_n \cos n\theta + b_n \sin n\theta\right)$$

which is identical to the basic Fourier series upon the substitution of $\theta = \pi x/l$. We have used the results of parts (a) and (b) in equation (1). The sign of the argument of the first exponential in equation (1) changes because we have changed the sign of the index of the summation. The signs of the fourth and eighth terms in the summation of equation (2) are correct because both include factors of $i \cdot i = -1$.

Postscript: The cosine and sine functions are orthogonal over a finite interval, say -l < x < l, and can be made orthonormal on that interval as demonstrated in problem 21. Orthonormal vectors or orthonormal functions constitute a basis. Any function can be expressed in terms of a linear combination of the vectors, or in this case, the functions that constitute the basis.

The infinite square well, also known as a particle in a box, uses the orthogonal cosine and sine functions as a basis.

The exponential format of the Fourier series is often called **complex Fourier series**. We are interested in the complex Fourier series because it is the form that is most easily generalized to the **Fourier integral**.

23. Sketch the graphs of the following functions and their the Fourier transforms.

(a)
$$f(x) = \begin{cases} 1, & -a < x < a, \\ 0, & \text{elsewhere,} \end{cases}$$
 and (b) $f_1(x) = \begin{cases} 1/2, & -b < x < b, \\ 0, & \text{elsewhere,} \end{cases}$ where $b = 2a$

Fourier integrals are generalizations of Fourier series. A Fourier integral is a representation of a non-periodic function that may be regarded as the limit of the Fourier series as the period approaches infinity. Two Fourier transforms compose the Fourier integral. Fourier transforms are the objects that we want to develop further for quantum mechanical calculation. We refer the reader to Byron and Fuller⁶, or your favorite text on mathematical physics for greater depth. In the limit of $l \to \infty$, the complex Fourier series becomes

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

The function f(x) is the Fourier transform of g(k), and g(k) is the Fourier transform of f(x). Substitution of one transform into the other expressing the combination as one relation, *i.e.*,

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x') e^{-ikx'} dx' \right) e^{ikx} dk$$
$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} f(x') e^{ik(x-x')} dx' \quad \text{is the Fourier integral}$$

The functions given for parts (a) and (b) are constants for specified intervals and zero elsewhere which means that you can find g(k) and $g_1(k)$ by integrating between -a and a, and -b and b instead of using infinite limits. Express your answer for part (b) in terms of the constant a and look for relations between the graphs of parts (a) and (b). This problem uses constant functions which are among the easiest functions to integrate both as an appropriate place to start and to highlight relations between parts (a) and (b) for which we provide comment in the postscript.

(a)
$$g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \int_{-a}^{a} f(x) e^{-ikx} dx$$
$$= \frac{1}{\sqrt{2\pi}} \frac{1}{(-ik)} e^{-ikx} \Big|_{-a}^{a} = \frac{1}{\sqrt{2\pi}} \frac{e^{-ika} - e^{ika}}{-ik}$$
$$= \frac{2}{\sqrt{2\pi} k} \frac{e^{-ika} - e^{ika}}{-2i} = \frac{2}{\sqrt{2\pi} k} \frac{e^{ika} - e^{-ika}}{2i} = \frac{2}{\sqrt{2\pi}} \frac{\sin(ka)}{k}.$$

The graphs of f(x) and g(k), are

⁶ Byron and Fuller, *Mathematics of Classical and Quantum Physics* (Dover Publications, Inc., New York, 1970), pp. 239–253, 566–570.

Graph of f(x) Graph of g(k)

(b) The Fourier transform of the given function where b = 2a, double the width and half the height, so that the area under the curve is equal for both f(x) and $f_1(x)$, is

$$g_1(k) = \frac{1}{\sqrt{2\pi}} \frac{\sin(kb)}{k} = \frac{1}{\sqrt{2\pi}} \frac{\sin(2ka)}{k}$$

Graph of $f_1(x)$

Graph of $g_1(k)$

Postscript: The graph of $f_1(x)$ is broader than the graph of f(x), but the graph of $g_1(k)$ is sharper than the graph of g(k). If one of the Fourier transforms is distributed and broad, the other will be localized and sharp. This phenomena is a precursor of the Heisenberg uncertainty relations.

While $f_i(x)$ has a limited domain, the domain of $g_i(k)$ is infinite. This is another general feature of Fourier transforms.

24. Derive the Fourier transforms from the complex Fourier series.

The basic Fourier series is useful for introductions and many applications, but the complex Fourier series is the form from which Fourier transforms are most easily attained. This is a challenging problem but provides an opportunity to deepen your understanding of Fourier transforms.

Start with the notation

$$F(y) = \sum_{-\infty}^{\infty} c_n e^{in\pi y/l}, \quad \text{where} \quad c_n = \frac{1}{2l} \int_{-l}^{l} F(y) e^{-in\pi y/l} dy.$$

Substitute the integral form of c_n into the summation. Symmetrize the factor of 1/2l. This means to rearrange the summation so a factor of $1/\sqrt{2l}$ is in both the F(y) and the c_n . You now have F(y) and c_n that are different than originally defined. Change variables by letting $x = \sqrt{\frac{\pi}{l}} y$. Also, let $k_n = n\sqrt{\frac{\pi}{l}}$. You can now find that $\Delta k_n = \sqrt{\frac{\pi}{l}}$ and $\frac{n\pi y}{l} = k_n x$. Redefine $F\left(\sqrt{\frac{l}{\pi}} x\right) = f(x)$. Introduce a new symbol for the coefficients that indicates the

index k_n replaces n', so $c_n \to g_{k_n}$. Finally, let $l \to \infty$, so that the Fourier transforms

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{ikx} dk \quad \text{and} \quad g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \quad \text{are exposed.}$$

$$F(y) = \sum_{n = -\infty}^{\infty} \left(\frac{1}{2l} \int_{-l}^{l} F(y) e^{-in\pi y/l} \, dy \right) e^{in\pi y/l} = \sum_{n = -\infty}^{\infty} \left(\frac{1}{\sqrt{2l}} \int_{-l}^{l} F(y) e^{-in\pi y/l} \, dy \right) \frac{1}{\sqrt{2l}} e^{in\pi y/l}$$

We can now identify a symmetrized function and coefficient as

$$F(y) = \sum_{n = -\infty}^{\infty} c_n \frac{1}{\sqrt{2l}} e^{in\pi y/l} \quad \text{and} \quad c_n = \frac{1}{\sqrt{2l}} \int_{-l}^{l} F(y) e^{-in\pi y/l} \, dy \,. \tag{1}$$

We are going to change variables to $\sqrt{\frac{\pi}{l}}y = x \Rightarrow y = \sqrt{\frac{l}{\pi}}x \Rightarrow dy = \sqrt{\frac{l}{\pi}}dx$. We are also going to use $k_n = n\sqrt{\frac{\pi}{l}} \Rightarrow \Delta k_n = k_{n+1} - k_n = (n+1)\sqrt{\frac{\pi}{l}} - n\sqrt{\frac{\pi}{l}} = \sqrt{\frac{\pi}{l}}$. These substitutions allow us to rewrite a portion of the argument of the exponentials, $\frac{n\pi y}{l} = n\sqrt{\frac{\pi}{l}}\sqrt{\frac{\pi}{l}}y = k_n x$. The difference in the new index is $\Delta k_n = \sqrt{\frac{\pi}{l}} \Rightarrow \frac{\Delta k_n}{\sqrt{2\pi}} = \frac{1}{\sqrt{2l}}$. The limits of the integral become $y = l \Rightarrow x = \sqrt{\frac{\pi}{l}}l = \sqrt{\pi l}$, and $y = -l \Rightarrow x = -\sqrt{\pi l}$. We finally introduce a new symbol for the coefficients that indicates the index is now k_n vice n so $c_n \to g_{k_n}$. Using these substitutions and developments in equation (1),

$$F(y) = F\left(\sqrt{\frac{l}{\pi}}x\right) = \sum_{k_n = -\infty}^{\infty} g_{k_n} \frac{1}{\sqrt{2\pi}} e^{ik_n x} \Delta k_n = \frac{1}{\sqrt{2\pi}} \sum_{k_n = -\infty}^{\infty} g_{k_n} e^{ik_n x} \Delta k_n$$

and
$$g_{k_n} = \frac{1}{\sqrt{2l}} \int_{-\sqrt{\pi l}}^{\sqrt{\pi l}} F\left(\sqrt{\frac{l}{\pi}}x\right) e^{-ik_n x} \sqrt{\frac{l}{\pi}} dx = \frac{1}{\sqrt{2\pi}} \int_{-\sqrt{\pi l}}^{\sqrt{\pi l}} F\left(\sqrt{\frac{l}{\pi}}x\right) e^{-ik_n x} dx$$

define
$$F\left(\sqrt{\frac{l}{\pi}}x\right) = f(x)$$
. Now let the period d were $x = \Delta h = \sqrt{\frac{\pi}{\pi}} + 0$. The

