Physics 221A
Fall 2010
Notes 4
Spatial Degrees of Freedom

1. Introduction

In these notes we develop the theory of wave functions in configuration space, building it up from the ket formalism and the postulates of quantum mechanics. We assume the particle has no spin or other internal degrees of freedom, or that if such degrees of freedom exist they can be ignored. As pointed out in Sec. 2.5, it is partly a matter of choice of where to stop when looking for a complete set of commuting observables, and in these notes we shall stop with the spatial coordinates $\mathbf{x} = (x, y, z)$, or, in one dimension, simply x.

We then introduce translation operators and use them and the classical correspondence to motivate the definition of momentum in quantum mechanics. We then explore the two representations, position and momentum, and the relationship between them. Finally, we discuss minimum uncertainty wave packets.

2. The Position Representation; Wave Functions

For simplicity we begin with the one-dimensional case. We assume the position x of a particle in one dimension can be measured, and that the results of the measurement are continuous. Thus, we are dealing with the case of the continuous spectrum. We denote the operator corresponding to measuring x by $\hat{x}$, so the eigenvalue-eigenket problem is

$$\hat{x}|x\rangle = x|x\rangle. \tag{1}$$

Here $\hat{x}$ is the operator, x is the eigenvalue, and $|x\rangle$ is the eigenket with eigenvalue x. We are assuming that $\hat{x}$ by itself forms a complete set of commuting observables. Since x belongs to the continuous spectrum, the eigenkets $|x\rangle$ are not normalizable and lie outside Hilbert space.

Since $\hat{x}$ is a complete set of commuting observables, the eigenkets $|x\rangle$ are nondegenerate and form a basis in the Hilbert space in the continuum sense. These eigenkets are only defined by Eq. (1) to within a normalization and a phase. We fix the normalization by requiring

$$\langle x_1|x_2\rangle = \delta(x_1 - x_2). \tag{2}$$

The phase conventions for the eigenkets $|x\rangle$ are a question we shall return to later. Under these assumptions, the resolution of the identity takes the form

$$1 = \int_{-\infty}^{+\infty} dx\, |x\rangle\langle x|. \tag{3}$$

Now let $|\psi\rangle$ represent a normalized (pure) state of the system, let $I = [x_0, x_1]$ be an interval on the x-axis, and let P_I be the corresponding projection operator,

$$P_I = \int_{x_0}^{x_1} dx\, |x\rangle\langle x|. \tag{4}$$

Then, according to the postulates of quantum mechanics (Sec. 2.2), we have

$$\text{Prob}(x_0 \le x \le x_1) = \langle\psi|P_I|\psi\rangle = \int_{x_0}^{x_1} dx\, \langle\psi|x\rangle\langle x|\psi\rangle. \tag{5}$$

We now introduce the definition,

$$\boxed{\psi(x) = \langle x|\psi\rangle,} \tag{6}$$

of the *wave function* $\psi(x)$, whereupon the probability (5) can be written,

$$\text{Prob}(x_0 \le x \le x_1) = \int_{x_0}^{x_1} dx\, |\psi(x)|^2. \tag{7}$$

Since the interval $[x_0, x_1]$ is arbitrary, we see that $|\psi(x)|^2$ must be interpreted as the *probability density* of finding the particle on the x-axis. We have derived wave functions from the ket formalism plus the postulates of quantum mechanics, as promised in Notes 1.

Equation (6) is important because it shows how to go from kets to wave functions. It takes the place of sloppy notation such as Eq. (1.7). To go the other direction, we multiply $|\psi\rangle$ on the left by the resolution of the identity (3),

$$|\psi\rangle = \int dx\, |x\rangle\langle x|\psi\rangle, \tag{8}$$

which, by using Eq. (6), becomes

$$\boxed{|\psi\rangle = \int dx\, |x\rangle\psi(x).} \tag{9}$$

This is the inverse of Eq. (6), allowing one to go from a wave function $\psi(x)$ to the corresponding ket $|\psi\rangle$. We see that $\psi(x)$ is the set of expansion coefficients of the ket $|\psi\rangle$ in the position eigenbasis.

Another consequence of this formalism follows easily. Suppose we have two kets $|\psi\rangle$ and $|\phi\rangle$, and we wish to compute the scalar product $\langle\psi|\phi\rangle$ in wave function language. We simply insert the resolution of the identy (3) between the bra and the ket to obtain,

$$\langle\psi|\phi\rangle = \int dx\, \langle\psi|x\rangle\langle x|\phi\rangle = \int dx\, \psi^*(x)\phi(x), \tag{10}$$

a familiar formula.

This formalism is easily generalized to three dimensions. Let $\mathbf{x}$ be a position vector in three-dimensional space, with components (x, y, z) or (x_1, x_2, x_3). The measurement of the three components of position corresponds to a vector of operators, which we denote by $\hat{\mathbf{x}}$ (with a hat), to distinguish the operators from their eigenvalues (the results of the position measurement). In quantum mechanics, when we speak of a "vector operator" we usually mean a *vector of operators*, in this case three operators $\hat{\mathbf{x}} = (\hat{x}, \hat{y}, \hat{z}) = (\hat{x}_1, \hat{x}_2, \hat{x}_3)$. We assume that the components of $\hat{\mathbf{x}}$ commute with one another,

$$[\hat{x}_i, \hat{x}_j] = 0, \tag{11}$$

which as explained in Notes 2 can be tested experimentally. For example, if we filter a beam in x and then y by means of small slits, or do it in the reverse order, we find that the statistical results of arbitrary measurements on the filtered beam are the same in both cases.

As above we assume that we can ignore any internal degrees of freedom of the particle, so that the three operators $\hat{\mathbf{x}}$ by themselves form a complete set of commuting observables. Then the simultaneous eigenkets of $\hat{\mathbf{x}}$ are nondegenerate and form a basis by themselves. The eigenket-eigenvalue problem is

$$\hat{x}_i|\mathbf{x}\rangle = x_i|\mathbf{x}\rangle, \tag{12}$$

for $i = 1, 2, 3$, a set of three simultaneous equations satisfied by an single eigenket $|\mathbf{x}\rangle = |x, y, z\rangle$, labeled by the three eigenvalues of the three commuting operators. In obvious generalizations of the one-dimensional case, we normalize these kets according to

$$\langle\mathbf{x}_1|\mathbf{x}_2\rangle = \delta^3(\mathbf{x}_1 - \mathbf{x}_2) = \delta(x_1 - x_2)\delta(y_1 - y_2)\delta(z_1 - z_2), \tag{13}$$

we have a resolution of the identity,

$$1 = \int d^3\mathbf{x}\,|\mathbf{x}\rangle\langle\mathbf{x}|, \tag{14}$$

and the transformation between wave functions and kets is given by

$$\psi(\mathbf{x}) = \langle\mathbf{x}|\psi\rangle, \tag{15}$$

and

$$|\psi\rangle = \int d^3\mathbf{x}\,|\mathbf{x}\rangle\psi(\mathbf{x}). \tag{16}$$

Also, the probability that the particle will be found in a region R of three-dimensional space is

$$\int_R d^3\mathbf{x}\,|\psi(\mathbf{x})|^2, \tag{17}$$

so $|\psi(\mathbf{x})|^2$ must be interpreted as the probability density.

