<u>Introduction to Symmetries</u>

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Lecture 1:

Translations and Linear Momentum.

We start by considering a very simple example of a "continuous symmetry" - that of one-dimensional translations. The basic idea is that physics should not depend on our particular choice of coordinate system - for instance, as we shall discuss in this Lecture, where we choose to locate the origin (or, in the next Lecture, how we choose to orientate the axes).

Suppose, then, that we have one coordinate system S and a physical point P whose coordinates in S are (x, y, z). And suppose we have another coordinate system S' whose origin is shifted by a along the x- axis of S , so that the coordinates of the same physical point P referred to the new system S' are (x', y', z') where $x' = x - a, y' = y, z' = z$. We shall now forget about the x- and y- dimensions, which are unaffected by this one-dimensional translation, and deal only with the x coordinates. People in system S will use a wavefunction $\psi(x)$ to describe physics, and will calculate a physical probability density $\mid \psi(x) \mid^2$. How about people using the system S'? It must be the case that their description, in terms of their wavefunction and their coordinate x', must represent the same "objective physics"as is represented by $\mid \psi(x) \mid^2$. This is a physical "lump of probability" sitting someplace - it is *here* and not somewhere else, and all observers have got to agree on where as a matter of fact it is, what shape it is, etc. So our basic question is this: *what wavefunction ψ' must people in S' use, with their coordinate x', so that they are consistently describing the same physical situation as the people in S, using coordinate x ?*

Let's take a concrete example:

$$\psi(x) = Ne^{-x^2/x_0^2}.$$

This of course is just a Gaussian, centred on the origin $x = 0$ of system S. N is a normalisation constant and x_0 controls the width of the Gaussian. So $\mid \psi(x) \mid^2$ is a lump of probability sitting at the place called $x = 0$ according to people in S. The people in S' had better give a *true* representation of it, using their coordinate x' and their wavefunction ψ'. How can they ensure this? Let's make a (wrong) guess - let's guess that you don't need to change the functional form of the wavefunction, all you have to do is use the same wavefunction but make its argument x' rather than x. In other words, our guess is that the S' people should use $\psi(x')$. What does this look like? Well, we know that $x' = x - a$. So

$$\psi(x') = \psi(x - a) = Ne^{-(x-a)^2/x_0^2}$$

which is a Gaussian centred on $x = a$, not on $x = 0$! So this is an *incorrect* representation of the physics as described by people in S. We have to change the functional form of the wavefunction, when changing coordinate system, as well as the actual coordinates.

The right answer to the question "what wavefunction should people in S' use?" is : they must use a *different* wavefunction, ψ', such that when ψ' is evaluated at x' it does produce the same physical probability distribution as ψ does when evaluated at x. The simplest way to arrange this is obviously to demand that

$$\psi'(x') = \psi(x)$$

which is a very important equation!

[Aside: you may be wondering.... couldn't there be a phase factor of the form $e^{i\delta}$ on the RHS? This would cancel out in the modulus squared giving the probability distribution... And another thing - couldn't ψ on the RHS be replaced by ψ^* , because this too would give the same probability distribution...Yes to both! Wigner sorted all this out a long time ago. The complex conjugate is needed only if our transformation involves time-reversal; otherwise, it is ψ, and the phase factor can be chosen to be unity.]

OK, so what is this ψ' ? we have $\psi'(x') = \psi(x)$ with $x' = x - a$. So the equation $\psi'(x-a) = \psi(x)$ has to be true for all values of x. Let's replace " x " by " $x+a$ ". Then we must have

$$\psi'(x) = \psi(x+a).$$

This equation tells us what the function $\psi'(x)$ *is*, namely

$$\psi'(x) = Ne^{-(x+a)^2/x_0^2}$$

Compare this with the definition of $\psi(x)$, above; it is clearly *not* the same function of x as ψ is. Fine; so what is $\psi'(x')$? It is plainly

$$\psi'(x') = Ne^{-(x'+a)^2/x_0^2}.$$

Does this do the job we want it to? i.e. does it correctly describe, for the S' people, the right lump of probability? Well,

$$\psi'(x') = Ne^{-(x'+a)^2/x_0^2} = Ne^{-(x-a+a)^2/x_0^2} = Ne^{-x^2/x_0^2} = \psi(x)$$

as required, where we just substituted $x' = x - a$. In pictures, $\psi'(x')$ is a Gaussian centred on the point $x' = -a$, which is of course exactly the same physical pooint as $x = 0$. So it works.