Redefine $F\left(\sqrt{\frac{\iota}{\pi}}x\right) = f(x)$. Now, let the period $l \to \infty \Rightarrow \Delta k_n = \sqrt{\frac{\pi}{l}} \to 0$. The difference between successive $k_n \to 0$ so that k_n assumes all real values and thus becomes a

continuous variable. The summation over discrete k_n becomes an integral over the continuous variable k, the coefficient g_{k_n} becomes a continuous function g(k), the difference Δk_n becomes the differential dk, and

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{ikx} dk \quad \text{and} \quad g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$$

Postscript: The factor of $1/2\pi$ must be in the Fourier integral but it does not need to be symmetrized in the Fourier transforms. Some authors and tables place the entire factor $1/2\pi$ with one integral so that there is no coefficient in front of the other integral. Also, some authors and tables will change the signs of the exponentials from what we have presented. Asymmetric treatment of the factor of $1/2\pi$ and/or use of a different sign convention result in slightly different functional forms for resulting Fourier transforms.

25. Find the momentum space wavefunction corresponding to a position space wavefunction that is Gaussian.

Gaussian wavefunctions are foundational as you will find in chapter 3 and elsewhere. But first, what does it mean to change a wavefunction in position space to a wavefunction in momentum space? It means find the description of a system using an unknown function of the continuous variable momentum starting with the description of the system that is a known function of the continuous variable position. It is a change of basis in the realm of continuous variables. Quantum mechanical Fourier transforms are the means to change from position space to momentum space and vice versa for continuous variables.

The de Broglie relation associates wavelength or wavenumber, and momentum,

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

Substitute p/\hbar for k in both Fourier transforms. This means the differential $dk = dp/\hbar$ in the integral for f(x). Symmetrize the $1/\hbar$ from this differential by placing a factor $1/\sqrt{\hbar}$ in both integrals, and the result is the quantum mechanical form of the Fourier transforms,

$$f(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \widehat{g}(p) e^{ipx/\hbar} dp, \qquad \widehat{g}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} f(x) e^{-ipx/\hbar} dx.$$

The usual use of these relations is to transform a wave function in position space to momentum space (or vice versa), so will be applied

$$\psi\left(x\right) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \widehat{\psi}\left(p\right) e^{ipx/\hbar} \, dp, \qquad \widehat{\psi}\left(p\right) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi\left(x\right) e^{-ipx/\hbar} \, dx.$$

There are a number of subtleties associated with the quantum mechanical analog of the Fourier transforms, so our heuristic argument should be regarded as nothing more than a useful mnemonic.

Use $\psi(x) = A e^{-bx^2}$, b > 0, as your position space wavefunction that is Gaussian. Form 3.323.2 from Gradshteyn and Ryzhik,

$$\int_{-\infty}^{\infty} e^{-\alpha^2 x^2 - \beta x} \, dx = \frac{\sqrt{\pi}}{\alpha} \, e^{\beta^2 / 4\alpha^2},$$

should be useful. Do you recognize the functional form of the momentum space wavefunction?

$$\begin{split} \widehat{\psi}\left(p\right) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi\left(x\right) e^{-ipx/\hbar} \, dx = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} A \, e^{-bx^2} \, e^{-ipx/\hbar} \, dx \\ &= \frac{A}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-bx^2 - ipx/\hbar} \, dx \, . \end{split}$$

Using $\alpha = \sqrt{b}$, and $\beta = ip/\hbar$, our integral is

$$\widehat{\psi}(p) = \frac{A}{\sqrt{2\pi\hbar}} \frac{\sqrt{\pi}}{\sqrt{b}} \exp\left(\frac{(ip/\hbar)^2}{4(\sqrt{b})^2}\right) = \frac{A}{\sqrt{2\hbar b}} e^{-p^2/4b\hbar^2}.$$

Postscript: Notice that $\hat{\psi}(p)$ is also an exponential function with a negative argument that is a constant times the independent variable squared. In fact, $\hat{\psi}(p)$ is also a Gaussian wavefunction. The Fourier transform of a Gaussian function is another Gaussian function.

21. (a) Show that

$$\psi_n(x) = \cos\left(\frac{n\pi x}{l}\right)$$
 and $\psi_m(x) = \sin\left(\frac{m\pi x}{l}\right)$ are orthogonal on the interval $-l < x < l$.

(b) Orthonormalize $\psi_n(x)$ and $\psi_m(x)$.

There are many reasons for this problem at this point. Part (a) is an application of an inner product in position space. Cosines, sines, and orthogonality are intrinsic to the discussion of Fourier series that follows. Finally, we will see these wave functions again when discussing the infinite square well, meaning that they are realistic enough to be useful. A substantial portion of the reason that they are useful is the property of orthonormality addressed in part (b).

To show orthogonality for part (a), you must find that the inner product of each wavefunction with itself is non-zero, *i.e.*, $\langle \psi_n | \psi_n \rangle \neq 0$ and $\langle \psi_m | \psi_m \rangle \neq 0$. Then you must show that

$$<\psi_{n_i} | \psi_{n_j} > = <\psi_{m_i} | \psi_{m_j} > = <\psi_n | \psi_m > = 0.$$

Here are some indefinite integrals taken from the 30th edition of CRC Standard Mathematical Tables and Formulae that you should find useful.

$$\int \cos^2 ax \, dx = \frac{x}{2} + \frac{1}{4a} \sin 2ax \,, \qquad \int \sin^2 ax \, dx = \frac{x}{2} - \frac{1}{4a} \sin 2ax \,,$$
$$\int (\sin ax) (\cos ax) \, dx = \frac{1}{2a} \sin^2 ax \,,$$

and some others from Gradshteyn and Ryzhik,

$$\int (\cos ax) (\cos bx) dx = \frac{\sin (a-b)x}{2(a-b)} + \frac{\sin (a+b)x}{2(a+b)}, \quad a^2 \neq b^2,$$
$$\int (\sin ax) (\sin bx) dx = \frac{\sin (a-b)x}{2(a-b)} - \frac{\sin (a+b)x}{2(a+b)}, \quad a^2 \neq b^2,$$
$$\int (\sin ax) (\cos bx) dx = -\frac{\cos (a-b)x}{2(a-b)} - \frac{\cos (a+b)x}{2(a+b)}, \quad a^2 \neq b^2.$$

The appropriate limits on these integrals are -l and l. Indices are used only to enumerate eigenstates, thus, all n and m are positive integers. Also remember that cosine is an even function and sine is an odd function.

$$\langle \psi_n | \psi_n \rangle = \int_{-l}^{l} \left(\cos\left(\frac{n\pi x}{l}\right) \right)^* \left(\cos\left(\frac{n\pi x}{l}\right) \right) dx = \int_{-l}^{l} \cos^2\left(\frac{n\pi x}{l}\right) dx$$
$$= \left[\frac{x}{2} + \frac{l}{4n\pi} \sin\frac{2n\pi x}{l} \right]_{-l}^{l} = \frac{l}{2} - \frac{-l}{2} + \frac{l}{4n\pi} \sin\frac{2n\pi l}{l} - \frac{l}{4n\pi} \sin\frac{-2n\pi l}{l}$$
$$= l + \frac{l}{4n\pi} \left(\sin 2n\pi + \sin 2n\pi \right) = l + \frac{l}{2n\pi} \sin 2n\pi = l \neq 0 ,$$

where the sine is struck because the sine of any integral multiple of π is zero. Similarly

$$\langle \psi_m | \psi_m \rangle = \int_{-l}^{l} \left(\sin\left(\frac{m\pi x}{l}\right) \right)^* \left(\sin\left(\frac{m\pi x}{l}\right) \right) dx = \int_{-l}^{l} \sin^2\left(\frac{m\pi x}{l}\right) dx$$
$$= \left[\frac{x}{2} - \frac{l}{4m\pi} \sin\frac{2m\pi x}{l} \right]_{-l}^{l} = \frac{l}{2} - \frac{-l}{2} - \frac{l}{4m\pi} \sin\frac{2m\pi l}{l} + \frac{l}{4m\pi} \sin\frac{-2m\pi l}{l}$$
$$= l - \frac{l}{4m\pi} \left(\sin 2m\pi + \sin 2m\pi \right) = l - \frac{l}{2m\pi} \sin^2 2m\pi = l \neq 0 .$$