Equations (6) or (15) define the *wave function* $\psi(x)$ or $\psi(\mathbf{x})$, respectively, in quantum mechanics. A question that arises sometimes when solving the Schrödinger equation is whether ψ is single-valued. But by our definitions, $\psi(x)$ or $\psi(\mathbf{x})$ is automatically single-valued, since it is just the expansion coefficient of the state $|\psi\rangle$ with respect to the basis $|x\rangle$ or $|\mathbf{x}\rangle$.

Equations (6) and (9) (in one dimension) or (15) and (16) (in three dimensions) make explicit the transformations back and forth between the Hilbert space of ket vectors $|\psi\rangle$ and the Hilbert space of wave functions $\psi(x)$ or $\psi(\mathbf{x})$. As discussed in Sec. 1.3, we regard these two Hilbert spaces as isomorphic but distinct, and we say that the space of wave functions $\psi(x)$ or $\psi(\mathbf{x})$ forms the *configuration representation* of the space of kets $|\psi\rangle$. There are other representations, and while the configuration representation is often used in practice one should note that in the postulates of quantum mechanics there is no privileged role assigned to it. Any calculation that can be carried out in the configuration representation can be carried out in any other representation with the same results from a physical standpoint.

In effect, a representation is merely a choice of basis, allowing one to work with the expansion coefficients of a state vector $|\psi\rangle$ with respect to the chosen basis instead of the abstract ket vectors themselves. As noted below Eq. (9), the configuration space wave function $\psi(x)$ or $\psi(\mathbf{x})$ is the expansion coefficients of the state ket $|\psi\rangle$ with respect to the basis of position eigenkets $\{|x\rangle\}$ or $\{|\mathbf{x}\rangle\}$. In quantum mechanics we frequently choose as a basis the simultaneous eigenkets of a complete set of commuting observables; thus, the basis is labeled by the observables in question, and we speak, for example, of the position representation, momentum representation, etc. Nothing prevents us from using other bases, however (which have no correspondence with any simple set of commuting observables).

Just as the wave function $\psi(x)$ represents the ket vector $|\psi\rangle$ in the configuration representation, so also is there a representation of various operators that act on ket vectors. Consider, for example, the operator $\hat{x}$ (working in one dimension for simplicity). Multiplying Eq. (9) by $\hat{x}$ gives

$$\hat{x}|\psi\rangle = \int dx\, \hat{x}|x\rangle\psi(x) = \int dx\, |x\rangle x\psi(x), \tag{18}$$

showing that the effect of multiplying a ket vector $|\psi\rangle$ by the operator $\hat{x}$ is to multiply the corresponding configuration wave function $\psi(x)$ by x. That is, we can write

$$(\hat{x}\psi)(x) = x\psi(x). \tag{19}$$

As we say, the operator $\hat{x}$ is *represented* by multiplication by x in the configuration representation. It is represented by other operations in other representations. Similarly, in three dimensions we have

$$(\hat{x}_i\psi)(\mathbf{x}) = x_i\psi(\mathbf{x}). \tag{20}$$

You may worry about the physical meaning of the unnormalizable eigenkets $|x\rangle$ or $|\mathbf{x}\rangle$. In reality we never measure the position of a particle exactly, instead the best we can do is to localize it in some small region of space. The eigenkets $|x\rangle$ or $|\mathbf{x}\rangle$ are an idealization of this process, in which the size of the region is allowed to approach zero. This limit also leads to singular mathematics, since the eigenkets $|x\rangle$ or $|\mathbf{x}\rangle$ have infinite norm and do not belong to Hilbert space.

Measuring the position of a particle is really a nonrelativistic concept, because as we localize a particle to smaller and smaller regions, by the uncertainty principle the momentum increases, ultimately taking on relativistic values. Then processes such as the creation of particle-antiparticle pairs come into play, and we are really dealing with a multi-particle situation, which is properly handled by the methods of quantum field theory. We will find in Physics 221B that the position operator for a particle in relativistic quantum mechanics is one that is fraught with difficulties. The position operator is really a nonrelativistic concept.

3. Translation Operators

We now develop translation operators, working initially in one dimension for simplicity. Let a be a displacement. We imagine a displacement operation as one that acts on a physical system, moving all particles from their initial positions (say, x) to their new positions $(x+a)$. This is sometimes called the *active* point of view, because our operations take a given physical system and transform it into a new system, in this case in a different location in space.

In quantum mechanics, we can define a *translation operator* which carries out this operation on a physical system. The translation operator $T(a)$ is a linear operator acting on the Hilbert space of a physical system, parameterized by the displacement a. We define the translation operator in one dimension by

$$T(a)|x\rangle = |x+a\rangle. \tag{21}$$

This definition makes sense, because physically $|x\rangle$ is the state of the system after a measurement has placed the particle in a small region around position x, and similarly for $|x+a\rangle$. Equation (21) is actually a definition of the operators $T(a)$ because the kets $|x\rangle$ form a basis. If we specify the action of a linear operator on a set of basis vectors, then by linear superposition its action on an arbitrary vector becomes known.

Equation (21) gives the action of the translation operator on the position eigenkets. Let us also work out its action on wave functions. Let $|\psi\rangle$ be a state with wave function $\psi(x) = \langle\psi|x\rangle$, and let $|\phi\rangle = T(a)|\psi\rangle$ be the translated state with wave function $\phi(x) = \langle x|\phi\rangle$. What is the relationship between the old wave function $\psi(x)$ and the new one $\phi(x)$? We answer this by writing

$$\begin{aligned}\phi(x) = \langle x|\phi\rangle = \langle x|T(a)|\psi\rangle &= \int dx'\, \langle x|T(a)|x'\rangle\langle x'|\psi\rangle = \int dx'\, \langle x|x'+a\rangle\langle x'|\psi\rangle \\ &= \int dx'\, \delta(x-x'-a)\psi(x') = \psi(x-a),\end{aligned} \tag{22}$$

where we have inserted a resolution of the identity, used Eqs. (21) and (2), and carried out the integral. We write the result as

$$\bigl(T(a)\psi\bigr)(x) = \psi(x-a), \tag{23}$$

where we have replaced ϕ by $T(a)\psi$. This is a companion to Eq. (21), which gives the action of translation operators on the basis kets; this gives their action on wave functions.