Next we consider a very important special case of the above - namely, a translation through a very small (infinitesimal) distance ϵ. We shall see, remarkably, how infinitesimal translations are closely connected to the momentum operators in quantum mechanics....and from this will follow the deep connection between *translation invariance* and *momentum conservation.* We shall consider many other examples of such *infinitesimal transformations* in the later lectures. Note that this kind of analysis can only be done for *continuous transformations* i.e. those that can be built up, precisely, from a series of (infinitely many, in the limit) tiny infinitesimal steps - not like Parity, for instance, which is the transformation $\mathbf{r}' = -\mathbf{r}$ and which is a *discrete* transformation (as opposed to continuous).

Consider then the fundamental relation $\psi'(x') = \psi(x)$(which defines the function ψ') . Written differently, this is $\psi'(x) = \psi(x+a)$ as we saw. Now take $a \to \epsilon$. We have

$$\begin{aligned}
\psi'(x) &= \psi(x+\epsilon) \\
&= \psi(x) + \epsilon\frac{\partial\psi}{\partial x} \quad \text{expanding by Taylor's theorem to first order} \\
&= \psi(x) + \frac{i\epsilon}{\hbar}. - i\hbar\frac{\partial}{\partial x}\psi \\
&= \psi(x) + \frac{i\epsilon}{\hbar}\hat{p}_x\psi(x) \\
&= \left(1 + \frac{i\epsilon}{\hbar}\hat{p}_x\right)\psi(x)
\end{aligned}$$

where $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$ is the familiar quantum-mechanical momentum operator. The last equality is very important - it tells us the answer to our question "what is the function ψ' ? " (at least, for this infinitesimal translation). To get ψ' in this case, the answer is you operate on ψ with the indicated operator $\left(1 + \frac{i\epsilon}{\hbar}\hat{\psi}_x\right)$. This is of course just a fancy way of saying the operator $\left(1 + \epsilon\frac{\partial}{\partial x}\right)$, as in the second line....but the connection to the q.m. mementum operator is crucial, physically. Note also that, as expected, the "new" wavefunction ψ' is infinitesimally close to the "old" one ψ.

Now let's go back to a finite translation a. In this case we can't cut off the Taylor expansion at just the first order term, but must (formally) keep all the terms:

$$\begin{aligned}
\psi'(x) = \psi(x+a) &= \psi(x) + a\frac{\partial\psi(x)}{\partial x} + \frac{a^2}{2}\frac{\partial^2\psi(x)}{\partial x^2} + ... \\
&= \left(1 + a\frac{\partial}{\partial x} + \frac{a^2}{2}\frac{\partial^2}{\partial x^2} + ...\right)\psi(x) \\
&= \left(e^{a\frac{\partial}{\partial x}}\right)\psi(x) \quad \text{check by re-expanding the exponential, formally!} \\
&= \left(e^{a.\frac{i}{\hbar}.-i\hbar\frac{\partial}{\partial x}}\right)\psi(x)
\end{aligned}$$

or equivalently

$$\psi'(x) = e^{ia\hat{p}_x/\hbar}\psi(x).$$

Note particularly that the *arguments* are the same, namely x, on both sides of this last equation. It therefore tells us directly the relation between the function ψ' and the function ψ: namely (rather formally, it must be admitted) ψ' is that function which is obtained by applying the operator $e^{ia\hat{p}_x/\hbar}$ to ψ. So this answers our question about what wavefunction the S' people should use.

Let's introduce a special notation for this important operator that constructs ψ' for us:

$$\hat{U}_x(a) = e^{ia\hat{p}_x/\hbar}.$$

Then, it is easy to see that it is a *unitary operator*:

$$\hat{U}_x^\dagger(a) = e^{-ia\hat{p}_x^\dagger/\hbar} = e^{-ia\hat{p}_x/\hbar}$$

using the fact that $\hat{p}_x$ is Hermitian: $(\hat{p}_x)^\dagger = \hat{p}_x$. And it's clear that $e^{-ia\hat{p}_x/\hbar}$ is the operator appropriate to a displacement of $-a$, so it must be just the *inverse* of $\hat{U}_x(a)$:

$$\hat{U}_x^\dagger(a) = \hat{U}_x^{-1}(a)$$

and so

$$\hat{U}_x^\dagger(a).\hat{U}_x(a) = I$$

which is the statement that $\hat{U}_x(a)$ is unitary (" $U^\dagger.U = I$ ").