Conjugation is cosmetic when functions are real so is hereafter suppressed. Then

$$\begin{aligned} <\psi_{n_{i}} |\psi_{n_{j}}> &= \int_{-l}^{l} \left(\cos \frac{n_{i}\pi x}{l}\right) \left(\cos \frac{n_{j}\pi x}{l}\right) \, dx \\ &= \left[\frac{\sin \left(\frac{n_{i}\pi x}{l} - \frac{n_{j}\pi x}{l}\right)}{2\left(\frac{n_{i}\pi}{l} - \frac{n_{j}\pi}{l}\right)} + \frac{\sin \left(\frac{n_{i}\pi x}{l} + \frac{n_{j}\pi x}{l}\right)}{2\left(\frac{n_{i}\pi}{l} + \frac{n_{j}\pi}{l}\right)}\right]_{-l}^{l} \\ &= \frac{l}{2\pi} \frac{\sin \left(n_{i} - n_{j}\right) \pi}{\left(n_{i} - n_{j}\right)} - \frac{l}{2\pi} \frac{\sin \left(-n_{i} + n_{j}\right) \pi}{\left(n_{i} - n_{j}\right)} + \frac{l}{2\pi} \frac{\sin \left(n_{i} + n_{j}\right) \pi}{\left(n_{i} + n_{j}\right)} - \frac{l}{2\pi} \frac{\sin \left(-n_{i} - n_{j}\right) \pi}{\left(n_{i} + n_{j}\right)}. \end{aligned}$$

Remember that $n_i \neq n_j$, because the case $n_i = n_j = n$ is covered by $\langle \psi_n | \psi_n \rangle$. The arguments of all the sine functions are sums and differences of integers times π , so are integral multiples of π . The numerators of all terms are therefore zero, so $\langle \psi_{n_i} | \psi_{n_j} \rangle = 0$. Next

$$<\psi_{m_{i}} | \psi_{m_{j}} > = \int_{-l}^{l} \left(\sin \frac{m_{i}\pi x}{l} \right) \left(\sin \frac{m_{j}\pi x}{l} \right) dx$$
$$= \left[\frac{\sin \left(\frac{m_{i}\pi x}{l} - \frac{m_{j}\pi x}{l} \right)}{2 \left(\frac{m_{i}\pi}{l} - \frac{m_{j}\pi}{l} \right)} - \frac{\sin \left(\frac{m_{i}\pi x}{l} + \frac{m_{j}\pi x}{l} \right)}{2 \left(\frac{m_{i}\pi}{l} + \frac{m_{j}\pi}{l} \right)} \right]_{-l}^{l}$$
$$= \frac{l}{2\pi} \frac{\sin (m_{i} - m_{j})\pi}{(m_{i} - m_{j})} - \frac{l}{2\pi} \frac{\sin (-m_{i} + m_{j})\pi}{(m_{i} - m_{j})} - \frac{l}{2\pi} \frac{\sin (m_{i} + m_{j})\pi}{(m_{i} + m_{j})} + \frac{l}{2\pi} \frac{\sin (-m_{i} - m_{j})\pi}{(m_{i} + m_{j})}.$$

Again, $m_i \neq m_j$, because the case $m_i = m_j = m$ is addressed by $\langle \psi_m | \psi_m \rangle$. Again, the arguments of all the sine functions are sums and differences of integers times π , so are integral

multiples of π . The numerators of all terms are again zero, so $\langle \psi_{m_i} | \psi_{m_i} \rangle = 0$. Then

$$<\psi_{m} | \psi_{n} > = \int_{-l}^{l} \left(\sin \frac{m\pi x}{l} \right) \left(\cos \frac{n\pi x}{l} \right) dx$$
$$= \left[-\frac{\cos \left(\frac{m\pi x}{l} - \frac{n\pi x}{l} \right)}{2 \left(\frac{m\pi}{l} - \frac{n\pi}{l} \right)} - \frac{\cos \left(\frac{m\pi x}{l} + \frac{n\pi x}{l} \right)}{2 \left(\frac{m\pi}{l} + \frac{n\pi}{l} \right)} \right]_{-l}^{l}$$
$$\frac{l}{2\pi} \frac{\cos (m-n)\pi}{(m-n)} + \frac{l}{2\pi} \frac{\cos (-m+n)\pi}{(m-n)} - \frac{l}{2\pi} \frac{\cos (m+n)\pi}{(m+n)} + \frac{l}{2\pi} \frac{\cos (-m-n)\pi}{(m+n)}$$

The cosine is an even function, so $\cos(-m+n)\pi = \cos(m-n)\pi$ and $\cos(-m-n)\pi = \cos(m+n)\pi$. Substituting in the last line,

$$\langle \psi_m \, | \, \psi_n \rangle = -\frac{l}{2\pi} \frac{\cos\left(m-n\right)\pi}{(m-n)} + \frac{l}{2\pi} \frac{\cos\left(m-n\right)\pi}{(m-n)} - \frac{l}{2\pi} \frac{\cos\left(m+n\right)\pi}{(m+n)} + \frac{l}{2\pi} \frac{\cos\left(m+n\right)\pi}{(m+n)} \,,$$

and the first and second terms are identical except they have opposite signs so sum to zero, similarly, the third and fourth terms sum to zero, so we conclude $\langle \psi_m | \psi_n \rangle = 0$, $m \neq n$. The qualification $m \neq n$ applies to the last calculation because m = n is not covered by any previous case. Since both indices are equal for this calculation, let m = n = k

$$\langle \psi_{k} | \psi_{k} \rangle = \int_{-l}^{l} \left(\sin \frac{k\pi x}{l} \right) \left(\cos \frac{k\pi x}{l} \right) dx = \frac{l}{2k\pi} \sin^{2} \frac{k\pi x}{l} \Big|_{-l}^{l}$$
$$= \frac{l}{2k\pi} \left(\sin^{2} k\pi - \sin^{2} (-k\pi) \right) = \frac{l}{2k\pi} \left(\sin^{2} k\pi - \sin^{2} k\pi \right) = 0$$

since \sin^2 is an even function. Also, the sine of an integral multiple of π is zero so the squares of integral multiples of π are zero. This exhausts all possibilities for indices that are positive integers. Therefore,

$$\psi_n(x) = \cos\left(\frac{n\pi x}{l}\right)$$
 and $\psi_m(x) = \sin\left(\frac{m\pi x}{l}\right)$ are orthogonal on the interval $-l < x < l$.

(b) In the first two calculations we found $\langle \psi_n | \psi_n \rangle = \langle \psi_m | \psi_m \rangle = l$, so

$$\langle \psi_n | \mathbf{A}^* \mathbf{A} | \psi_n \rangle = | \mathbf{A} |^2 \langle \psi_n | \psi_n \rangle = | \mathbf{A} |^2 l = 1 \quad \Rightarrow \quad \mathbf{A} = \frac{1}{\sqrt{l}}$$
$$\Rightarrow \quad \psi_n(x) = \frac{1}{\sqrt{l}} \cos\left(\frac{n\pi x}{l}\right) \quad \text{and} \quad \psi_m(x) = \frac{1}{\sqrt{l}} \sin\left(\frac{n\pi x}{l}\right)$$

are orthonormal on the interval -l < x < l.

22. (a) Show that if indices of n < 0 where to apply, $a_{-n} = a_n$, and that $a_0 = \frac{1}{l} \int_{-l}^{l} f(x) dx$ for a basic Fourier series.