There are several remarks concerning Eq. (23). First, notice the minus sign in this equation, compared to the plus sign in Eq. (21). The minus sign is necessary to get a wave function that has been moved forward under the displacement operation, as illustrated in Fig. 1. To remember the signs it helps to write Eq. (22) in the form, $\bigl(T(a)\psi\bigr)(x+a) = \psi(x)$ and to say, "the value of the new wave function at the new point equals the value of the old wave function at the old point."

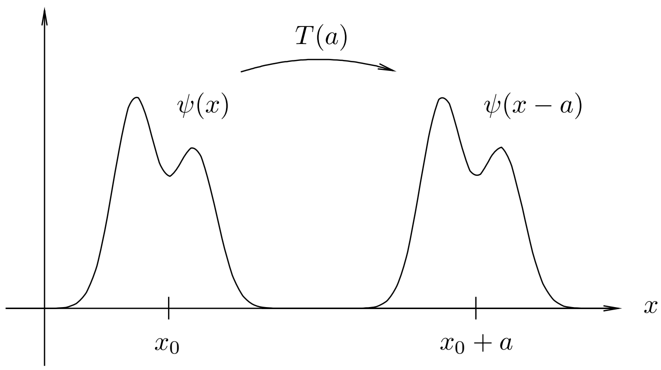

Fig. 1. The action of the translation operator $T(a)$ on a wave function $\psi(x)$.

Another remark is that that Eq. (23) uses the translation operator $T(a)$ in a different sense from its original definition, because it is acting on a configuration space wave function ψ instead of a ket $|\psi\rangle$. As we say, Eq. (23) gives the *representation* of the operator $T(a)$ on configuration space wave functions.

Finally, we remark that many books would write Eq. (23) without the parentheses, that is, as

$$T(a)\psi(x) = \psi(x-a). \tag{24}$$

The problem with this notation is that it is not clear what $T(a)$ acts on. ψ is a function, and $\psi(x)$ is the value of that function at a point x, that is, it is a number. Does $T(a)$ act on the function or the value of the function? Obviously, it acts on the function, which is what the extra parentheses in Eq. (23) make explicit.

The translation operator is easily generalized to three dimensions, where the displacement $\mathbf{a}$ is a vector, and the translation operator is defined by

$$T(\mathbf{a})|\mathbf{x}\rangle = |\mathbf{x}+\mathbf{a}\rangle. \tag{25}$$

The other formulas and results of this section are easily generalized to the three-dimensional case.

4. Properties of the Translation Operators

The translation operators in one dimension satisfy the following properties:

$$T(0) = 1, \tag{26a}$$

$$T(a)T(b) = T(a+b) = T(b)T(a), \tag{26b}$$

$$T(a)^{-1} = T(-a), \tag{26c}$$

$$T(a)^{-1} = T(a)^\dagger. \tag{26d}$$

Property (26a) follows immediately from the definition (21). Property (26b) is the composition law that is also obvious from the definition (21); it can be proved explicitly by writing

$$T(a)T(b)|x\rangle = T(a)|x+b\rangle = |x+b+a\rangle = T(a+b)|x\rangle. \tag{27}$$

Note that the parameter $x+b+a$ of the ket $|x+b+a\rangle$ is just a label of the ket, so these labels obey the usual (commutative) rules for addition. This implies that the translation operators are commutative, as indicated in Eq. (26*b*). The third property (26*c*) is proved by setting $b=-a$ in Eq. (26*b*). The translation operators are invertible. The last property (26*d*) states that the translation operators are unitary. We prove this by letting $\psi(x)$ be an arbitrary wave function, and $|\phi\rangle = T(a)|\psi\rangle$, so that $\phi(x)=\psi(x-a)$. Then

$$\int dx\,|\psi(x)|^2 = \int dx\,|\phi(x)|^2 = \int dx\,|\psi(x-a)|^2, \tag{28}$$

as we prove by substituting $x'=x-a$ in the last integral. Thus, $T(a)$ preserves the norm of arbitrary states. But a linear operator that does this is necessarily unitary (see Prob. 1.5(c)).

Altogether, properties (26*a*)–(26*d*) qualify the set of translation operators as a group of unitary operators. Unitary operators appear frequently in symmetry operations because these are the only linear operators that preserve probabilities (hence, the results of physical measurements). In this case, the group is *Abelian*, which simply means that the translation operators commute with one another (property (26*b*)).

5. The Generator of Translations

A simple idea that arises in symmetry operations is that a given, finite symmetry operation can be built up as a composition of smaller symmetry operations. For example, a displacement of one meter is the composition of a thousand displacements of one millimeter. In the limit we can imagine a finite symmetry operation as being built up out of an infinite number of infinitesimal symmetry operations. For this reason, special attention is attached to infinitesimal symmetry operations. It turns out that infinitesimal versions of unitary symmetry operators in quantum mechanics are always expressible in terms of certain Hermitian operators, which are called the *generators* of the symmetry. We will now see how this works out in the case of translations.

Thinking of a small displacement a, we expand the translation operator $T(a)$ in a Taylor series in powers of a. This series begins with

$$T(a) = T(0) + a\frac{dT}{da}(0) + \ldots. \tag{29}$$

The first (zeroth order) term is $T(0)=1$, and as for the second (first order) term, we notice that $dT/da|_{a=0}$ does not depend on a so it is some operator with no parameters. We put this into a more convenient form by defining

$$\hat{k} = i\frac{dT}{da}(0), \tag{30}$$

where the hat emphasizes that $\hat{k}$ is an operator (in contrast to a, which is a number).

In these notes we frequently use a hat to distinguish an operator from an ordinary number, or from the classical counterpart of the operator. We normally omit the hat when there is no danger of confusion (for example, T above is an operator, but we put no hat on it). But we also use the hat for unit vectors, and certain other purposes. It is hoped that the meaning of the hat in any individual case will be clear from the context.

Through first order, we can write the expansion of the translation operator as

$$T(a) = 1 - ia\hat{k} + \ldots. \tag{31}$$

We have split off a factor of i in the definition (30) so that $\hat{k}$ will be Hermitian. This follows when we use Eq. (31) to write out the series for $T(a)^\dagger$ and $T(-a) = T(a)^{-1}$:

$$\begin{aligned} T(a)^\dagger &= 1 + ia\hat{k}^\dagger + \ldots, \\ T(-a) &= 1 + ia\hat{k} + \ldots, \end{aligned} \tag{32}$$

which by Eqs. (26c) and (26d) must be equal. But this implies

$$\hat{k} = \hat{k}^\dagger. \tag{33}$$

The Hermitian operator $\hat{k}$ appears in the first correction term in Eq. (31), which, when a is small, is an infinitesimal translation. For this reason $\hat{k}$ is regarded as the *generator* of translations in one dimension. As yet we have no physical interpretation for $\hat{k}$, but since it is Hermitian it must correspond to the measurement of some physical quantity. We will see in a moment what that is.

