

1 Transformations and Dirac

Certain operations are required to preserve probability *amplitudes*. Examples are spacial translations and rigid rotations. Regardless of the fact that classical and quantum mechanics are different, we demand that physics be unchanged upon carrying out certain simple operations. The way this is implemented is what is different between classical and quantum mechanics. Preservation of probability amplitudes is the quantum requirement.

Spacial Translations We will start with spacial translations as the simplest case. Suppose we have a quantum state $|\Psi\rangle$ for which $\langle x|\Psi\rangle$ is a “lump” centered at $x = 0$. We want to perform a spacial translation by a , giving a transformed state $|\Psi'\rangle$. We write

$$|\Psi'\rangle = U(a)|\Psi\rangle, \quad (1)$$

where $U(a)$ is a *unitary* transformation. The unitary property of U will guarantee preservation of probability amplitudes. We require

$$\langle \Phi|\Psi\rangle = \langle \Phi|\Psi'\rangle. \quad (2)$$

Now if

$$\begin{aligned} |\Psi'\rangle &= U(a)|\Psi\rangle \\ |\Phi'\rangle &= U(a)|\Phi\rangle, \end{aligned} \quad (3)$$

we have

$$\langle \Phi'|\Psi'\rangle = \langle \Phi|U^\dagger U|\Psi\rangle = \langle \Phi|\Psi\rangle, \quad (4)$$

where we used

$$\langle \Phi'| = \langle U\Phi| = \langle \Phi|U^\dagger,$$

which easily follows from the definition of adjoint.

We want to investigate the translation operator $U(a)$. This operator must satisfy the following requirements:

$$U(a) \longrightarrow I, \quad a \rightarrow 0,$$

and

$$U(a_1 + a_2) = U(a_1)U(a_2).$$

Together these two requirements are demanding that a translation can be built up out of smaller steps, e.g. to translate $1nm$ we can do 10 steps, each of one \AA .

Let us return to our lump. How are $\langle x|\Psi\rangle$ and $\langle x|\Psi'\rangle$ related? We can see what the result must be by simply drawing a picture, with $\langle x|\Psi\rangle$ a blob centered near $x = 0$ and $\langle x|\Psi'\rangle$ a blob centered near $x = a$. We satisfy the common sense requirement of a rigid translation by writing the following equation,

$$\langle x - a|\Psi\rangle = \langle x|\Psi'\rangle. \quad (5)$$

To see that Eq.(5) is correct, substitute $x = a$ in both sides. In both cases, we are at the center of the “lump.” Note that Eq.(5) is really a common sense requirement. If $|\Psi' \rangle$ is really a rigid translation of $|\Psi \rangle$ by an amount a , then Eq.(5) has to hold.

As to the *form* of $U(a)$, all of our requirements on $U(a)$ will be satisfied if we write

$$U(a) = \exp(-i\frac{a}{\hbar}P), \quad (6)$$

where P is a self-adjoint operator. It is generally true that if

$$T = \exp(A),$$

then

$$T^\dagger = \exp(A^\dagger).$$

This can be shown by expanding T out in an exponential series, and taking the adjoint term by term. Let us write a few terms for U and U^\dagger . We have

$$\begin{aligned} U(a) &= I - i\frac{a}{\hbar}P + \frac{1}{2}\left(\frac{-ia}{\hbar}\right)^2 PP + \dots \\ U^\dagger(a) &= I + i\frac{a}{\hbar}P + \frac{1}{2}\left(\frac{ia}{\hbar}\right)^2 PP + \dots \end{aligned} \quad (7)$$

In going from U to U^\dagger we have used two properties of adjoints; $(\alpha T)^\dagger = \alpha^* T^\dagger$, and $(T_1 T_2)^\dagger = T_2^\dagger T_1^\dagger$. Let us quickly show the latter using old notation. We have

$$(\phi, T_1 T_2 \psi) = (T_1^\dagger \phi, T_2 \psi) = (T_2^\dagger T_1^\dagger \phi, \psi) = ((T_1 T_2)^\dagger \phi, \psi).$$

The last equality gives the desired result. So we have that

$$U^\dagger(a) = \exp(i\frac{a}{\hbar}P). \quad (8)$$

But comparing to $U(a)$, we see that $U^\dagger(a)$ just has the sign in front of a reversed, meaning the inverse of $U(a)$, so we have

$$U^\dagger(a)U(a) = I, \quad (9)$$

which is the unitarity requirement.