(b) Show that if indices of n < 0 where to apply, $b_{-n} = -b_n$, and that $b_0 = 0$ for a basic Fourier series.

(c) Express the c_n that are the coefficients of the exponential format of the Fourier series in terms of the basic Fourier coefficients a_n and b_n , and show that $c_0 = a_0/2$.

(d) Demonstrate the equivalence of the basic Fourier series and the exponential format of the Fourier series.

the same period? A Fourier series is a representation of a periodic function as a linear combination of all cosine and sine functions that have the same period. The periodic function f(x) = f(x+2l), has a period of 2l, or repeats itself every 2l. In a basic Fourier series,

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

where the coefficients are

$$a_n = \frac{1}{l} \int_{-l}^{l} f(x) \cos\left(\frac{n\pi x}{l}\right) dx$$
, and $b_n = \frac{1}{l} \int_{-l}^{l} f(x) \sin\left(\frac{n\pi x}{l}\right) dx$,

given that the period is 2l. The Fourier series in a exponential format for a function that is periodic over the length 2l is

$$f(x) = \sum_{-\infty}^{\infty} c_n e^{in\pi x/l}, \quad \text{where} \quad c_n = \frac{1}{2l} \int_{-l}^{l} f(x) e^{-in\pi x/l} dx.$$

Use the defining integrals for a_n , b_n , and c_n , for parts (a), (b), and (c). Cosines are even functions and sines are odd functions. Substituting these results into the summation that defines the exponential form yields the basic Fourier series required for part (d). It is wise to divide the summation into three parts that coincide with the three cases, namely: n < 0 implies a summation from $-\infty$ to -1, n = 0 is one term of the summation, and n > 0 implies a summation from 1 to ∞ . The tricky part is switching the indices on the summation from $-\infty$ to -1. It may require some reflection, but realize that

$$\sum_{-\infty}^{-1} \frac{1}{2} (a_n - ib_n) e^{in\pi x/l} = \sum_{1}^{\infty} \frac{1}{2} (a_n + ib_n) e^{-in\pi x/l}.$$

(a)
$$a_{-n} = \frac{1}{l} \int_{-l}^{l} f(x) \cos\left(\frac{-n\pi x}{l}\right) dx = \frac{1}{l} \int_{-l}^{l} f(x) \cos\left(\frac{n\pi x}{l}\right) dx = a_{n},$$

and $a_{0} = \frac{1}{l} \int_{-l}^{l} f(x) \cos(0) dx = \frac{1}{l} \int_{-l}^{l} f(x) dx.$
(b) $b_{-n} = \frac{1}{l} \int_{-l}^{l} f(x) \sin\left(\frac{-n\pi x}{l}\right) dx = -\frac{1}{l} \int_{-l}^{l} f(x) \sin\left(\frac{n\pi x}{l}\right) dx = -b_{n},$

(c)
$$c_{n} = \frac{1}{2l} \int_{-l}^{l} f(x) e^{-in\pi x/l} dx = \frac{1}{2l} \int_{-l}^{l} f(x) \sin(0) dx = 0.$$

$$= \frac{1}{2l} \int_{-l}^{l} f(x) e^{-in\pi x/l} dx = \frac{1}{2l} \int_{-l}^{l} f(x) \left[\cos\left(\frac{n\pi x}{l}\right) - i\sin\left(\frac{n\pi x}{l}\right) \right] dx$$

$$= \frac{1}{2l} \int_{-l}^{l} f(x) \cos\left(\frac{n\pi x}{l}\right) dx - \frac{i}{2l} \int_{-l}^{l} f(x) \sin\left(\frac{n\pi x}{l}\right) dx = \frac{1}{2} (a_{n} - ib_{n})$$
Where $n = 0$, the component of the componential is zero.

When n = 0, the argument of the exponential is zero, so

$$c_0 = \frac{1}{2l} \int_{-l}^{l} f(x) e^0 dx = \frac{1}{2l} \int_{-l}^{l} f(x) dx = \frac{1}{2} a_0$$

(d) For convenience, let $\theta = \pi x/l$. The summation is

$$f(x) = \sum_{-\infty}^{\infty} c_n e^{in\theta} = \sum_{-\infty}^{-1} \frac{1}{2} (a_n - ib_n) e^{in\theta} + \frac{1}{2} a_0 + \sum_{1}^{\infty} \frac{1}{2} (a_n - ib_n) e^{in\theta}$$

$$= \frac{1}{2} a_0 + \sum_{1}^{\infty} \left(\frac{a_n}{2} + \frac{ib_n}{2}\right) e^{-in\theta} + \sum_{1}^{\infty} \left(\frac{a_n}{2} - \frac{ib_n}{2}\right) e^{in\theta}$$
(1)

$$= \frac{1}{2} a_0 + \sum_{1}^{\infty} \left(\frac{a_n}{2} e^{-in\theta} + \frac{ib_n}{2} e^{-in\theta} + \frac{a_n}{2} e^{in\theta} - \frac{ib_n}{2} e^{in\theta}\right)$$

$$= \frac{1}{2} a_0 + \sum_{1}^{\infty} \left(\frac{a_n}{2} \cos n\theta - \frac{a_n}{2} i \sin/n\theta + \frac{ib_n}{2} \cos/n\theta + \frac{b_n}{2} \sin n\theta + \frac{a_n}{2} \cos n\theta + \frac{a_n}{2} i \sin/n\theta - \frac{ib_n}{2} \cos/n\theta + \frac{b_n}{2} \sin n\theta\right)$$
(2)

$$= \frac{1}{2} a_0 + \sum_{1}^{\infty} (a_n \cos n\theta + b_n \sin n\theta)$$

which is identical to the basic Fourier series upon the substitution of $\theta = \pi x/l$. We have used the results of parts (a) and (b) in equation (1). The sign of the argument of the first exponential in equation (1) changes because we have changed the sign of the index of the summation. The signs of the fourth and eighth terms in the summation of equation (2) are correct because both include factors of $i \cdot i = -1$.

Postscript: The cosine and sine functions are orthogonal over a finite interval, say -l < x < l, and can be made orthonormal on that interval as demonstrated in problem 21. Orthonormal vectors or orthonormal functions constitute a basis. Any function can be expressed in terms of a linear combination of the vectors, or in this case, the functions that constitute the basis.

The infinite square well, also known as a particle in a box, uses the orthogonal cosine and sine functions as a basis.

The exponential format of the Fourier series is often called **complex Fourier series**. We are interested in the complex Fourier series because it is the form that is most easily generalized to the **Fourier integral**.

23. Sketch the graphs of the following functions and their the Fourier transforms.

(a)
$$f(x) = \begin{cases} 1, & -a < x < a, \\ 0, & \text{elsewhere,} \end{cases}$$
 and (b) $f_1(x) = \begin{cases} 1/2, & -b < x < b, \\ 0, & \text{elsewhere,} \end{cases}$ where $b = 2a$

Fourier integrals are generalizations of Fourier series. A Fourier integral is a representation of a non-periodic function that may be regarded as the limit of the Fourier series as the period approaches infinity. Two Fourier transforms compose the Fourier integral. Fourier transforms are the objects that we want to develop further for quantum mechanical calculation. We refer the reader to Byron and Fuller⁶, or your favorite text on mathematical physics for greater depth. In the limit of $l \to \infty$, the complex Fourier series becomes

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

The function f(x) is the Fourier transform of g(k), and g(k) is the Fourier transform of f(x). Substitution of one transform into the other expressing the combination as one relation, *i.e.*,

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x') e^{-ikx'} dx' \right) e^{ikx} dk$$
$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} f(x') e^{ik(x-x')} dx' \quad \text{is the Fourier integral}$$

The functions given for parts (a) and (b) are constants for specified intervals and zero elsewhere which means that you can find g(k) and $g_1(k)$ by integrating between -a and a, and -b and b instead of using infinite limits. Express your answer for part (b) in terms of the constant a and look for relations between the graphs of parts (a) and (b). This problem uses constant functions which are among the easiest functions to integrate both as an appropriate place to start and to highlight relations between parts (a) and (b) for which we provide comment in the postscript.