We have only written out the first two terms in the Taylor series (31) for $T(a)$, but the entire series can be summed and put into a neat form. To do this we will obtain a differential equation for $T(a)$ and then solve it. We first write out the definition of the derivative of $T(a)$ as a limit,

$$\frac{dT(a)}{da} = \lim_{\epsilon\to 0} \frac{T(a+\epsilon) - T(a)}{\epsilon}. \tag{34}$$

By Eq. (26b), the first term in the numerator can be written as $T(\epsilon)T(a)$, which allows the operator $T(a)$ to be factored out of the entire numerator to the right:

$$\frac{dT(a)}{da} = \Bigl(\lim_{\epsilon\to 0} \frac{T(\epsilon) - 1}{\epsilon}\Bigr) T(a). \tag{35}$$

But the remaining limit is just the derivative $dT(a)/da$ evaluated at $a = 0$, which by Eq. (30) is $-i\hat{k}$. Altogether, we obtain

$$\frac{dT(a)}{da} = -i\hat{k}\,T(a), \tag{36}$$

a differential equation that we must solve subject to the initial conditions $T(0) = 1$. The solution is immediate,

$$T(a) = \exp(-ia\hat{k}). \tag{37}$$

Now we can easily extend the power series (31) to higher order,

$$T(a) = 1 - ia\hat{k} - \frac{1}{2}a^2\hat{k}^2 + \ldots. \tag{38}$$

We see that the generator of translations $\hat{k}$, which first appeared in infinitesimal translation operators, also appears in the exponential form for finite translation operators.

It is easy to work out the action of $\hat{k}$ on the basis kets $|x\rangle$. We simply write

$$\hat{k}|x\rangle = i\frac{dT(a)}{da}|x\rangle\Big|_{a=0} = i\frac{d}{da}|x+a\rangle\Big|_{a=0} = i\frac{d}{dx}|x\rangle. \tag{39}$$

The derivative of the ket $|x\rangle$ may look strange. In wave function language it is the derivative of a δ-function.

We obtain an equivalent result that looks more familiar by working out the action of $\hat{k}$ on a wave function. The procedure is the same:

$$(\hat{k}\psi)(x) = i\Big(\frac{dT(a)}{da}\psi\Big)(x)\Big|_{a=0} = i\frac{d}{da}\psi(x-a)\Big|_{a=0} = -i\frac{d\psi(x)}{dx}. \tag{40}$$

We start to see the appearance of the usual momentum operator on wave functions.

6. Translations in Three Dimensions, and Commutation Relations

In a similar manner, for translation operators in three dimensions we define

$$\hat{k}_i = i\frac{\partial T(\mathbf{a})}{\partial a_i}\Big|_{\mathbf{a}=0}, \tag{41}$$

where $i = 1, 2, 3$. This gives us a Hermitian vector operator (that is, a vector of Hermitian operators) $\hat{\mathbf{k}}$, with components $\hat{k}_i$, $i = 1, 2, 3$. Now the exponential form of the translation operator is

$$T(\mathbf{a}) = \exp(-i\mathbf{a}\cdot\hat{\mathbf{k}}) = 1 - i\mathbf{a}\cdot\hat{\mathbf{k}} - \frac{1}{2}(\mathbf{a}\cdot\hat{\mathbf{k}})^2 + \ldots. \tag{42}$$

This series can be used to obtain the commutation relations of the operators $\hat{\mathbf{k}} = (\hat{k}_1, \hat{k}_2, \hat{k}_3)$. We expand the product $T(\mathbf{a})T(\mathbf{b})$ in power series, carrying everything to second order,

$$\begin{aligned} T(\mathbf{a})T(\mathbf{b}) &= \Big[1 - i(\mathbf{a}\cdot\hat{\mathbf{k}}) - \frac{1}{2}(\mathbf{a}\cdot\hat{\mathbf{k}})^2 + \ldots\Big]\Big[1 - i(\mathbf{b}\cdot\hat{\mathbf{k}}) - \frac{1}{2}(\mathbf{b}\cdot\hat{\mathbf{k}})^2 + \ldots\Big] \\ &= 1 - i(\mathbf{a}+\mathbf{b})\cdot\hat{\mathbf{k}} - \frac{1}{2}(\mathbf{a}\cdot\hat{\mathbf{k}})^2 - (\mathbf{a}\cdot\hat{\mathbf{k}})(\mathbf{b}\cdot\hat{\mathbf{k}}) - \frac{1}{2}(\mathbf{b}\cdot\hat{\mathbf{k}})^2 + \ldots. \end{aligned} \tag{43}$$

But since $T(\mathbf{a})T(\mathbf{b}) = T(\mathbf{b})T(\mathbf{a})$, the answer must be the same if we swap $\mathbf{a}$ and $\mathbf{b}$. Most of the series is obviously symmetric in $\mathbf{a}$ and $\mathbf{b}$, but the one term $(\mathbf{a}\cdot\hat{\mathbf{k}})(\mathbf{b}\cdot\hat{\mathbf{k}})$ is not. When we subtract the swapped series from the original series, we obtain a vanishing commutator,

$$[\mathbf{a}\cdot\hat{\mathbf{k}}, \mathbf{b}\cdot\hat{\mathbf{k}}] = 0. \tag{44}$$

Since this is true for all choices of $\mathbf{a}$ and $\mathbf{b}$, we can choose each of these vectors to be one of the unit vectors along the coordinate axes (nine choices in all), and we find

$$[\hat{k}_i, \hat{k}_j] = 0. \tag{45}$$

We see that $\hat{\mathbf{k}}$ is a vector of commuting, Hermitian operators.