So if we take U in the form of Eq.(6), we have unitarity and $U(a) \rightarrow I$, as $a \rightarrow 0$. Finally let us write out $U(a_1 + a_2) = U(a_1)U(a_2)$. We have

$$\exp(-i\frac{a_1}{\hbar}P) \exp(-i\frac{a_2}{\hbar}P) = \exp(-i\frac{a_1 + a_2}{\hbar}P). \quad (10)$$

This equation looks OK if we can add exponents as we do with numbers. Since both exponentials involve the *same operator* P , adding exponents *is valid* here. When the operators in the exponents are *different*, simply adding exponents is *not valid* in general, but if the operators are the same as they are here, it is valid.

So our proposed form for $U(a)$ satisfies all the general requirements we can impose. We can learn more by returning to Eq.(5) and taking a small and working to linear order in a . We may write

$$\langle x - a | \Psi \rangle = \langle x | \Psi \rangle - a \frac{\partial}{\partial x} \langle x | \Psi \rangle + \dots \quad (11)$$

and

$$\langle x | \Psi' \rangle = \langle x | I - i \frac{a}{\hbar} P + \dots | \Psi \rangle = \langle x | \Psi \rangle - i \frac{a}{\hbar} \langle x | P | \Psi \rangle + \dots \quad (12)$$

Matching $O(a)$ terms, we have

$$\langle x | P | \Psi \rangle = \frac{\hbar}{i} \frac{\partial}{\partial x} \langle x | \Psi \rangle. \quad (13)$$

This is a familiar looking equation. So far we have said nothing about the physical meaning of the operator P . Instead, we have imposed general requirements. Before further discussion of the physical meaning of P , let us generalize to more than one dimension.

Suppose we have a particle moving in two dimensions, the x and y directions. We can now translate in either or both directions. A basic fact about translations is that translations in different directions *commute*. Let a_x be the amount of the translation in the x -direction, and a_y for the y -direction. We must have

$$U(a_x)U(a_y) = U(a_y)U(a_x), \quad (14)$$

where now each direction has its own generator;

$$\begin{aligned} U(a_x) &= \exp(-i \frac{a_x}{\hbar} P_x) \\ U(a_y) &= \exp(-i \frac{a_y}{\hbar} P_y). \end{aligned} \quad (15)$$

Now we said previously that it was OK to add exponents if we have the same operator in the two exponents. Here we have two different operators. The more general statement is

$$\exp(A) \exp(B) = \exp(A + B) \quad (16)$$

iff $AB = BA$, or A and B *commute*. Now if $P_x P_y = P_y P_x$, we will have the desired property

$$U(a_x)U(a_y) = U(a_y)U(a_x) = \exp(-\frac{i}{\hbar}(a_x P_x + a_y P_y)) \quad (17)$$

so we can translate in different orders, or just perform one direct translation.

Now by studying small a_y and expanding to linear order, we can find that

$$\langle x, y | P_y | \Psi \rangle = \frac{\hbar}{i} \frac{\partial}{\partial y} \langle x, y | \Psi \rangle \quad (18)$$

along with

$$\langle x, y | P_x | \Psi \rangle = \frac{\hbar}{i} \frac{\partial}{\partial x} \langle x, y | \Psi \rangle \quad (19)$$

Clearly in three dimensions, we will have

$$\langle \vec{x} | \vec{P} | \Psi \rangle = \frac{\hbar}{i} \vec{\nabla} \langle \vec{x} | \Psi \rangle \quad (20)$$