There is an important point to note here about the relationship between the *unitary* operator $\hat{U}_x(a)$ and the *Hermitian* operator $\hat{p}_x$. Basically, we can always make a unitary operator $\hat{U}$ by writing

$$\hat{U} = e^{i\hat{h}}$$

where $\hat{h}$ is Hermitian (try taking the dagger of both sides). And we can slip in a real parameter in front of the $\hat{h}$ without altering the unitarity property. So something of the form $e^{i\alpha\hat{h}}$ where $\hat{h}$ is Hermitian and α is real will always get us a unitary operator. Just as this kind of thing "does the job" for translations (in the sense that $\hat{U}_x(a)$ acting on ψ produces ψ'), so we will see in the other lectures exactly the same kind of operators arising in the case of other transformations. In this context, the operator up in the exponent, namely $\hat{h}$, is called the *generator* of the transformation, or more pedantically the *infinitesimal generator*, or the *generator of infinitesimal transformations*. You can see the sense of this language in the case (translation) that we have just done: $\hat{p}_x$ was indeed the operator that appeared when we did the infinitesimal translation. And we "exponentiated" it to get the operator for the finite translation case. So with the unitary operators effecting finite transformations there will be associated Hermitian operators effecting (or generating) infinitesimal ones....and since in quantum mechanics Hermitian operators represent *observables* these "generators" must have an important physics role to play! (as of course we have already noted in the case of the translation generator, which is precisely the momentum).

So far, we have discussed only the question of how to ensure consistency between the *wavefunctions* used by S and S'. How about the *Hamiltonians* in the two systems? Consider the time-independent Schrodinger equation (in one dimension for simplicity) as written by the people in S:

$$\hat{H}(x)\psi(x) = E\psi(x).$$

The people in S' will write their own Schrodinger equation:

$$\hat{H}'(x')\psi'(x') = E\psi'(x')$$

but they had better use the same E!! the value of which must be independent of which set of coordinates is used. So, just as the S' people must use a different wavefunction $\psi'(x')$, so must they also (in general) use a different Hamiltonian $\hat{H}'(x')$. What is this different Hamiltonian? Well, look at the last two equations, remembering that we have already decided that $\psi'(x') = \psi(x)$: for consistency, we must require

$$\hat{H}'(x') = \hat{H}(x),$$

very much as for the wavefunctions.

Let's see the consequence of this for our particular case $x' = x-a$. We require $\hat{H}'(x-a) = \hat{H}(x)$, or $\hat{H}'(x) = \hat{H}(x+a)$. This says that $\hat{H}'$ evaluated at x has to equal $\hat{H}$ evaluated at $x+a$. Now, what kinds of Hamiltonian might we be considering? Take for example the Hamiltonian for a free particle in 1-D:

$$\hat{H}(x) = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}.$$

What would $\hat{H}(x+a)$ be? Note that

$$\frac{\partial}{\partial(x+a)} = \frac{\partial}{\partial x}$$

and

$$\frac{\partial^2}{(\partial(x+a))^2} = \frac{\partial^2}{\partial x^2}$$

so that, in this case,

$$*\hat{H}'(x) = \hat{H}(x+a) = \hat{H}(x)* .$$

[Aside: Would this be true if we added in a potential $V(x)$?] The last equation tells us that, in this case,

$$\hat{H}'(x) = \hat{H}(x)$$

which is saying that this free-particle $\hat{H}$ does *not*, in fact, change its functional form "under a translation" - i.e. it is *invariant*. Any of the equalities contained in the equation *.......* above are equally good statements of this invariance.

Now let's see what follows from this invariance of the free Hamiltonian under translations. Consider an infinitesimal displacement. We have

$$\hat{H}(x) = \hat{H}(x+\epsilon) = \hat{H}(x) + \epsilon\frac{\partial \hat{H}}{\partial x} \quad \text{expanding to first order}$$

from which it follows that

$$\frac{\partial \hat{H}(x)}{\partial x} = 0.$$

This means that $\hat{H}$ does not have any *explicit* dependence on x (what if we had a $V(x)$?)