The relations (39) and (40) are also easily generalized to three dimensions. These give

$$\hat{k}_i|\mathbf{x}\rangle = i\frac{\partial}{\partial x_i}|\mathbf{x}\rangle, \tag{46}$$

and

$$\big(\hat{k}_i\psi\big)(\mathbf{x}) = -i\frac{\partial\psi(\mathbf{x})}{\partial x_i}, \tag{47}$$

or, in vector notation,

$$\big(\hat{\mathbf{k}}\psi\big)(\mathbf{x}) = -i\nabla\psi(\mathbf{x}). \tag{48}$$

It is also easy to work out the commutation relations among the operators $\hat{x}_i$ and $\hat{k}_j$. We just apply them to a wave function in opposite orders, obtaining

$$\begin{aligned} \hat{x}_i\hat{k}_j\psi &= x_i\Big(-i\frac{\partial}{\partial x_j}\Big)\psi = -ix_i\frac{\partial\psi}{\partial x_j}, \\ \hat{k}_j\hat{x}_i\psi &= \Big(-i\frac{\partial}{\partial x_j}\Big)x_i\psi = -i\,\delta_{ij}\,\psi - ix_i\frac{\partial\psi}{\partial x_j}. \end{aligned} \tag{49}$$

Subtracting these, we find

$$[\hat{x}_i, \hat{k}_j] = i\,\delta_{ij}. \tag{50}$$

Combined with Eqs. (11) and (45), this gives a complete set of commutation relations among the components of the operators $\hat{\mathbf{x}}$ and $\hat{\mathbf{k}}$.

7. The Momentum in Classical Mechanics

We shall make a few remarks about the momentum in classical mechanics, in preparation for our discussion of the momentum in quantum mechanics.

As explained in Sec. B.12, there is more than one definition of the momentum of classical mechanics. One is the *kinetic momentum*,

$$\mathbf{p} = m\dot{\mathbf{x}}, \tag{51}$$

and the other is the *canonical momentum*,

$$\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{x}}}, \tag{52}$$

where L is the Lagrangian. In the case of a particle of charge q moving in static electric and magnetic fields $\mathbf{E} = -\nabla\phi$ and $\mathbf{B} = \nabla\times\mathbf{A}$, the Lagrangian is given by Eq. (B.44), reproduced here,

$$L(\mathbf{x}, \dot{\mathbf{x}}) = \frac{m}{2}|\dot{\mathbf{x}}|^2 - q\phi(\mathbf{x}) + \frac{q}{c}\dot{\mathbf{x}}\cdot\mathbf{A}(\mathbf{x}), \tag{53}$$

so the canonical momentum is given by Eq. (B.48), reproduced here,

$$\mathbf{p} = m\dot{\mathbf{x}} + \frac{q}{c}\mathbf{A}(\mathbf{x}). \tag{54}$$

In the presence of a magnetic field (more precisely, in the presence of a vector potential) the definitions of the classical momentum (51) and (52) are not the same. We have not defined the momentum operator in quantum mechanics yet, but before we do, we must ask which of these two classical momenta will it correspond to, the kinetic or the canonical?

In several respects the canonical momentum can be regarded as more fundamental than the kinetic momentum. For example, the momentum $\mathbf{p}$ that occurs in classical Hamiltonians $H(\mathbf{x},\mathbf{p})$ is the canonical momentum. For another example, in classical mechanics there is a general relationship between symmetries and invariants (that is, constants of the motion), called *Noether's theorem*. According to this theorem, a system whose Lagrangian is invariant under translations in a direction $\mathbf{n}$ (a unit vector) possesses a conserved quantity, which is the component of the momentum in the given direction, $\mathbf{n}\cdot\mathbf{p}$. If the Lagrangian is invariant under all translations, then the entire momentum $\mathbf{p}$ is conserved (all three components). But it is the canonical momentum, not the kinetic, that is conserved (in cases where it makes a difference).

For yet another example, it is customary to regard the momentum in classical mechanics as the *generator* of translations. For example, if $f(\mathbf{x},\mathbf{p})$ is a function on phase space (a classical observable), then we can define a classical translation operator $T_{\rm cl}(\mathbf{a})$, parameterized by a displacement $\mathbf{a}$, by

$$\big(T_{\rm cl}(\mathbf{a})f\big)(\mathbf{x},\mathbf{p}) = f(\mathbf{x}-\mathbf{a},\mathbf{p}). \tag{55}$$

This operator moves the function $f(\mathbf{x},\mathbf{p})$ forward in $\mathbf{x}$ while leaving $\mathbf{p}$ alone. If $\mathbf{a}$ is an infinitesimal displacement, then the result can be expanded to first order,

$$\big(T_{\rm cl}(\mathbf{a})f\big)(\mathbf{x},\mathbf{p}) = f(\mathbf{x},\mathbf{p}) - \mathbf{a}\cdot\frac{\partial f}{\partial \mathbf{x}}. \tag{56}$$

But the correction term can be written as a Poisson bracket,

$$-\mathbf{a}\cdot\frac{\partial f}{\partial \mathbf{x}} = \{\mathbf{a}\cdot\mathbf{p}, f\}. \tag{57}$$

Thus, the effect of the infinitesimal translation $\mathbf{a}$ on a function can be obtained by forming the Poisson bracket of $\mathbf{a}\cdot\mathbf{p}$ with that function, and adding to the original function. Since a finite displacement can be regarded as being built up out of a large number of infinitesimal displacements, the function $\mathbf{a}\cdot\mathbf{p}$ is regarded as the generator of displacements in the $\mathbf{a}$ direction. But the use of the Poisson bracket in Eq. (57) requires that the momentum be the canonical momentum, not the kinetic.

If $\mathbf{a}$ is not small, then the translation operator $T_{\rm cl}(\mathbf{a})$ can be represented by an exponential series of iterated Poisson brackets. One notation for this is

$$T_{\rm cl}(\mathbf{a}) = e^{:\mathbf{a}\cdot\mathbf{p}:}, \tag{58}$$

where the notation $:A:$ (for any classical observable A) means the operator that acts on function $B(\mathbf{x},\mathbf{p})$ by forming the Poisson bracket:

$$:A:B = \{A, B\}. \tag{59}$$

The Poisson bracket representation for the translation operators and Noether's theorem for systems invariant under translations are closely related. It would take us too far afield (into classical mechanics) to go into these matters here, but there are some lessons we should take away from this discussion for the development of quantum mechanics. First, the momentum in quantum mechanics should correspond to the canonical momentum in classical mechanics, not the kinetic. Second, it is desirable in building up the structure of quantum mechanics to preserve as much of the classical relationship between symmetries and invariants as possible. For example, this will mean that the momentum is conserved in the case of a free particle (because the system is invariant under translations). Thus we will require that the momentum in quantum mechanics be the generator of translations in quantum mechanics, in some appropriate sense.