Finally for many particles, we must translate *all* of them, and we have

$$\langle \vec{x}_1, \vec{x}_2, \dots | \vec{P} | \Psi \rangle = \frac{\hbar}{i} \left(\sum_{j=1}^n \vec{\nabla}_j \right) \langle \vec{x}_1, \vec{x}_2, \dots | \Psi \rangle . \quad (21)$$

Finally, let us convince ourselves that \vec{P} is in fact the total linear momentum. We will carry out the discussion for one particle in three dimensions. We again invoke experiment and de Broglie's ideas to say we can expand in plane waves of definite momentum, so

$$\langle \vec{x} | \Psi \rangle = \int \langle \vec{x} | \vec{p} \rangle \langle \vec{p} | \Psi \rangle d^3 \vec{p} \quad (22)$$

Here \vec{p} is really momentum, following the chain of logic that experiments like Davisson Germer imply that $\vec{p} = \hbar \vec{k}$. Let us use our results on \vec{P} to write

$$\langle \vec{x} | \vec{P} | \Psi \rangle = \frac{\hbar}{i} \vec{\nabla} \int \langle \vec{x} | \vec{p} \rangle \langle \vec{p} | \Psi \rangle d^3 \vec{p} = \int \langle \vec{x} | \vec{p} \rangle \vec{p} \langle \vec{p} | \Psi \rangle d^3 \vec{p} \quad (23)$$

Inserting a complete set of momentum eigenstates on the left hand side, we have

$$\int \langle \vec{x} | \vec{P} | \vec{p} \rangle \langle \vec{p} | \Psi \rangle d^3 \vec{p} = \int \langle \vec{x} | \vec{p} \rangle \vec{p} \langle \vec{p} | \Psi \rangle d^3 \vec{p} \quad (24)$$

which implies that

$$\vec{P} | \vec{p} \rangle = \vec{p} | \vec{p} \rangle, \quad (25)$$

so in fact \vec{P} is the linear momentum after all.

Time Translation Time translation is one case where we do want to take the *passive* viewpoint. That is, we simply want to let the system evolve in time,

$$| \Psi \rangle \longrightarrow | \Psi(t) \rangle .$$

As before, we want to preserve probability amplitudes, or

$$\langle \Phi | \Psi \rangle = \langle \Phi(t) | \Psi(t) \rangle .$$

What we are saying here is, if we have an undisturbed system, the amplitude to find $|\Phi\rangle$ in $|\Psi\rangle$ at time t must be the same as it is now. A unitary operator will guarantee that property. If we have

$$\begin{aligned} |\Psi(t)\rangle &= U(t)|\Psi\rangle \\ |\Phi(t)\rangle &= U(t)|\Phi\rangle, \end{aligned} \tag{26}$$

then

$$\langle \Phi(t)|\Psi(t)\rangle = \langle U\Phi|U\Psi\rangle = \langle \Phi|U^\dagger U|\Psi\rangle = \langle \Phi|\Psi\rangle.$$

We again use the general form

$$U(t) = \exp\left(-\frac{i}{\hbar}Ht\right) \tag{27}$$

where H is a self-adjoint operator. This form will guarantee that $U(t) \rightarrow I$ as $t \rightarrow 0$, and

$$U(t_1 + t_2) = U(t_1)U(t_2).$$

Let us derive a differential equation by considering small times. For simplicity, we consider a system with only one coordinate, x . We have

$$\langle x|\Psi(t + \epsilon)\rangle = \langle x|U(\epsilon)|\Psi(t)\rangle,$$

where $|\Psi(t)\rangle = U(t)|\Psi\rangle$. Expanding to $O(\epsilon)$, we have

$$\langle x|\Psi(t)\rangle + \epsilon \frac{\partial}{\partial t} \langle x|\Psi(t)\rangle + \dots = \langle x|\Psi(t)\rangle - \frac{i}{\hbar} \epsilon \langle x|H|\Psi(t)\rangle.$$

Matching the coefficient of ϵ on both sides, we have

$$i\hbar \frac{\partial}{\partial t} \langle x|\Psi(t)\rangle = \langle x|H|\Psi(t)\rangle. \tag{28}$$