(a)
$$g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \int_{-a}^{a} f(x) e^{-ikx} dx$$
$$= \frac{1}{\sqrt{2\pi}} \frac{1}{(-ik)} e^{-ikx} \Big|_{-a}^{a} = \frac{1}{\sqrt{2\pi}} \frac{e^{-ika} - e^{ika}}{-ik}$$
$$= \frac{2}{\sqrt{2\pi} k} \frac{e^{-ika} - e^{ika}}{-2i} = \frac{2}{\sqrt{2\pi} k} \frac{e^{ika} - e^{-ika}}{2i} = \frac{2}{\sqrt{2\pi}} \frac{\sin(ka)}{k}.$$

The graphs of f(x) and g(k), are

⁶ Byron and Fuller, *Mathematics of Classical and Quantum Physics* (Dover Publications, Inc., New York, 1970), pp. 239–253, 566–570.

Graph of f(x) Graph of g(k)

(b) The Fourier transform of the given function where b = 2a, double the width and half the height, so that the area under the curve is equal for both f(x) and $f_1(x)$, is

$$g_1(k) = \frac{1}{\sqrt{2\pi}} \frac{\sin(kb)}{k} = \frac{1}{\sqrt{2\pi}} \frac{\sin(2ka)}{k}$$

Graph of $f_1(x)$

Graph of $g_1(k)$

Postscript: The graph of $f_1(x)$ is broader than the graph of f(x), but the graph of $g_1(k)$ is sharper than the graph of g(k). If one of the Fourier transforms is distributed and broad, the other will be localized and sharp. This phenomena is a precursor of the Heisenberg uncertainty relations.

While $f_i(x)$ has a limited domain, the domain of $g_i(k)$ is infinite. This is another general feature of Fourier transforms.

24. Derive the Fourier transforms from the complex Fourier series.

The basic Fourier series is useful for introductions and many applications, but the complex Fourier series is the form from which Fourier transforms are most easily attained. This is a challenging problem but provides an opportunity to deepen your understanding of Fourier transforms.

Start with the notation

$$F(y) = \sum_{-\infty}^{\infty} c_n e^{in\pi y/l}, \quad \text{where} \quad c_n = \frac{1}{2l} \int_{-l}^{l} F(y) e^{-in\pi y/l} dy.$$

Substitute the integral form of c_n into the summation. Symmetrize the factor of 1/2l. This means to rearrange the summation so a factor of $1/\sqrt{2l}$ is in both the F(y) and the c_n . You now have F(y) and c_n that are different than originally defined. Change variables by letting $x = \sqrt{\frac{\pi}{l}} y$. Also, let $k_n = n\sqrt{\frac{\pi}{l}}$. You can now find that $\Delta k_n = \sqrt{\frac{\pi}{l}}$ and $\frac{n\pi y}{l} = k_n x$. Redefine $F\left(\sqrt{\frac{l}{\pi}} x\right) = f(x)$. Introduce a new symbol for the coefficients that indicates the

index k_n replaces n', so $c_n \to g_{k_n}$. Finally, let $l \to \infty$, so that the Fourier transforms

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{ikx} dk \quad \text{and} \quad g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \quad \text{are exposed.}$$

$$F(y) = \sum_{n = -\infty}^{\infty} \left(\frac{1}{2l} \int_{-l}^{l} F(y) e^{-in\pi y/l} \, dy \right) e^{in\pi y/l} = \sum_{n = -\infty}^{\infty} \left(\frac{1}{\sqrt{2l}} \int_{-l}^{l} F(y) e^{-in\pi y/l} \, dy \right) \frac{1}{\sqrt{2l}} e^{in\pi y/l}$$

We can now identify a symmetrized function and coefficient as

$$F(y) = \sum_{n = -\infty}^{\infty} c_n \frac{1}{\sqrt{2l}} e^{in\pi y/l} \quad \text{and} \quad c_n = \frac{1}{\sqrt{2l}} \int_{-l}^{l} F(y) e^{-in\pi y/l} \, dy \,. \tag{1}$$

We are going to change variables to $\sqrt{\frac{\pi}{l}}y = x \Rightarrow y = \sqrt{\frac{l}{\pi}}x \Rightarrow dy = \sqrt{\frac{l}{\pi}}dx$. We are also going to use $k_n = n\sqrt{\frac{\pi}{l}} \Rightarrow \Delta k_n = k_{n+1} - k_n = (n+1)\sqrt{\frac{\pi}{l}} - n\sqrt{\frac{\pi}{l}} = \sqrt{\frac{\pi}{l}}$. These substitutions allow us to rewrite a portion of the argument of the exponentials, $\frac{n\pi y}{l} = n\sqrt{\frac{\pi}{l}}\sqrt{\frac{\pi}{l}}y = k_n x$. The difference in the new index is $\Delta k_n = \sqrt{\frac{\pi}{l}} \Rightarrow \frac{\Delta k_n}{\sqrt{2\pi}} = \frac{1}{\sqrt{2l}}$. The limits of the integral become $y = l \Rightarrow x = \sqrt{\frac{\pi}{l}}l = \sqrt{\pi l}$, and $y = -l \Rightarrow x = -\sqrt{\pi l}$. We finally introduce a new symbol for the coefficients that indicates the index is now k_n vice n so $c_n \to g_{k_n}$. Using these substitutions and developments in equation (1),

$$F(y) = F\left(\sqrt{\frac{l}{\pi}}x\right) = \sum_{k_n = -\infty}^{\infty} g_{k_n} \frac{1}{\sqrt{2\pi}} e^{ik_n x} \Delta k_n = \frac{1}{\sqrt{2\pi}} \sum_{k_n = -\infty}^{\infty} g_{k_n} e^{ik_n x} \Delta k_n$$

and
$$g_{k_n} = \frac{1}{\sqrt{2l}} \int_{-\sqrt{\pi l}}^{\sqrt{\pi l}} F\left(\sqrt{\frac{l}{\pi}}x\right) e^{-ik_n x} \sqrt{\frac{l}{\pi}} dx = \frac{1}{\sqrt{2\pi}} \int_{-\sqrt{\pi l}}^{\sqrt{\pi l}} F\left(\sqrt{\frac{l}{\pi}}x\right) e^{-ik_n x} dx$$

define
$$F\left(\sqrt{\frac{l}{\pi}}x\right) = f(x)$$
. Now let the period d were $x = \Delta h = \sqrt{\frac{\pi}{\pi}} + 0$. The

Redefine $F\left(\sqrt{\frac{\iota}{\pi}}x\right) = f(x)$. Now, let the period $l \to \infty \Rightarrow \Delta k_n = \sqrt{\frac{\pi}{l}} \to 0$. The difference between successive $k_n \to 0$ so that k_n assumes all real values and thus becomes a

continuous variable. The summation over discrete k_n becomes an integral over the continuous variable k, the coefficient g_{k_n} becomes a continuous function g(k), the difference Δk_n becomes the differential dk, and

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{ikx} dk \quad \text{and} \quad g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$$

Postscript: The factor of $1/2\pi$ must be in the Fourier integral but it does not need to be symmetrized in the Fourier transforms. Some authors and tables place the entire factor $1/2\pi$ with one integral so that there is no coefficient in front of the other integral. Also, some authors and tables will change the signs of the exponentials from what we have presented. Asymmetric treatment of the factor of $1/2\pi$ and/or use of a different sign convention result in slightly different functional forms for resulting Fourier transforms.

25. Find the momentum space wavefunction corresponding to a position space wavefunction that is Gaussian.

Gaussian wavefunctions are foundational as you will find in chapter 3 and elsewhere. But first, what does it mean to change a wavefunction in position space to a wavefunction in momentum space? It means find the description of a system using an unknown function of the continuous variable momentum starting with the description of the system that is a known function of the continuous variable position. It is a change of basis in the realm of continuous variables. Quantum mechanical Fourier transforms are the means to change from position space to momentum space and vice versa for continuous variables.