We're now going to show that this last result is equivalent to saying that the momentum operator $\hat{p}_x$ commutes with $\hat{H}$. Consider $[\hat{p}_x, \hat{H}(x)]\psi(x)$ for any wavefunction $\psi(x)$. This equals

$$\begin{aligned} & -i\hbar\tfrac{\partial}{\partial x}\left(\hat{H}(x)\psi(x)\right) - \left(\hat{H}(x). - i\hbar\tfrac{\partial\psi}{\partial x}\right) \\ = \quad & -i\hbar\left(\tfrac{\partial \hat{H}(x)}{\partial x}\right)\psi(x) - i\hbar\hat{H}(x)\tfrac{\partial\psi}{\partial x} + i\hbar\hat{H}(x)\tfrac{\partial\psi}{\partial x} \end{aligned} .$$

The last two terms cancel leaving the result

$$[\hat{p}_x, \hat{H}(x)]\psi(x) = -i\hbar\frac{\partial \hat{H}(x)}{\partial x}\psi(x).$$

Since this holds for any ψ, we can interpret it as the operator equation (true acting on any function)

$$[\hat{p}_x, \hat{H}(x)] = -i\hbar\frac{\partial \hat{H}(x)}{\partial x}.$$

But we had $\frac{\partial \hat{H}(x)}{\partial x} = 0$ if $\hat{H}(x)$ was invariant under translations. So such invariance implies that

$$[\hat{p}_x, \hat{H}(x)] = 0$$

i.e. *$\hat{p}_x$ commutes with $\hat{H}(x)$*. Now, from general quantum mechanics we should know that *the eigenvalues of operators which commute with the Hamiltonian are constants of the motion i.e. are conserved, and their values can be specified simultaneously with the energy eigenvalue.* So in this case invariance under translations in the x-direction implies that the x-component of momentum p_x (the number, not the operator) is conserved. [What if we had a $V(x)$?]

There is a more formal way of writing much of this, that we shall use more of in later examples. Let's go back to the time-independent Schrodinger equation in system S:

$$\hat{H}(x)\psi(x) = E\psi(x).$$

We know that

$$\psi'(x) = \hat{U}_x(a)\psi(x).$$

It follows that

$$\hat{U}_x(a)\left(\hat{H}(x)\psi(x)\right) = \hat{U}_x(a)E\psi(x) = E\hat{U}_x(a)\psi(x) = E\psi'(x).$$

Now the term on the extreme left can be written as

$$\hat{U}_x(a)\hat{H}(x)\hat{U}_x^{-1}(a)\hat{U}_x(a)\psi(x) = \left[\hat{U}_x(a)\hat{H}(x)\hat{U}_x^{-1}(a)\right]\psi'(x).$$

Hence

$$\left[\hat{U}_x(a)\hat{H}(x)\hat{U}_x^{-1}(a)\right]\psi'(x) = E\psi'(x).$$

But the Schrodinger equation in S' is, as we have seen,

$$\hat{H}'(x)\psi'(x') = E\psi'(x'),$$

and this is true for all x', so there is nothing to stop us writing it as

$$\hat{H}'(x)\psi'(x) = E\psi'(x).$$

Comparing with the previous equation we can identify

$$\hat{H}'(x) = \hat{U}_x(a)\hat{H}(x)\hat{U}_x^{-1}(a).$$

We see that while wavefunctions transform by $\hat{U}$ *,operators transform by* $\hat{U}\widehat{Op}\hat{U}^{-1}$.

Furthermore, if $\hat{H}$ is invariant under these translations, then as we have seen

$$\hat{H}'(x) = \hat{H}(x).$$

This immediately gives

$$\hat{U}_x(a)\hat{H}(x)\hat{U}_x^{-1}(a) = \hat{H}(x)$$

or

$$\hat{U}_x(a)\hat{H}(x) = \hat{H}(x)\hat{U}_x(a)$$

so that $\hat{U}_x(a)$ commutes with the Hamiltonian. Recalling that

$$\hat{U}_x(a) = e^{ia\hat{p}_x/\hbar},$$

we deduce that $\hat{p}_x$ must commute with the Hamiltonian in this case (of invariance), as before.

Note that all of this generalises immediately to three dimensions via the operator

$$\hat{U}_x(a_x).\hat{U}_y(a_y).\hat{U}_z(a_z) = exp(i\boldsymbol{a}.\hat{\boldsymbol{p}}/\hbar),$$

where, since any $\hat{p}_i$ commutes with any $\hat{p}_j$, it does not matter in which order we write the terms on the LHS, and so the RHS is uniquely defined (this will not be quite the same for rotations!).