The argument just given is *very general*. It is based solely on conservation of probability amplitudes. No matter how complicated our system is, we can assert that

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H|\Psi(t)\rangle.$$

There is nothing in the above that requires that H be independent of time. Conservation of probability amplitudes has nothing to do with conservation of energy, so H can have explicit dependence on time. This would occur for example in a system acted upon by an external, time-dependent field. **NOTE** When there is explicit time dependence in H , Eq.(28) continues to hold, but Eq.(27) needs generalization. For now, we will assume no external forces on our system, so we have a closed system. For this case, H will be an operator with no explicit time dependence.

The line of argument just presented does not specify what H is, it merely says if we are going to preserve probability amplitudes, a self-adjoint H must exist. Further, it does not (yet) relate H to the physical quantity, energy. Here appeal to experiment must be used. Einstein-Planck tell us that frequency is related to energy up to a factor of Planck's constant. From our equation, an eigenstate of H will produce a term in $|\Psi(t)\rangle$ which moves with a definite frequency, and we then can conclude that H must be an operator whose eigenstates have definite *energy*. More explicitly, suppose we have an eigenstate of H ,

$$H|\Psi\rangle = E|\Psi\rangle,$$

with $\langle\Psi|\Psi\rangle = 1$, and of course E is real since H is self-adjoint. Then $U(t)$ acting on this state gives

$$U(t)|\Psi\rangle = \exp(-\frac{i}{\hbar}Ht)|\Psi\rangle = \exp(-\frac{i}{\hbar}Et)|\Psi\rangle,$$

so this state moves with a definite frequency $\hbar\omega = E$, and Einstein-Planck tell us that E is indeed the energy.

Finding H What is H ? None of the above discussion actually tells us what to use for the operator H . We generally have three routes to discovering H :

- A classical H exists, which is then “quantized.”
- Symmetry arguments can be used. For example Dirac discovered his famous equation by looking for a relativistically invariant equation that could handle spin 1/2.
- Experiment may reveal new degrees of freedom. For example the Stern-Gerlach experiment revealed the existence of electron spin.

Let us review the first method. Suppose we have a classical particle moving in one dimension under a potential $V(x)$. The Lagrangian is

$$L = \frac{m}{2}(\frac{dx}{dt})^2 - V(x)$$

The generalized momentum is

$$p = \partial L / \partial(\dot{x}) = m\dot{x} = m\frac{dx}{dt},$$

and the classical Hamiltonian is

$$H = p\frac{dx}{dt} - L = \frac{1}{2m}p^2 + V(x).$$

For the quantum Hamiltonian, we simply replace the classical momentum and coordinate by the corresponding quantum operators, so as a quantum operator we have

$$H = \frac{1}{2m}P^2 + V(X).$$

Using the quantum form of H we have

$$\langle x|H|\Psi \rangle = \langle x|\frac{1}{2m}P^2 + V(X)|\Psi \rangle = \langle x|\frac{1}{2m}P^2|\Psi \rangle + \langle x|V(X)|\Psi \rangle .$$

Now $\langle x|V(X) = V(x) \langle x|$, so $\langle x|V(X)|\Psi \rangle = V(x) \langle x|\Psi \rangle$. Further,

$$\langle x|P|\Psi \rangle = \frac{\hbar}{i} \frac{\partial}{\partial x} \langle x|\Psi \rangle ,$$

so we finally have

$$\langle x|H|\Psi \rangle = \langle x|\frac{1}{2m}P^2 + V(X)|\Psi \rangle = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)\right) \langle x|\Psi \rangle$$

so the time-dependent equation becomes

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

the familiar form of the time-dependent Schrödinger equation.

NOTE: This is an easy route to the Schrödinger equation. However, at the time Schrödinger discovered his equation, the idea of conservation of probability amplitudes had yet to be formulated.