8. The Momentum in Quantum Mechanics

The operator $\hat{\mathbf{k}}$ is regarded as the generator of displacements in quantum mechanics, since by Eq. (31) it provides the small correction necessary when an infinitesimal displacement is carried out. Finite displacements can be regarded as the composition of a large number of infinitesimal displacements. Also, as noted, $\hat{\mathbf{k}}$ corresponds to the measurement of some physical quantity, and both $\hat{\mathbf{k}}$ and $\mathbf{p}$ (the latter being the generator of translations in classical mechanics) are vectors. So the suspicion arises that $\hat{\mathbf{k}}$ is related to the momentum operator in quantum mechanics, call it $\hat{\mathbf{p}}$ (as yet undefined, but the hat means "operator"). The vector operators $\hat{\mathbf{k}}$ and $\hat{\mathbf{p}}$ cannot be equal, however, because they have different units: $\hat{\mathbf{k}}$ has units of inverse length, and $\hat{\mathbf{p}}$ has units of momentum. To make the units come out right we guess that there is a proportionality factor between $\hat{\mathbf{p}}$ and $\hat{\mathbf{k}}$ with units of action, a constant that we call $\hbar$:

$$\hat{\mathbf{p}} = \hbar\hat{\mathbf{k}}. \tag{60}$$

We take this as the definition of momentum in quantum mechanics.

The postulates of quantum mechanics do not tell us what quantum operator corresponds to a given classical quantity, so we must not think that the definition of momentum $\hat{\mathbf{p}}$ is engraved in stone. The best we can do is to find a vector of operators in quantum mechanics that has properties similar to the classical momentum and that goes over to the classical momentum in the classical limit. In fact, the similarity with the classical momentum (as the generator of translations) has motivated the definition (60), and, as for the classical limit and the other expected properties of momentum, they will be laid bare as we proceed.

9. The Constant $\hbar$

Notice that $\hbar$ did not appear in the postulates of quantum mechanics; it appears for the first time in our development of the formalism in Eq. (60). The value of $\hbar$ must be determined experimentally. The discussion so far has been based on the analysis of a single particle moving in three-dimensional space, so one might question whether different particles have different values of $\hbar$. We would not get the usual classical limit if this were so, so it seems theoretically doubtful that there are different values of $\hbar$, but it is a question that can be tested experimentally (all the $\hbar$'s turn out to be the same to within experimental accuracy). The relation (60) implies the usual de Broglie relation connecting momentum and wavelength,

$$\lambda = \frac{2\pi\hbar}{p}, \tag{61}$$

as we shall show momentarily, so the value of $\hbar$ can be determined by measuring the de Broglie wavelength of a particle of a known momentum. The most elegant experiments along these lines have involved Bragg diffraction of a neutron beam from a single, large (about 10cm) silicon crystal with no dislocations or grain boundaries. The manufacture of such crystals has become feasible with modern semiconductor technology. The predictions of the relation (60) are fully confirmed. Actually, if Eq. (60) were not correct, there are very few of the theoretical predictions of quantum mechanics that would agree with experiment.

The silicon neutron interferometer just mentioned was used in the 1970's to measure the phase shift of neutron wave functions as the neutrons fall in the earth's gravitational field. The experiment and results are discussed in Sakurai. This was the first demonstration that gravitational potentials enter the Schrödinger equation in the same manner as other potentials.

The fact that $\hbar$ is a universal constant was known to Planck and others in the 1890's, even before quantum mechanics existed. Planck knew that a constant with dimensions of action must occur in the expression for the spectrum of black body radiation, even before the correct expression was known. He also realized that $h = 2\pi\hbar$, c and G (Newton's constant of gravitation) could be combined to create a natural system of units for distance, time and mass. The Planck unit of distance is

$$L_{\text{Planck}} = \sqrt{\frac{\hbar G}{c^3}} = 1.6 \times 10^{-33}\text{cm}. \tag{62}$$

It is the length scale at which the effects of both quantum mechanics and gravity are expected to be important. Physics at such scales is currently a matter of much speculation, and is likely to remain so for some time, in view of the near impossibility of direct experimental tests. Nevertheless the importance of the length scale itself has been known for a long time.

10. Properties of the Momentum

We will provisionally accept the definition (60) of the momentum operator in quantum mechanics, and proceed to examine the consequences. First, the translation operators can now be written in the form,

$$T(\mathbf{a}) = \exp\Big[-\frac{i}{\hbar}(\mathbf{a}\cdot\hat{\mathbf{p}})\Big] = 1 - \frac{i}{\hbar}(\mathbf{a}\cdot\hat{\mathbf{p}}) + \ldots. \tag{63}$$

The various commutation relations we have evaluated may now be expressed in terms of $\hat{\mathbf{p}}$ instead of $\hat{\mathbf{k}}$ and gathered together in one place,

$$[\hat{x}_i, \hat{x}_j] = 0, \tag{64a}$$

$$[\hat{x}_i, \hat{p}_j] = i\hbar\, \delta_{ij}, \tag{64b}$$

$$[\hat{p}_i, \hat{p}_j] = 0. \tag{64c}$$

These are the Heisenberg-Born commutation relations. They may be compared to the classical canonical Poisson bracket relations, Eqs. (B.82).

Also, the properties (46) and (48) of the operators $\hat{\mathbf{k}}$ are easily translated into the properties of the momentum. We have

$$\hat{\mathbf{p}}|\mathbf{x}\rangle = i\hbar\nabla|\mathbf{x}\rangle, \tag{65}$$

and

$$(\hat{\mathbf{p}}\psi)(\mathbf{x}) = -i\hbar\nabla\psi(\mathbf{x}), \tag{66}$$

Equation (65) gives the action of the momentum operator in ket language, whereas Eq. (66) gives it in the position representation. It has other forms in other representations.

11. The Momentum Representation

Because $\hat{\mathbf{p}}$ is a vector of commuting, Hermitian operators, these operators possess a simultaneous eigenbasis. We write the eigenvalue-eigenket problem for momentum in the form,

$$\hat{\mathbf{p}}|\mathbf{p}\rangle = \mathbf{p}|\mathbf{p}\rangle. \tag{67}$$

We solve this in the configuration representation, that is, we multiply Eq. (67) on the left by the bra $\langle\mathbf{x}|$, define the wave function of the momentum eigenket $|\mathbf{p}\rangle$ by

$$\psi_{\mathbf{p}}(\mathbf{x}) = \langle\mathbf{x}|\mathbf{p}\rangle, \tag{68}$$

and use Eq. (66) to obtain

$$-i\hbar\nabla\psi_{\mathbf{p}}(\mathbf{x}) = \mathbf{p}\psi_{\mathbf{p}}(\mathbf{x}). \tag{69}$$

