Supplementary Notes for lecture 17 for McGill Phys 357.

1. Unitary Operators and Generators of Translation

Unitary operators play an incredibly important role in quantum mechanics. If I want to turn a state into another state, and keep those states normalized, then the operator must be unitary. That follows because if $|\Phi\rangle = \mathrm{A}\,|\Psi\rangle$, then

$$\langle\Phi|\Phi\rangle = \langle\Psi|\mathrm{A}^\dagger\mathrm{A}|\Psi\rangle = 1 \tag{1}$$

That is only true if $\mathrm{A}^\dagger\mathrm{A} = \mathrm{I}$, or $\mathrm{A}^{-1} = \mathrm{A}^\dagger$. From now on, if a matrix is unitary, we'll call it U.

Right away, we know several properties of a unitary operator. The columns of U must be orthogonal $U[:,i]^\dagger U[:,j] = \delta_{ij}$, because the rows of the inverse must be orthogonal to the columns of the original matrix. Since inverses commute, the rows of A are also orthogonal, because the columns of $\mathrm{U}^\dagger$ have to be orthogonal. The eigenvectors also have to be orthogonal, because if $\mathrm{U} = \mathrm{V}\Lambda\mathrm{V}^{-1}$ then because $\mathrm{U}^{-1} = \mathrm{U}^\dagger$ we know

$$\mathrm{V}\Lambda^{-1}\mathrm{V}^{-1} = \mathrm{V}^{-1\dagger}\Lambda^\dagger\mathrm{V}^\dagger \tag{2}$$

For that to hold generally requires that $\mathrm{V}^{-1} = \mathrm{V}^\dagger$ so the eigenvectors themselves form a unitary matrix. We also know that $\Lambda^{-1} = \Lambda^\dagger$, or $\Lambda^\dagger\Lambda = \mathrm{I}$, that is the absolute value of each eigenvalue is 1.

We can write any complex number down as $c\exp(i\theta)$ where c is the magnitude of the number, and θ is a real angle. Since the magnitude of the eigenvalues is one for a unitary matrix, we can write them as $\exp(i\theta)$ and so the general form for a unitary matrix is

$$\mathrm{U} = \mathrm{V}\exp(i\Theta)\mathrm{V}^\dagger \tag{3}$$

for real-valued diagonal matrix Θ and orthogonal eigenvector V. Because Hermitian matrices have real eigenvalues and orthogonal eigenvectors, there's a unique mapping from every Hermitian matrix A (we aren't calling it H so as to not be confused with the Hamiltonian) to a unitary matrix:

$$\mathrm{U} = \exp(i\mathrm{A}) \tag{4}$$

Similarly, modulo branch cuts, there's a unique mapping from every unitary matrix to a Hermitian matrix.

One final piece really locks in the form of evolution operators. Let's say I want to evolve a wave function that is a function of some value x. We then want to be able to go from $|\Psi(x)\rangle$ to $|\Psi(x+dx)\rangle$. If we zoom in far enough, so nothing else in the system is changing, then whatever operator U takes $|\Psi(x)\rangle$ to $|\Psi x + dx\rangle$ also will take $|\Psi(x+dx)\rangle$ to $|\Psi(x+2dx)\rangle$. Intuitively this makes sense - two rotations about the same axis by angle $d\theta$ is the same as a rotation by angle $2d\theta$, or moving forward by dt twice is the same as moving forward by $2dt$. That leaves us with $\mathrm{U}(ndx) = \mathrm{U}(dx)^n$. That works if the eigenvalues of U are proportional to dx. That leaves us with the general form of a unitary operator that translates a wave function by some small amount dx:

$$\mathrm{U}_x(dx) = \mathrm{V}\exp(i\Lambda_x dx)\mathrm{V}^\dagger \tag{5}$$

I've added the subscript x to emphasize that over different ranges where we might want to carry out translations, the eigenvalues can change, hence the translation operator changes. We'll indeed see cases where this happens, but if we make dx small enough, we can always treat Λ as constant over a region. Since $\mathrm{V}\Lambda_x\mathrm{V}^\dagger$ is a Hermitian matrix, we can write

$$\mathrm{U}_x(dx) = \exp(i\mathrm{A}_x dx) \tag{6}$$

If I've zoomed in even further, I can expand the right-hand side of Equation 6 to first order to get:

$$\mathrm{U}_x(dx) = 1 + i\mathrm{A}_x dx \tag{7}$$

This is the fundamental reason why the generator of rotations looked the way it did, and that the generator of time translations looks the same way. If we have a unitary operator that continuously transforms a state into another state, you *have* to be able to write it down as a generator of translations, as in Equation 7. We can often give Equation 7 more physical meaning by introducing constants. For rotations, we set $\mathrm{A} = -\mathrm{J}/\hbar$ because it turned out that writing things that way meant we could generate rotations with the angular momentum operator. For time evolution, we'll write the generator of time translations as

$$\mathrm{U}_t(dt) = \mathrm{I} - i\mathrm{H}dt/\hbar \tag{8}$$

because it will turn out the operator H is the Hamiltonian of the system when we write things this way. We haven't shown that, of course, but at this point we do know that there exists some operator H that has the *units* of energy that will translate a wave function forward in time.