Momentum Representation We have given the discussion in terms of the x -representation. However, we can be in any representation. Let us explore using the momentum or wave-number representation. Consider

$$\langle p|X|\Psi \rangle = \int dp \langle p|X|x \rangle \langle x|\Psi \rangle = \int dp \langle p|x \rangle x \langle x|\Psi \rangle .$$

Now

$$\langle p|x \rangle = (\langle x|p \rangle)^* = \frac{1}{\sqrt{2\pi\hbar}} \exp(-\frac{1}{\hbar}px).$$

We can pull down a factor x with $-(\hbar/i)\partial/\partial p$, so

$$\langle p|X|\Psi \rangle = -\frac{\hbar}{i} \frac{\partial}{\partial p} \langle p|\Psi \rangle$$

As an example, take a harmonic oscillator. We have

$$\langle p|H|\Psi \rangle = \langle p|(\frac{PP}{2m} + \frac{1}{2}m\omega^2 X^2)|\Psi \rangle = \left(\frac{p^2}{2m} - \frac{1}{2}m\omega^2 \hbar^2 \frac{\partial^2}{\partial p^2}\right) \langle p|\Psi \rangle .$$

We note that for the harmonic oscillator, the Hamiltonian looks quite similar in x and p representations.

Examples of $U(t)$ The easiest case we can study is a free particle in one dimension. Here $H = P^2/2m$ so

$$U(t) = \exp(-\frac{i}{\hbar} \frac{P^2}{2m} t)$$

To see what this really is more concretely, let us sandwich the identity to the right of $U(t)$. The identity is

$$I = \int dp |p\rangle \langle p|,$$

and $P|p\rangle = p|p\rangle$, so we have

$$U(t) = \int dp |p\rangle \exp(-\frac{i}{\hbar} \frac{p^2}{2m} t) \langle p|,$$

so $U(t)$, like I is diagonal in a *continuous* index. This is still a bit abstract. We can make it more concrete by taking a coordinate space matrix element, $\langle x|U(t)|x'\rangle$. This is an *amplitude* not an actual *probability amplitude*, but an interesting quantity nevertheless. To visualize it, imagine we have a particle at x' at $t = 0$. We wait for a time t and ask what is the amplitude for it to be at x ? We are considering a free particle, but in general the matrix element

$$\langle x|U(t)|x'\rangle$$

is an example of Feynman's propagator. Returning to the free particle, we can write

$$\begin{aligned} \langle x|U(t)|x'\rangle &= \int dp \langle x|p\rangle \exp(-\frac{i}{\hbar} \frac{p^2}{2m} t) \langle p|x'\rangle \\ &= \int \frac{dp}{2\pi\hbar} \exp(i\frac{p(x-x')}{\hbar}) \exp(-\frac{i}{\hbar} \frac{p^2}{2m} t) \langle p|x'\rangle, \end{aligned}$$

where we used

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp(i\frac{px}{\hbar})$$

Evaluating the integral for $\langle x|U(t)|x'\rangle$ is an exercise in Gaussian integration, which we will come back to later.

The harmonic oscillator gives another example where we can see the structure of $U(t)$. We know from undergrad QM that for the harmonic oscillator, H has a purely discrete spectrum. There are eigenstates $|n\rangle$, satisfying

$$H|n\rangle = (\frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2)|n\rangle = \hbar\omega(n + \frac{1}{2})|n\rangle.$$

The $|n\rangle$ are a complete set, so

$$I = \sum_n |n\rangle \langle n|,$$

and

$$U(t) = \exp(-\frac{i}{\hbar}Ht)I = \sum_n |n\rangle \exp(-i\omega(n + \frac{1}{2})) \langle n|$$

Both I and $U(t)$ are diagonal matrices, now in a *discrete* index. We again may get to a more concrete object by taking coordinate matrix elements. We have

$$\langle x|U(t)|x'\rangle = \sum_n \langle x|n\rangle \exp(-i\omega(n + \frac{1}{2})) \langle n|x'\rangle .$$

The $\langle x|n\rangle$ are just the familiar harmonic oscillator wave functions. Evaluating $U(t)$ does not look easy in this form, but turns out to be another exercise in Gaussian integrals.