Thus, $\psi_{\mathbf{p}}(\mathbf{x})$ is the eigenfunction of the differential operator $-i\hbar\nabla$ (really three commuting differential operators) with eigenvalue $\mathbf{p}$. The solution exists for all values of $\mathbf{p}$ and is unique to within a constant,

$$\psi_{\mathbf{p}}(\mathbf{x}) = Ae^{i\mathbf{p}\cdot\mathbf{x}/\hbar}, \tag{70}$$

where A is a normalization and a phase. Thus, momentum has a continuous spectrum, so we normalize the eigenstates according to

$$\langle\mathbf{p}_1|\mathbf{p}_2\rangle = \delta^3(\mathbf{p}_1 - \mathbf{p}_2). \tag{71}$$

Using the integral

$$\int d^3\mathbf{x}\, e^{i(\mathbf{p}_2-\mathbf{p}_1)\cdot\mathbf{x}/\hbar} = (2\pi\hbar)^3\delta(\mathbf{p}_1 - \mathbf{p}_2), \tag{72}$$

the normalization constant A in Eq. (70) is determined to within a phase, which we fix by demanding that A be real and positive. The result is

$$\boxed{\langle \mathbf{x}|\mathbf{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}}\, e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}.} \tag{73}$$

The eigenfunctions of momentum are plane waves, whose wave length is given by the de Broglie relation (61).

Since the momentum eigenstates are nondegenerate, the momentum operators $\hat{\mathbf{p}}$ form a complete set of commuting observables, and we may speak of the *momentum representation.* The resolution of the identity in this representation is

$$1 = \int d^3\mathbf{p}\, |\mathbf{p}\rangle\langle\mathbf{p}|. \tag{74}$$

We will denote the wave function of the state $|\psi\rangle$ in the momentum representation by

$$\phi(\mathbf{p}) = \langle \mathbf{p}|\psi\rangle \tag{75}$$

(compare Eq. (15) for the configuration representation), so that by multiplying Eq. (74) onto the ket $|\psi\rangle$ we obtain

$$|\psi\rangle = \int d^3\mathbf{p}\, |\mathbf{p}\rangle\phi(\mathbf{p}), \tag{76}$$

similar to Eq. (16) in the configuration representation. The wave function $\phi(\mathbf{p})$ is the expansion coefficients of the state $|\psi\rangle$ with respect to the momentum eigenbasis $\{|\mathbf{p}\rangle\}$.

By using Eq. (73) and resolutions of the identity it is easy to switch back and forth between wave functions $\psi(\mathbf{x})$ and $\phi(\mathbf{p})$, representing the same quantum state in two different representations. For example, we have

$$\psi(\mathbf{x}) = \langle \mathbf{x}|\psi\rangle = \int d^3\mathbf{p}\, \langle\mathbf{x}|\mathbf{p}\rangle\langle\mathbf{p}|\psi\rangle = \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^{3/2}}\, e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}\, \phi(\mathbf{p}), \tag{77}$$

and its inverse,

$$\phi(\mathbf{p}) = \int \frac{d^3\mathbf{x}}{(2\pi\hbar)^{3/2}}\, e^{-i\mathbf{p}\cdot\mathbf{x}/\hbar}\, \psi(\mathbf{x}). \tag{78}$$

The wave functions $\psi(\mathbf{x})$ and $\phi(\mathbf{p})$ are Fourier transforms of one another, modulo the insertion of factors of $\hbar$ to account for the physical units.

In the momentum representation, the operator $\hat{\mathbf{p}}$ is represented simply by multiplication by $\mathbf{p}$, the vector of c-numbers. That is, if $\phi(\mathbf{p})$ is given in terms of the state $|\psi\rangle$ by Eq. (75), then the momentum space wave function of the state $\hat{\mathbf{p}}|\psi\rangle$ is

$$\langle\mathbf{p}|\hat{\mathbf{p}}|\psi\rangle = \mathbf{p}\langle\mathbf{p}|\psi\rangle = \mathbf{p}\,\phi(\mathbf{p}), \tag{79}$$

where we have allowed $\hat{\mathbf{p}}$ to act to the left on the bra $\langle\mathbf{p}|$, bringing out the eigenvalue $\mathbf{p}$. We can write this as

$$(\hat{\mathbf{p}}\phi)(\mathbf{p}) = \mathbf{p}\phi(\mathbf{p}). \tag{80}$$

Similarly, the operator $\hat{\mathbf{x}}$ in the momentum representation is given by

$$(\hat{\mathbf{x}}\phi)(\mathbf{p}) = i\hbar \frac{\partial \phi(\mathbf{p})}{\partial \mathbf{p}}. \tag{81}$$

Compare this to Eq. (66), and notice the difference in sign. This follows since if $\phi(\mathbf{p})$ is related to $|\psi\rangle$ by Eq. (75), then what we mean by the left-hand side of Eq. (81) is

$$\begin{aligned}\langle \mathbf{p}|\hat{\mathbf{x}}|\psi\rangle &= \int d^3\mathbf{x}\, \langle \mathbf{p}|\mathbf{x}\rangle\langle \mathbf{x}|\hat{\mathbf{x}}|\psi\rangle = \int \frac{d^3\mathbf{x}}{(2\pi\hbar)^{3/2}}\, e^{-i\mathbf{p}\cdot\mathbf{x}/\hbar}\, \mathbf{x}\psi(\mathbf{x}) \\ &= i\hbar \frac{\partial}{\partial \mathbf{p}} \int \frac{d^3\mathbf{x}}{(2\pi\hbar)^{3/2}}\, \psi(\mathbf{x}) = i\hbar \frac{\partial \phi(\mathbf{p})}{\partial \mathbf{p}}.\end{aligned} \tag{82}$$

12. Multiparticle Wave Functions

In a system of N particles, the positions of the individual particles are independent observables that commute with one another, so a complete set (ignoring spin for now) consists of the operators $(\hat{\mathbf{x}}_1, \ldots, \hat{\mathbf{x}}_N)$, with eigenvalues $(\mathbf{x}_1, \ldots, \mathbf{x}_N)$. In this case the wave function is defined by

$$\psi(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \langle \mathbf{x}_1, \ldots, \mathbf{x}_N|\psi\rangle. \tag{83}$$

The wave function is defined over configuration space, that is, the space in which a single point specifies the positions of all the particles. This is the same configuration space as in classical mechanics, which is discussed in Sec. B.3. Configuration space coincides with physical space only in the case of a single particle. Similarly, one can define a multiparticle, momentum space wave function $\phi(\mathbf{p}_1, \ldots, \mathbf{p}_N)$.

13. The Sign of i

The following is a remark concerning the the definition of $\hat{\mathbf{k}}$ in Eq. (30), which led to the definition of momentum in Eq. (60). We split off a factor of i in Eq. (30) to make $\hat{\mathbf{k}}$ Hermitian, but the same would have been achieved if we had split off $-i$ (thereby changing the definition of $\hat{\mathbf{k}}$ by a sign). This would lead to the opposite sign in the definition of $\hat{\mathbf{p}}$, and changes in signs in many of the subsequent formulas. Would this change lead to any physical consequences or contradictions with experiment?