2. Conservation and Eigenstates

Let's consider the class of translation operators that don't explicitly depend on the particular spot we're doing the translation, *i.e.*

$$\mathrm{U}_x(dx) = \mathrm{U}(dx) \tag{9}$$

In the case of time translations, that means that U does not *explicitly* depend on time. Right away, from Equation 6, we see that we can generate large translations as well as small ones. If we know that our starting wave function is $|\Psi(x=0)\rangle \equiv |\Psi_0\rangle$, then

$$|\Psi(x)\rangle = \exp(i\mathrm{A}x)\,|\Psi_0\rangle \tag{10}$$

If pick our starting state to be an eigenvector of A, with eigenvalue λ, then we know that

$$\exp(i\mathrm{A}x)\,|\Psi_0\rangle = \exp(i\lambda x)\,|\Psi_0\rangle \tag{11}$$

since the we saw that the eigenvalues of unitary matrix $\mathrm{U} = \exp(i\mathrm{A})$ for Hermitian matrix A are $\exp(i\lambda)$, and the eigenvectors stay the same. The important thing to take away is that the left side of Equation 11 has an operator, but in the right side that has turned into a scalar. Because it's an eigenstate, our wave function has picked up an overall phase, but remains an eigenstate. That

means if we go out and measure our Hermitian operator A in the new state, we have to get the same answer. This follows from:

$$\langle\Psi(x)|\,\mathrm{A}\,|\Psi(x)\rangle = \langle\Psi_0|\exp(-i\lambda x)\mathrm{A}\exp(i\lambda x)\,|\Psi_0\rangle = \lambda \tag{12}$$

Whatever value of A we measure *does not change* as we evolve our system. It is *conserved*. Even more generally, if we let $|\Psi\rangle$ be a superposition of states, the expectation value of our operator won't change. If we have a mixed state, each component picks up a different phase, but the expectation of an operator doesn't depend on the relative phases of the eigenstates of that operator (they all just drop out when we form *e.g.* $c_+^* c_+$ and $c_-^* c_-$ for a spin-1/2 system). Equivalently, since U and A commute (because U consists of powers of A), $\langle\Psi_0|\,\mathrm{U}^\dagger\mathrm{AU}\,|\Psi_0\rangle = \langle\Psi_0|\,\mathrm{AU}^\dagger\mathrm{U}\,|\Psi_0\rangle = \langle\Psi_0|\,\mathrm{A}\,|\Psi_0\rangle$.

This is really a remarkable conclusion. Simply by requiring that probability is conserved, we see that if we want to evolve a wave function, there's a unitary operator that does that. That unitary operator has an associated Hermitian operator, and the expectation of that operator does not depend on the wave function's evolution, as long as the evolution does not depend explicitly on our variable. For the particular case of translations in time, there's an associated Hermitian operator with units of energy, the expectation of which does not change with time (again, as long as there is no explicit time dependence, so H is not $\mathrm{H}(t)$). It's a small (but important!) leap to say that operator *is* the energy of the system, but that is indeed true and so the time evolution operator is the Hamiltonian H.

3. The Schrodinger Equation(s)

Let's go back to Equation 6, and insert a wave function on the right. That leaves us with

$$|\Psi(x_0+x)\rangle = \mathrm{U}_{x_0}(x)\,|\Psi(x_0)\rangle = \exp(i\mathrm{A}_{x_0}x)\,|\Psi(x_0)\rangle \tag{13}$$

where we've changed variables to say we're starting at some value x_0 and shifting by x (I'm doing this mainly to avoid writing ddx). If we differentiate this with respsect to x, we have

$$\frac{d\Psi}{dx} = i\mathrm{A}\,|\Psi\rangle \tag{14}$$

I've dropped the explicit dependence on x_0 because we're now assuming you're evaluating A for the same value of x where you're evaluating your wave function. Of course, A may well be constant (and indeed will be for most of the examples we look at), but now it doesn't *have* to be. We're now left with the quite general theorem that for a wave function that depends on parameter x, any continuous[1] unitary transformation of our wave function can be described by Equation 14. The operator A is Hermitian, and is related to our unitary transform by $\mathrm{U} = \exp(i\mathrm{A})$. If we take the special case of evolving with time, and letting $\mathrm{A} = -\mathrm{H}/\hbar$, Equation 14 turns into the Schrodinger equation:

$$\frac{d\,|\Psi\rangle}{dt} = -i\mathrm{H}\,|\Psi\rangle\,/\hbar \tag{15}$$

[1]Because we do absolutely need that $\mathrm{A}(2dx) = \mathrm{A}(dx)\mathrm{A}(dx)$.

Moving the i and $\hbar$ to the left side of the equation, we're left with the Schrodinger equation as it's normally written:

$$i\hbar\frac{d\left|\Psi\right\rangle}{dt} = \mathrm{H}\left|\Psi\right\rangle \tag{16}$$

Unitarity guarantees time evolution has to look like the Schrodinger equation, and for now since H is conserved and has units of energy, we'll take the leap of faith that it is the Hamiltonian. While we'll concentrate on solving Schrodinger's equation for much of the rest of the course, do please remember that there is a Schrodinger-like equation for *any* unitary evolution. We'll see this for several cases. If we replaced dt by $d\theta$ in Equation **??**, then the associated operator has the units of angular momentum, and indeed is J. The generator of rotations is simply the first-order expansion of Equation **??**. If we replace dt by dx, then the associated operator has units of momentum, and once again turns out to be the momentum operator (with a sign flip). If we replace dt by dp, then the associated operator is position (without a sign flip[2].

[2]It doesn't actually matter which of the momentum and position operators get the minus sign, but it's does very much matter that they have opposite signs. We'll see that position and momentum representations are forward/inverse Fourier transforms of each other. If you want to end up back where you started after a forward/inverse transform, then the operators have to have opposite signs.