The Case of Time-Dependent Hamiltonian If the time axis is uniform, we can write

$$U(t, t') = U(t - t'),$$

i.e. the U operator does not depend on where on the time axis the points t, t' are, only on the *difference* $t - t'$. However, there are certainly cases where this condition does not hold. A concrete example is a system where the potential depends explicitly on time. Suppose we have a classical system with classical Hamiltonian

$$H_c = \frac{\vec{p} \cdot \vec{p}}{2m} + V(\vec{x}, t).$$

How do we describe this system quantum mechanically? What is the Schrödinger equation for this system? We will come back to this specific case, but for now we will give a much more general discussion. Our basic requirement is unitarity. The state of the system at time t is related to the state at time t' by a unitary transformation,

$$|\Psi(t)\rangle = U(t, t')|\Psi(t')\rangle .$$

We require conservation of probability amplitudes,

$$\langle \Phi(t)|\Psi(t)\rangle = \langle \Phi(t')|\Psi(t')\rangle .$$

For this to hold for arbitrary states $|\phi\rangle$ and $|\Psi\rangle$, U must be unitary,

$$U^\dagger(t, t')U(t, t') = I. \tag{29}$$

What this requirement means is that the *system* is preserved as time evolves. The energy, linear momentum, angular momentum, etc all may change as time progresses, but the system remains so many particles of such and such type. (Actually the unitarity condition holds even when particles are created and destroyed. Some systems of that type will be covered in Physics 581.) Let us differentiate Eq.(29) with respect to t . We have

$$(\frac{\partial}{\partial t}U^\dagger(t, t'))U(t, t') + U^\dagger(t, t')\frac{\partial}{\partial t}U(t, t') = 0, \tag{30}$$

or applying $U^\dagger(t, t')$ on the left,

$$(U(t, t') \frac{\partial}{\partial t} U^\dagger(t, t')) U(t, t') + \frac{\partial}{\partial t} U(t, t') = 0. \quad (31)$$

Let us examine the operator multiplying $U(t, t')$, and in particular, see what its adjoint is. We have

$$(U(t, t') \frac{\partial}{\partial t} U^\dagger(t, t'))^\dagger = \frac{\partial}{\partial t} U(t, t') U^\dagger(t, t'). \quad (32)$$

Using Eq.(29), we can rewrite Eq.(32) as

$$(U(t, t') \frac{\partial}{\partial t} U^\dagger(t, t'))^\dagger = \frac{\partial}{\partial t} U(t, t') U^\dagger(t, t') = -U(t, t') \frac{\partial}{\partial t} U^\dagger(t, t'), \quad (33)$$

So if we set

$$U(t, t') \frac{\partial}{\partial t} U^\dagger(t, t') = -\frac{i}{\hbar} H(t), \quad (34)$$

then $H^\dagger(t) = H(t)$, and Eq.(31) becomes

$$i\hbar \frac{\partial}{\partial t} U(t, t') = H(t) U(t, t'). \quad (35)$$

Then if $|\Psi(t)\rangle = U(t, t') |\Psi(t')\rangle$, we have

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H(t) |\Psi(t)\rangle, \quad (36)$$

or taking the matrix element with the bra $\langle \vec{x}|$, we have

$$i\hbar \frac{\partial}{\partial t} \langle \vec{x} | \Psi(t) \rangle = \langle \vec{x} | H(t) | \Psi(t) \rangle. \quad (37)$$

Then if our quantum Hamiltonian is

$$H = \frac{1}{2m} \vec{P} \cdot \vec{P} + V(\vec{X}, t), \quad (38)$$

we have

$$i\hbar \frac{\partial}{\partial t} \langle \vec{x} | \Psi(t) \rangle = \langle \vec{x} | H(t) | \Psi(t) \rangle = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}, t) \right) \langle \vec{x} | \Psi(t) \rangle \quad (39)$$

Note We see that the Schrödinger equation really comes from unitarity, or conservation of probability amplitudes. The system may or may not conserve energy, linear momentum, or angular momentum, or any other quantum numbers. Even if none of these is conserved, there is still a Schrödinger equation describing the time evolution of the system.