The answer is no, but it would change most of the familiar formulas in quantum mechanics, by replacing i by $-i$. For example, a plane wave with wave vector $\mathbf{k}$ would become $e^{-i\mathbf{k}\cdot\mathbf{x}}$ instead of the usual $e^{i\mathbf{k}\cdot\mathbf{x}}$. It is a matter of convention to choose the sign of i in quantum mechanics, and our choice has been made in Eqs. (30) and (60). Once this choice has been made, however, then the sign of the Pauli matrix σ_y is determined, so that spin angular momentum has the same commutation relations as orbital angular momentum. This was a question addressed in Prob. 3.2(d).

14. Minimum Uncertainty Wave Packets

Let us loosely define a *wave packet* in one dimension as a wave function $\psi(x)$ whose dispersions Δx and Δp, defined as in Sec. 2.7 by

$$\begin{aligned}(\Delta x)^2 &= \langle \hat{x}^2\rangle - \langle \hat{x}\rangle^2,\\ (\Delta p)^2 &= \langle \hat{p}^2\rangle - \langle \hat{p}\rangle^2,\end{aligned} \tag{84}$$

are small, that is, close to the minimum values allowed by the inequality,

$$\Delta x \Delta p \ge \frac{\hbar}{2}. \tag{85}$$

See Eq. (2.50). Similarly, let us define a *minimum uncertainty wave packet* as one for which the product $\Delta x\Delta p$ takes on its minimum value of $\hbar/2$.

Let $\psi(x)$ be a normalized, minimum uncertainty wave packet with

$$\begin{aligned}\langle\psi|\hat{x}|\psi\rangle &= \langle\hat{x}\rangle = 0,\\ \langle\psi|\hat{p}|\psi\rangle &= \langle\hat{p}\rangle = 0,\end{aligned} \tag{86}$$

and let $\Delta x = L$, so that $\Delta p = \hbar/2L$. Now let

$$|\zeta\rangle = \Bigl(\hat{x} + \frac{2iL^2}{\hbar}\hat{p}\Bigr)|\psi\rangle. \tag{87}$$

The operator appearing on the right seems to have been pulled out of the air, but it is a version of an annihilation operator of the general form $\hat{x} + i\hat{p}$, with coefficients adjusted to make the following argument come out right. We will see such annihilation operators again when we discuss the harmonic oscillator. The result of Eq. (87) is

$$\langle\zeta|\zeta\rangle = \langle\hat{x}^2\rangle + \frac{2iL^2}{\hbar}\langle\hat{x}\hat{p} - \hat{p}\hat{x}\rangle + \frac{4L^2}{\hbar^2}\langle\hat{p}^2\rangle = L^2 - 2L^2 + L^2 = 0. \tag{88}$$

Then $|\zeta\rangle = 0$, so Eq. (87) in wave function language becomes

$$2L^2\frac{d\psi}{dx} + x\psi = 0, \tag{89}$$

which has the normalized solution,

$$\psi(x) = \frac{1}{\sqrt{L\sqrt{2\pi}}}\, e^{-x^2/4L^2}. \tag{90}$$

The minimum uncertainty wave packet is a Gaussian. If we allow $\langle\hat{x}\rangle = a$ and $\langle\mathbf{p}\rangle = b$ to take on arbitrary values a, b as shown, then we find

$$\psi(x) = \frac{1}{\sqrt{L\sqrt{2\pi}}}\exp\Bigl[-\frac{(x-a)^2}{4L^2} + i\frac{b(x-a)}{\hbar} + i\gamma\Bigr], \tag{91}$$

where γ is a phase. The wave packet is still a Gaussian, but it has been shifted in position and momentum.

Problems

1. In this problem we denote operators with a hat, as in $\hat{x}$ or $\hat{A}$, and we denote eigenvalues or classical quantities without a hat, as in x or $A(x,p)$. We work in one dimension, and think of a wave function $\psi(x)$ or $\psi(x,t)$.

If $\hat{A}$ is an operator, we define the *Weyl transform* of $\hat{A}$, denoted $A(x,p)$, by

$$A(x,p)=\int_{-\infty}^{+\infty} ds\, e^{-ips/\hbar}\,\langle x+s/2|\hat{A}|x-s/2\rangle. \tag{4}$$

Here the notation $|x-s/2\rangle$, for example, means the eigenket of $\hat{x}$ with eigenvalue $x-s/2$. It is useful to think of $A(x,p)$ as a function defined on the classical (x,p) phase space which is in some sense the classical observable corresponding to the quantum operator $\hat{A}$.

(a) Show that if $A(x,p)$ is the Weyl transform of operator $\hat{A}$, then $A(x,p)^*$ is the Weyl transform of $\hat{A}^\dagger$. In particular, this shows that the Weyl transform of a Hermitian operator is a real function on phase space.

(b) Show that if operators $\hat{A}$ and $\hat{B}$ have Weyl transforms $A(x,p)$ and $B(x,p)$, respectively, then

$$\mathrm{tr}(\hat{A}^\dagger\hat{B})=\int\frac{dx\,dp}{2\pi\hbar}\,A(x,p)^*B(x,p). \tag{5}$$

Notice how the right hand side looks like the "scalar product" of two classical observables on phase space.

(c) Find the Weyl transforms of the following operators: 1 (the identity operator); $\hat{x}$; $\hat{p}$; $\hat{x}\hat{p}$; $\hat{p}\hat{x}$; $\hat{p}^2/2m+V(\hat{x})$.

(d) Let $W(x,p)$ be the Weyl transform of the density operator $\hat{\rho}$. Since $\hat{\rho}$ is Hermitian, $W(x,p)$ is real. Interpret the integrals

$$\int_{-\infty}^{\infty} dx\,W(x,p) \qquad \text{and} \qquad \int_{-\infty}^{\infty} dp\,W(x,p), \tag{6}$$

physically and compare to the corresponding integrals of $\rho(x,p)$ in classical statistical mechanics, where ρ is the classical probability density in phase space.

Now some comments. These results suggest that $W(x,p)$ is a distribution function of particles in phase space whose statistics reproduces the statistics inherent in quantum measurement. Unlike a classical distribution function $\rho(x,p)$, however, $W(x,p)$ can take on negative values. These "negative probabilities" have no meaning in any statistical sense, but they only arise, in a certain sense, when we attempt to measure x and p simultaneously to a precision greater than that allowed by the uncertainty principle.