The de Broglie relation associates wavelength or wavenumber, and momentum,

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

Substitute p/\hbar for k in both Fourier transforms. This means the differential $dk = dp/\hbar$ in the integral for f(x). Symmetrize the $1/\hbar$ from this differential by placing a factor $1/\sqrt{\hbar}$ in both integrals, and the result is the quantum mechanical form of the Fourier transforms,

$$f(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \widehat{g}(p) e^{ipx/\hbar} dp, \qquad \widehat{g}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} f(x) e^{-ipx/\hbar} dx.$$

The usual use of these relations is to transform a wave function in position space to momentum space (or vice versa), so will be applied

$$\psi\left(x\right) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \widehat{\psi}\left(p\right) e^{ipx/\hbar} \, dp, \qquad \widehat{\psi}\left(p\right) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi\left(x\right) e^{-ipx/\hbar} \, dx \, .$$

There are a number of subtleties associated with the quantum mechanical analog of the Fourier transforms, so our heuristic argument should be regarded as nothing more than a useful mnemonic.

Use $\psi(x) = A e^{-bx^2}$, b > 0, as your position space wavefunction that is Gaussian. Form 3.323.2 from Gradshteyn and Ryzhik,

$$\int_{-\infty}^{\infty} e^{-\alpha^2 x^2 - \beta x} \, dx = \frac{\sqrt{\pi}}{\alpha} \, e^{\beta^2 / 4\alpha^2},$$

should be useful. Do you recognize the functional form of the momentum space wavefunction?

$$\begin{split} \widehat{\psi}\left(p\right) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi\left(x\right) e^{-ipx/\hbar} \, dx = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} A \, e^{-bx^2} \, e^{-ipx/\hbar} \, dx \\ &= \frac{A}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-bx^2 - ipx/\hbar} \, dx \, . \end{split}$$

Using $\alpha = \sqrt{b}$, and $\beta = ip/\hbar$, our integral is

$$\widehat{\psi}(p) = \frac{A}{\sqrt{2\pi\hbar}} \frac{\sqrt{\pi}}{\sqrt{b}} \exp\left(\frac{(ip/\hbar)^2}{4(\sqrt{b})^2}\right) = \frac{A}{\sqrt{2\hbar b}} e^{-p^2/4b\hbar^2}.$$

Postscript: Notice that $\hat{\psi}(p)$ is also an exponential function with a negative argument that is a constant times the independent variable squared. In fact, $\hat{\psi}(p)$ is also a Gaussian wavefunction. The Fourier transform of a Gaussian function is another Gaussian function.

26. Given $|\psi\rangle$ such that $\langle x | \psi \rangle = \psi(x) = A e^{ik_0 x}$, $-\frac{4\pi}{k_0} \langle x \langle \frac{4\pi}{k_0} \rangle$, and 0 otherwise,

- (a) normalize $\psi(x)$,
- (b) find $\widehat{\psi}(p)$, and
- (c) sketch $\psi(x)$ and $\widehat{\psi}(p)$.

The physical system described by $|\psi\rangle$ is a plane wave confined to a one dimensional "box," also known as a one-dimensional infinite square well. Part (a) means to solve for the constant A using the normalization condition on the interval to which the system is confined. In other words, the confinement allows you to use $-4\pi/k_0$ and $4\pi/k_0$ as the limits of integration. Of course, an unconfined plane wave cannot be normalized. Again, you need only to integrate between the limits of $-4\pi/k_0$ and $4\pi/k_0$ for part (b). "Sketch" means to understand the shape of the curves. Draw or plot only the real part of $\psi(x)$. Set the normalization constants, k_0 , and \hbar equal to 1 to get the shapes of $\psi(x)$ and $\hat{\psi}(p)$. You should find that the real part of $\psi(x)$ is an evenly distributed cosine curve but that $\hat{\psi}(p)$ is distinctly peaked.

(a) The calculus-based form of the normalization condition on the interval given is

$$\begin{split} 1 &= \int_{-4\pi/k_0}^{4\pi/k_0} \mathbf{A}^* \, e^{-ik_0 x} \, \mathbf{A} \, e^{ik_0 x} \, dx = \, |\mathbf{A}|^2 \int_{-4\pi/k_0}^{4\pi/k_0} e^0 \, dx = \, |\mathbf{A}|^2 \int_{-4\pi/k_0}^{4\pi/k_0} dx \\ &= |\mathbf{A}|^2 \left(x \Big|_{-4\pi/k_0}^{4\pi/k_0} \right) = \, |\mathbf{A}|^2 \left(\frac{4\pi}{k_0} - \frac{4\pi}{k_0} \right) = \, |\mathbf{A}|^2 \frac{8\pi}{k_0} \quad \Rightarrow \quad \mathbf{A} = \sqrt{\frac{k_0}{8\pi}} \\ \Rightarrow \quad \psi \left(x \right) = \sqrt{\frac{k_0}{8\pi}} \, e^{ik_0 x} = \frac{1}{2} \sqrt{\frac{k_0}{2\pi}} \, e^{ik_0 x} \, . \end{split}$$

(b)
$$\hat{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar} dx = \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{2} \sqrt{\frac{k_0}{2\pi}} \int_{-4\pi/k_0}^{4\pi/k_0} e^{ik_0 x} e^{-ipx/\hbar} dx$$

after substituting the results of part (a). So

$$\begin{split} \widehat{\psi}(p) &= \frac{1}{4\pi} \sqrt{\frac{k_0}{\hbar}} \int_{-4\pi/k_0}^{4\pi/k_0} e^{i(k_0 - p/\hbar)x} dx = \frac{1}{4\pi} \sqrt{\frac{k_0}{\hbar}} \frac{1}{i(k_0 - p/\hbar)} e^{i(k_0 - p/\hbar)x} \Big|_{-4\pi/k_0}^{4\pi/k_0} \\ &= \frac{1}{4\pi} \sqrt{\frac{k_0}{\hbar}} \frac{1}{i(k_0 - p/\hbar)} \left(e^{i(k_0 - p/\hbar)(4\pi/k_0)} - e^{i(k_0 - p/\hbar)(-4\pi/k_0)} \right) \\ &= \frac{1}{2\pi} \sqrt{\frac{k_0}{\hbar}} \frac{1}{2i(k_0 - p/\hbar)} \left(e^{i4\pi(1 - p/k_0\hbar)} - e^{-i4\pi(1 - p/k_0\hbar)} \right) \\ &= \frac{1}{2\pi} \sqrt{\frac{1}{k_0\hbar}} \frac{1}{(1 - p/k_0\hbar)} \frac{e^{i4\pi(1 - p/k_0\hbar)} - e^{-i4\pi(1 - p/k_0\hbar)}}{2i} \\ &= \frac{1}{2\pi} \sqrt{\frac{1}{k_0\hbar}} \frac{\sin 4\pi (1 - p/k_0\hbar)}{(1 - p/k_0\hbar)} \Rightarrow \quad \widehat{\psi}(p) = 2\sqrt{\frac{1}{k_0\hbar}} \frac{\sin \left(4\pi - \frac{4\pi p}{k_0\hbar}\right)}{\left(4\pi - \frac{4\pi p}{k_0\hbar}\right)}. \end{split}$$

The region of confinement is $-\infty in momentum space.$

(c)

Sketch of $\psi(x)$

Sketch of $\widehat{\psi}(p)$

Postscript: The advantage of casting $\widehat{\psi}(p)$ in this form is that a sine divided by the argument of the sine is a **sinc function**, which is used to model numerous systems.

- 27. Given $|\psi\rangle$ such that $\langle p|\psi\rangle = \widehat{\psi}(p) = \frac{\hbar \sin\left(\frac{ap}{\hbar}\right)}{p}$, $a \in \mathbf{R}$, (a) normalize $\widehat{\psi}(p)$, (b) find $\psi(x)$, and
- (c) sketch $\widehat{\psi}(p)$ and $\psi(x)$.

The only real difference in this problem from the last is that it emphasizes momentum space. Though most of the developments that you will encounter in this and other books are in position space, momentum space can be a preferred environment. It is useful to recognize even or odd functions and composite functions. Again, a function such that f(x) = f(-x), like a cosine, is said to be even. A function such that f(x) = -f(-x), like a sine, is said to be odd. An even function times another even function, or an odd function times another odd function is an even composite function. An even function times an odd function is an odd composite function. Most functions and composite functions are neither even nor odd, for instance, e^x is neither even nor odd. However, when this even/odd type of symmetry does exist, there are some useful techniques that are applicable. For instance, the integral of an odd function is is twice the same integral between the limits of zero and the upper limit.