Equations of Motion for Expected Values Consider an operator O which does not depend on time. The expected value of O is then

$$\langle O \rangle(t) = \langle \Psi(t) | O | \Psi(t) \rangle. \quad (40)$$

Setting $t' = 0$ as is usually done, we have

$$\langle O \rangle(t) = \langle \Psi | \exp(\frac{i}{\hbar} H t) O \exp(-\frac{i}{\hbar} H t) | \Psi \rangle. \quad (41)$$

Taking the partial derivative with respect to t , we have

$$\frac{\partial}{\partial t} \langle O \rangle(t) = \frac{-i}{\hbar} \langle \Psi(t) | [O, H] | \Psi(t) \rangle. \quad (42)$$

Let us apply Eq.(42) to components of \vec{X} and \vec{P} . We will need to evaluate the commutators,

$$[X_l, H], \text{ and } [P_l, H],$$

where l labels a particular component. We have

$$[X_l, H] = \frac{1}{2m} [X_l, \vec{P} \cdot \vec{P}] = \frac{i\hbar}{m} P_l, \quad (43)$$

where we used $[X_m, P_n] = i\hbar\delta_{mn}$. Similarly, the same commutator is used to show that

$$[P_l, H] = [P_l, V(\vec{X})] = \frac{\hbar}{i} \frac{\partial}{\partial X_l} V(\vec{X}). \quad (44)$$

Exercise 1 Derive Eq.(44) when

$$V(X) = \sum_{n=0}^{\infty} a_n X^n,$$

where a_n are constants. Use only the commutator $[X, P] = i\hbar$.

Using these equations we have

$$\frac{\partial}{\partial t} \langle X_l \rangle(t) = \frac{1}{m} \langle P_l \rangle, \quad \frac{\partial}{\partial t} \langle P_l \rangle(t) = - \langle \frac{\partial}{\partial X_l} V(\vec{X}) \rangle. \quad (45)$$

By inserting the identity as $I = \int d^3x |\vec{x}\rangle \langle \vec{x}|$, we may also write

$$- \langle \frac{\partial}{\partial X_l} V(\vec{X}) \rangle = - \int d^3x \langle \Psi(t) | \vec{x} \rangle \frac{\partial}{\partial x_l} V(\vec{x}) \langle \vec{x} | \Psi(t) \rangle$$

Eqs.(45) are just the classical equations of motion applied to expected values. (Since the expected values depend only on time, the partial derivatives with respect to time are the same as ordinary derivatives.) Further, the above derivation extends to the case where the potential is time dependent, so the quantum equations for expected values agree with the corresponding classical equations for that case as well.

Rotations As our last example of Dirac's transformation theory, we consider rotations. Our system will be one particle in three dimensions, but the method is completely general. Imagine we have a state $|\Psi\rangle$ and we want to perform a rigid rotation around the 3-axis by angle ϕ , to give a rotated state $|\Psi'\rangle$. The rotated vector \vec{x} will be denoted by $R(\phi)\vec{x}$, and is given by

$$\begin{pmatrix} \cos(\phi) & -\sin(\phi) & 0 \\ \sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \cos(\phi) - y \sin(\phi) \\ y \cos(\phi) + x \sin(\phi) \\ z \end{pmatrix}$$

As in previous cases, we will generate $|\Psi'\rangle$ by a unitary transformation,

$$|\Psi'\rangle = U(\phi)|\Psi\rangle$$

where

$$U(\phi) = \exp(-\frac{i}{\hbar}J_3)$$

where J_3 as a self-adjoint operator. Based upon purely classical or common sense reasoning, we have

$$\langle R^{-1}\vec{x}|\Psi\rangle = \langle \vec{x}|U(\phi)|\Psi\rangle. \quad (46)$$

Note the presence of R^{-1} on the left hand side. To see that this equation is correct, imagine that $|\Psi\rangle$ corresponds to a "lump" on the x -axis. Rotating it by angle ϕ around the 3 or z -axis, we it will now be a lump at centered about a point in the first quadrant. If we evaluate $\langle \vec{x}|\Psi'\rangle$ at a point \vec{x} right in the middle of the rotated state, this will give the same value on $|\Psi\rangle$ if we are at $R^{-1}\vec{x}$. (Draw a picture to see this clearly.)