Two integrals are of interest. Form 611 from the 30th edition of the CRC tables,

$$\int_0^\infty \frac{\sin\left(ax\right)}{x^2} \, dx = \frac{\pi \left|a\right|}{2}$$

for part (a). Assume that a > 0 so that you do not have to carry the absolute value symbols. If you change variables to $y = \frac{ap}{\hbar}$, you will find that the above integral is useful for application of the normalization condition, given that you have used the even/odd function arguments correctly. The second integral of interest is

$$\int_0^\infty \frac{\sin bx \cos cx}{x} \, dx = \begin{cases} 0, & c > b > 0, \\ \pi/2, & b > c > 0, \\ \pi/4, & b = c > 0, \end{cases}$$

from the 30th edition of the CRC tables, form 615. If you correctly apply the quantum mechanical Fourier transform, the Euler equation $e^{i\theta} = \cos \theta + i \sin \theta$, and the even/odd function arguments for the integrals, you should find

$$\psi\left(x\right) = \frac{1}{\pi\hbar} \sqrt{\frac{2}{a}} \int_{0}^{\infty} \frac{\sin\left(\frac{ap}{\hbar}\right) \cos\left(\frac{px}{\hbar}\right)}{p/\hbar} dp$$

which can be caste into the desired form by changing variables using $y = p/\hbar$.

(a) The normalization condition in momentum space is

$$1 = \int_{-\infty}^{\infty} \widehat{\psi}^*(p) \operatorname{A}^* \operatorname{A} \widehat{\psi}(p) dp = |\operatorname{A}|^2 \int_{-\infty}^{\infty} \frac{\hbar \sin\left(\frac{ap}{\hbar}\right)}{p} \frac{\hbar \sin\left(\frac{ap}{\hbar}\right)}{p} dp$$
$$= |\operatorname{A}|^2 \int_{-\infty}^{\infty} \frac{\hbar^2 \sin^2\left(\frac{ap}{\hbar}\right)}{p^2} dp = |\operatorname{A}|^2 a^2 \int_{-\infty}^{\infty} \frac{\sin^2\left(\frac{ap}{\hbar}\right)}{\frac{a^2p^2}{\hbar^2}} dp.$$

Let $y = \frac{ap}{\hbar} \Rightarrow dy = \frac{a}{\hbar} dp \Rightarrow dp = \frac{\hbar}{a} dy$, and integral limits are identical,

$$\Rightarrow 1 = |\mathbf{A}|^2 a\hbar \int_{-\infty}^{\infty} \frac{\sin^2(y)}{y^2} dy = |\mathbf{A}|^2 2a\hbar \int_{0}^{\infty} \frac{\sin^2(y)}{y^2} dy = |\mathbf{A}|^2 2a\hbar \frac{\pi}{2} \Rightarrow \mathbf{A} = \frac{1}{\sqrt{a\pi\hbar}}$$

$$\widehat{\psi}(p) = \frac{1}{\sqrt{a\pi\hbar}} \frac{\hbar \sin\left(\frac{ap}{\hbar}\right)}{p}.$$

(b) The wavefunction in position space is

$$\begin{split} \psi\left(x\right) &= \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{\sqrt{a\pi\hbar}} \int_{-\infty}^{\infty} \frac{\hbar \sin\left(\frac{ap}{\hbar}\right)}{p} e^{ipx/\hbar} \, dp \\ &= \frac{1}{\pi\hbar} \frac{1}{\sqrt{2a}} \int_{-\infty}^{\infty} \frac{\sin\left(\frac{ap}{\hbar}\right)}{p/\hbar} \left[\cos\left(\frac{px}{\hbar}\right) + i\sin\left(\frac{px}{\hbar}\right)\right] \, dp \\ &= \frac{1}{\pi\hbar} \frac{1}{\sqrt{2a}} \int_{-\infty}^{\infty} \frac{\sin\left(\frac{ap}{\hbar}\right) \cos\left(\frac{px}{\hbar}\right)}{p/\hbar} \, dp + \frac{1}{\pi\hbar} \frac{1}{\sqrt{2a}} \int_{-\infty}^{\infty} \frac{\sin\left(\frac{ap}{\hbar}\right) \sin\left(\frac{px}{\hbar}\right)}{p/\hbar} \, dp \end{split}$$

where the last integral is zero because the product of three odd functions is an odd function, both sines and 1/p are odd functions, and the integral of an odd integrand between symmetric limits is zero. The other integrand is the product of two odd and one even function so is an even function. An even integrand between symmetric limits is twice the integral from zero to the upper limit so

$$\psi(x) = \frac{1}{\pi\hbar} \frac{2}{\sqrt{2a}} \int_0^\infty \frac{\sin\left(\frac{ap}{\hbar}\right)\cos\left(\frac{px}{\hbar}\right)}{p/\hbar} dp.$$

Changing variables to $y = \frac{p}{\hbar} \Rightarrow p = \hbar y \Rightarrow dp = \hbar dy$, so the limits are the same under the change of variables. Then

$$\psi(x) = \frac{1}{\pi\hbar} \frac{2}{\sqrt{2a}} \int_0^\infty \frac{\sin(ay)\cos(xy)}{y} \hbar \, dy = \begin{cases} 0, & x > a > 0, \\ \frac{1}{\sqrt{2a}}, & a > x > 0, \\ \frac{1}{2\sqrt{2a}}, & a = x > 0. \end{cases}$$

(c) The constant a has the dimension of length because the argument of a sine is dimensionless, which is pertinent to the graph of $\psi(x)$. Graphs look like

Sketch of
$$\widehat{\psi}(p)$$
 Sketch of $\psi(x)$

Postscript: Notice that the momentum space wavefunction given for problem 27 is a sinc function (or can be caste in the form of a sinc function by multiplying top and bottom by a). It shows

that the Fourier transform of a sinc function is a constant function. Constants and sinc functions are related by their Fourier transforms in general.

The position space wavefunction given in problem 26 is a plane wave. The only part that survives the integral transform is the periodic cosine portion. The cosine function is closely enough related to a constant function that its Fourier transform on a finite interval is also a sinc function.

Supplementary Problems

29. Form the outer product of

$$|v\rangle = \begin{pmatrix} 1\\ 2\\ 3 \end{pmatrix}$$
 and $< w | = (2, 3, 4).$

This problem is the mechanics of forming an outer product. See problem 1. Notice that an outer product is an operator.

30. Show that $\mathcal{P}_i^2 = \mathcal{P}_i$ using Dirac notation.

This problem should help familiarize you with both the projection operator and Dirac notation. First, the meaning of \mathcal{P}_i^2 is $\mathcal{P}_i^2 = \mathcal{P}_i \mathcal{P}_i$. An operator with an exponent means to apply that operator the exponent number of times consecutively. Secondly, a projection operator is an outer product, so simply form the outer products in Dirac notation. Lastly, recognize the orthonormality condition within the product that you have written. This "proof" is very short. The use of Dirac notation is often simply an exercise in recognizing the meaning of the symbols.

31. Show that $\langle f | g \rangle$ is invariant under unitary transformation where

$$|f\rangle = \begin{pmatrix} i\\0\\1+i \end{pmatrix} \text{ and } |g\rangle = \begin{pmatrix} 1\\1-i\\2i \end{pmatrix},$$

and the unitary transformation is made from the operator $\mathcal{L}_x = \begin{pmatrix} 0&1&0\\1&0&1\\0&1&0 \end{pmatrix}.$

Invariance is an important property. This problem should provide additional confidence that an inner product is invariant. It should also provide practice in self-consistently transforming vectors though the point of the problem is coordinate independence. This problem is the complex number

analogy of problem 6. You should find that $\langle f | g \rangle = 2 + i$. Problem 24 of part 2 provides the eigenvectors of \mathcal{L}_x which are

$$|-\sqrt{2}\rangle = \frac{1}{2} \begin{pmatrix} 1\\ -\sqrt{2}\\ 1 \end{pmatrix}, \quad |0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\ 0\\ -1 \end{pmatrix}, \quad \text{and} \quad |\sqrt{2}\rangle = \frac{1}{2} \begin{pmatrix} 1\\ \sqrt{2}\\ 1 \end{pmatrix}$$

Form the unitary transformation and its adjoint using these eigenvectors. Then find $\langle f' | = \langle f | \mathcal{U} \text{ and } | g' \rangle = \mathcal{U}^{\dagger} | g \rangle$. The inner product of these vectors is also 2 + i, so $\langle f' | g' \rangle = \langle f | g \rangle$.