Writing out Eq.(46) we have

$$\langle x \cos \phi + y \sin \phi, y \cos \phi - x \sin \phi, z|\Psi\rangle = \langle x, y, z, |U(\phi)|\Psi\rangle.$$

Taking $\phi \rightarrow 0$ and expanding we have

$$\langle x + y\phi, y - x\phi, z|\Psi\rangle \sim \langle x, y, z|\Psi\rangle + \phi(y\partial_x - x\partial_y) \langle x, y, z|\Psi\rangle,$$

and

$$\langle x, y, z|U(\phi)|\Psi\rangle \sim \langle x, y, z|\Psi\rangle - \frac{i}{\hbar}\phi \langle x, y, z|J_3|\Psi\rangle.$$

Matching coefficients of ϕ we have

$$\langle x, y, z|J_3|\Psi\rangle = (x\frac{\hbar}{i}\partial_y - y\frac{\hbar}{i}\partial_x) \langle x, y, z|\Psi\rangle = \langle x, y, z|(XP_y - YP_x)|\Psi\rangle$$

This shows that as an operator J_3 or J_z is given by

$$J_3 = J_z = (XP_y - YP_x),$$

and pulls out as the usual differential operator. **NOTE:** We have used J_3 here rather than L_3 to emphasize that this argument regarding rotations as preserving probability amplitudes will always involve the *total* angular momentum of the system. In the particular case we discussed the only form of angular momentum is the orbital angular momentum, so we could have used L_3 here.

We will delay a discussion of spin, but we can handle the case of n particles. If we have a system of n particles, we can write

$$\langle R^{-1}\vec{x}_1, \dots R^{-1}\vec{x}_n | \Psi \rangle = \langle \vec{x}_1, \dots \vec{x}_n | U(\phi) | \Psi \rangle,$$

that is, we must rotate all the particle coordinates. Expanding around $\phi = 0$ again, we obtain

$$\sum_{i=1}^n (xp_y - yp_x)_i \langle \vec{x}_1, \dots \vec{x}_n | \Psi \rangle = \langle \vec{x}_1, \dots \vec{x}_n | J_3 | \Psi \rangle,$$

and we can again write J_3 as an operator as

$$J_3 = \sum_{r=1}^n (XP_y - YP_x)_r,$$

which says that the total 3 or z component of the orbital angular momentum is the sum of the individual angular momenta for each particle in the system.

The generalization of the above for rotations around 1 and 2 axes is straightforward. For our n particle system we would obtain

$$J_l = \sum_{r=1}^n \epsilon_{jkl} (X_j P_k)_r.$$

(In this equation, j, k, l are Cartesian indices, while $r = 1, 2, \dots, n$ labels particles.) The commutation rules can be obtained by using the X and P commutation rules or by working to second order in small angles. They can be written

$$[J_j, J_k] = i\hbar \epsilon_{jkl} J_l.$$

Suppose we define a total coordinate and total momentum operator as

$$X_l = \sum_{r=1}^n (X_l)_r, \quad P_l = \sum_{r=1}^n (P_l)_r,$$

Then it is easy to show by using the commutation rules, that

$$[J_j, X_k] = i\hbar \epsilon_{jkl} X_l, \quad [J_j, P_k] = i\hbar \epsilon_{jkl} P_l.$$

What we are seeing here is the concept of **vector operator**. Suppose we have *any* 3-vector operator \vec{V} . Then the commutation rules of \vec{V} with \vec{J} are

$$[J_j, V_k] = i\hbar \epsilon_{jkl} V_l.$$

The origin of these commutation rules is the ultimately the fact that 3-vectors transform in a known way under rotations. The notion of vector operator plays an important role in advanced angular momentum theory.