32. Evaluate

(a)
$$\int_{-\pi}^{\pi} \sin(\theta) \,\delta\left(\theta - \frac{\pi}{6}\right) d\theta$$

(b)
$$2 \int_{0}^{\infty} \cos(x) \,e^{-x^{2}} \,\delta\left(\theta - \frac{\pi}{2}\right) dx$$

(c)
$$\int \frac{A}{x^{2} + b^{2}} \,\delta\left(x + 1\right) dx$$

(d)
$$\int \frac{\sin(p) \cos(p)}{p} \,\delta\left(p - \frac{\pi}{4}\right) dp$$

Per problem 11, an integral containing a delta function is the value of the integrand evaluated at the point that the argument of the delta function is equal to zero, provided that point is between the limits of the integral. The value of the integral is zero if that point is not within the limits of integration. The integral for parts (c) and (d) have no limits, but are not likely to be indefinite integrals because they contain a delta function. The usual convention is the limits are $-\infty$ and ∞ for a definite integral where the limits are not specified.

33. Show that
$$\int f(x) \delta\left(ax + b(x-c)\right) dx = \frac{1}{a+b} f\left(\frac{bc}{a+b}\right), \quad a, b > 0.$$

This problem is an extension of problem 12. As before, the limits of the integral are negative and positive infinity. Change variables to y = the argument of the delta function, and follow the procedures of problem 12. The qualification that the multiplicative constants are greater than zero means that you have only one case to consider.

There are basically two techniques that are applicable to delta functions—changing variables and integration by parts. Changing variables to make the argument of the delta function a single variable allows the definition and properties of the delta function to be clearly applied.

34. Show that $\delta(x-a)\delta(x-b) = \delta(a-b)$.

This problem should extend your understanding delta functions. The technique used for this problem is unusual. It is neither changing variables nor integrating by parts. It is posed partially to motivate you to visit the realm of the originator of the Dirac delta function⁷.

The delta function is even so $\delta(x-a) = \delta(a-x)$, for instance. Operate on the integral with $\int f(a) da$. Switch the order of integration so that you can do the integration over da which will yield an integral over dx. The resulting integral over dx can be true if and only if x = a, which is equivalent to integrating over a instead of x, so replace x with a. Compare this with the double integral formed by operating with $\int f(a) da$ and the result should emerge. It may be best to see the reference given in footnote 7.

35. Find
$$\int V_0 \left(e^{-2\alpha x} - 2e^{-\alpha x} \right) \delta'(x-a) \, dx$$
.

This problem includes the derivative of a delta function. This potential is realistic and is used to model diatomic molecules where $x = (r - r_0)/r_0$, where r_0 will depend upon the diatomic molecule being modeled. It is known as the **Morse potential**. Calculate the derivative of the function. The integral is the negative of this derivative evaluated at the point where the argument of δ' is zero. You should find that the value of this integral is $2V_0 \alpha \left(e^{-2\alpha a} - e^{-\alpha a}\right)$.

36. Show that

$$\mathcal{B} | a_j \rangle = \sum_{i}^{3} | a_i \rangle b_j \, \delta_{ij} \quad \Rightarrow \quad \mathcal{B} | a_j \rangle = b_j | a_j \rangle \quad \text{using explicit addition.}$$

This problem should increase your familiarity with Dirac notation and convey the fact that a Kronecker delta within a summation has the capability to make a summation "disappear." This technique is used frequently where Dirac notation is employed. Expand the finite summation. The index j can be 1, 2, or 3 in this three dimensional problem. The condition $\delta_{ij} = 1$ only when i = j forces all but one of the three possibilities to be zero for each value of j.

37. Show that

$$\sum_{i}^{2} \sum_{j}^{2} |a_{i}\rangle < a_{i} |\mathcal{B}| a_{j}\rangle < a_{j} |\delta_{ij} = \sum_{i}^{2} |a_{i}\rangle < a_{i} |\mathcal{B}| a_{i}\rangle < a_{i} |$$
 using explicit addition.

This is a toy problem intended to provide insight into how a summation that includes a Kronecker delta is simplified. It is similar to the previous problem. Explicit addition means to write out the terms of the finite sum. This problem may be easier than the last problem because both indices, i and j, are explicitly indicated in the summations so are explicitly indicated in the expansion. If you recognize that $\langle a_i | \mathcal{B} | a_j \rangle$ is a scalar, you can simplify the notation.

⁷ Dirac, The Principles of Quantum Mechanics (Clarendon Press, Oxford, England, 1958), 4th ed., pp. 60.

38. Show that if $|\psi\rangle$ is normalized, so is $|\psi'\rangle = e^{i\phi} |\psi\rangle$.

This problem reinforces the meaning of normalization but also introduces the concept of phase. The factor $e^{i\phi}$ is the phase and the scalar ϕ is the phase angle, though at times the scalar ϕ is called the phase because it is the only portion of the exponential that can vary. You are given $\langle \psi | \psi \rangle = 1$ to show that $\langle \psi' | \psi' \rangle = 1$. Form the bra $\langle \psi' |$ and then the braket $\langle \psi' | \psi' \rangle$ and you should see that the tenet is true.

39. Normalize $\psi(x) = \frac{A}{x^2 + b^2}$.

This problem is practice in the mechanics of normalization. The function is known as a Lorentzian function and has numerous applications. Use the normalization condition where A is a normalization constant. Form 3.249.1 on page 294 of Gradshteyn and Ryzhik is

$$\int_0^\infty \frac{dx}{(x^2 + a^2)^n} = \frac{(2n - 3s)!!}{2(2n - 2)!!} \frac{\pi}{a^{2n - 1}}$$

You need to recognize the even integrand between symmetric limits to use this integral. The double factorial is similar to a single factorial except the factors are reduced by two, that is

$$(2n)!! = (2n)(2n-2)(2n-4)...6 \cdot 4 \cdot 2$$
, or $(2n+1)!! = (2n+1)(2n-1)(2n-3)...5 \cdot 3 \cdot 1$.

The fact that factorials have precedence over multiplication may help with the reduction. You should find that $\psi(x) = \left(\frac{2b^3}{\pi}\right)^{1/2} \frac{1}{x^2 + b^2}$.

40. Show that

- (a) $\psi_n(\phi) = e^{in\phi}$ and $\psi_m(\phi) = e^{im\phi}$ are orthogonal on the interval $-\pi < \phi < \pi$ where n and m are integers.
- (b) Orthormalize $\psi_n(\phi)$ and $\psi_m(\phi)$.

The intent of this problem is similar to problem 21. You will likely find the exponentials easier than the sines and cosines. You need to show that $\langle \psi_n | \psi_n \rangle \neq 0$ and $\langle \psi_m | \psi_m \rangle \neq 0$. You also need to establish that $\langle \psi_n | \psi_m \rangle = 0$ for all integral n and m. Convert the inner products to integrals for the actual calculation since you have functional forms. The limits of the integration are $-\pi$ and π , because that is the region specified. Euler's equation is $e^{ix} = \cos x + i \sin x$, and if you subtract the same relation for the opposite argument $e^{-ix} = \cos x - i \sin x$, and divide by 2i you attain $\sin x = \frac{e^{ix} - e^{-ix}}{2i}$, which is an identity that should be useful.

^{41.} Given $\langle f | = (1, 2, 3)$ and $\langle g | = (4, 5, 6)$, show that $\langle f | g \rangle = 32$ after insertion of the identity two ways.

(a) Show that
$$< f \mid \left(\sum_{1}^{3} |i > < i| \right) \mid g > = 32$$
, and then
(b) show that $\sum_{1}^{3} < f \mid i > < i \mid g > = 32$.

This problem is a discrete space analog intended to persuade that bras and kets can be moved into or out of an integral as done in problem 18. Part (a) means to assemble the identity operator before multiplying by the vectors. Part (b) means to multiply each of the unit vectors that would compose the outer product in part (a) and sum the terms after multiplication is complete. After understanding the process in a three-dimensional space, imagine the same process in an infinite dimensional space where an integral instead of a summation is appropriate. Does the process change because the dimension of the space changes?