

Unitary Transformations

Unitary transformations are transformations of the matrices which maintain the Hermitian nature of the matrix, and the multiplication and addition relationship between the operators. They also maintain the eigenvalues of the matrix.

Consider a general Hermitian matrix A . This matrix has eigenvalues a_i and eigenvectors $|A, i\rangle$. We now want to find some transformation of the matrix A such that the new matrix \tilde{A} is Hermitian and has the same eigenvalues as A does. This new matrix will have eigenvectors $|\tilde{A}, a_i\rangle$. Let us assume that the transformation is linear—ie the transformation of a sum is the sum of the transformed vectors. Then we can write the transformation as

$$|\tilde{A}, a_i\rangle = U|A, a_i\rangle \quad (1)$$

where U is some matrix. Now, we want that a unit vector be taken to a unit vector. Thus,

$$\langle \tilde{A}, a_i | \tilde{A}, a_j \rangle = \langle A, a_i | U^\dagger U | A, a_j \rangle \quad (2)$$

but we want

$$\langle \tilde{A}, a_i | \tilde{A}, a_j \rangle = \langle A, a_i | A, a_j \rangle \quad (3)$$

This implies that

$$U^\dagger U = I \quad (4)$$

In the appendix, I will also argue that the requirement that U leave the eigenvalues of all Hermitian operators the same gives us in addition that

$$UU^\dagger = I \quad (5)$$

Furthermore, we know we can write

$$\tilde{A} = \sum_i a_i |\tilde{A}, a_i\rangle \langle \tilde{A}, a_i| = \sum_i a_i U |A, a_i\rangle \langle A, a_i| U^\dagger = UAU^\dagger \quad (6)$$

Thus, in order to preserve the Hermitian character and the eigenvalues of an arbitrary matrix A , we need that the transformation be of the form UAU^\dagger and that U be Unitary—ie $U^\dagger U = 1$.

Heisenberg's dynamic equations should preserve the eigenvalues of the matrix A since we are simply looking at the same attribute at different times. Thus, we should have that

$$A(t) = U(t)A_0U^\dagger(t) \quad (7)$$

Substituting this into the Heisenberg equation, we get

$$i\hbar \frac{dA(t)}{dt} = [A(t), H] \quad (8)$$

can be rewritten, using the product rule of differentiation

$$i\hbar \left(\frac{dU}{dt} A_0 U^\dagger + U A_0 \frac{dU^\dagger}{dt} \right) = AH - HA \quad (9)$$

or using the fact that $U^\dagger U = I$,

$$i\hbar \left(\frac{dU}{dt} U^\dagger A + AU \frac{dU^\dagger}{dt} \right) = AH - HA \quad (10)$$

Since

$$0 = \frac{dI}{dt} = \frac{dUU^\dagger}{dt} = \frac{dU}{dt} U^\dagger + U \frac{dU^\dagger}{dt} \quad (11)$$

we finally have

$$i\hbar \left(-U \frac{dU^\dagger}{dt} A + AU \frac{dU^\dagger}{dt} \right) = AH - HA \quad (12)$$

This can be solved only if

$$i\hbar U \frac{dU^\dagger}{dt} = H \quad (13)$$

or

$$i\hbar \frac{dU^\dagger}{dt} = U^\dagger H \quad (14)$$

or taking the Hermitean or Dirac adjoint of both sides

$$-i\hbar \frac{dU}{dt} = HU \quad (15)$$

Ie, we can solve the complete problem if we can solve this ordinary, but matrix, differential equation.

For our 2x2 matrices, this turns out to be easy to do. If

$$H = H_0 + \vec{H} \cdot \vec{\sigma} \quad (16)$$

then the exact solution to the above equation is

$$U = e^{i\frac{H_0}{\hbar}t} \left(\cos\left(\frac{|\vec{H}|}{\hbar}t\right) + i \sin\left(\frac{|\vec{H}|}{\hbar}t\right) \frac{\vec{H}}{|\vec{H}|} \cdot \sigma \right) \quad (17)$$

Schrödinger

There is an alternative way of finding the time dependence. Instead of having the matrices change with time, one can have the state change with time.

In the Heisenberg representation, the matrices and in particular their eigenvectors change in time

$$|A(t), a_i\rangle = U(t)|A_0, a_i\rangle \quad (18)$$

The inner product between the state of the system $|\psi\rangle$ and any eigenvector, which determines the probabilities is given by $\langle A(t), a_i | \psi \rangle$. However, we get the same amplitude if instead of having the eigenvectors evolve, we have the state evolve.

$$\langle A(t), a_i | \psi \rangle = (U(t)|A_0, a_i\rangle)^\dagger |\psi\rangle = \langle A_0, a_i | U(t)^\dagger |\psi\rangle \quad (19)$$

Ie, all of the amplitudes and probabilities remain the same if, instead of having the operators depend on time, we instead have the state evolve as $U(t)^\dagger |\psi\rangle$. We can write this as an equation for $|\psi, t\rangle$ by the equation

$$\begin{aligned} i\hbar \frac{d|\psi, t\rangle}{dt} &= i\hbar \frac{dU^\dagger}{dt} |\psi\rangle = i\hbar \frac{dU(t)^\dagger}{dt} U(t) U(t)^\dagger |\psi\rangle \\ &= (U^\dagger H U) |\psi, t\rangle \end{aligned} \quad (20)$$

The term $U^\dagger H U$ is the Schrödinger Hamiltonian. If H and U commute, which they will do if H is independent of time, then the Heisenberg and Schrödinger hamiltonians are the same.

This equation is the Schrödinger for the evolution of the system. In this case the matrices representing the attributes of the system remain constant, and the state changes with time. Especially for complex systems, this equation is often more easily solved than are the Heisenberg equations of motion.

Note that there is no classical analog for these two approaches. In classical physics, the state, the values which are associated with some attribute of the system are assumed to change in exactly the same way as do the variables which represent those attributes. Thus $x(t) = A\cos(\omega t)$ for a harmonic oscillator means that the attribute which is the position is a function of time in the same way as are the values which are actually ascribed to an attribute.

Appendix

We want to prove that if $U^\dagger U = I$ and that UAU^\dagger has the same eigenvalues as A for all matrices A then we also have $UU^\dagger = I$

One of the Hermitean matrices is the matrix I which has all of its eigenvalues equal to 1. Thus the matrix UIU^\dagger must also have all of its eigenvalues equal to 1 as well. Choosing a set of eigenvectors, $|i\rangle$ as the eigenvectors of UU^\dagger , and recalling that any vector $|\psi\rangle$ can be written as

$$|\psi\rangle = \sum_i \langle i|\psi\rangle |i\rangle \tag{21}$$

we see that $UU^\dagger|\psi\rangle = |\psi\rangle$, which is the definition of the identity matrix.

(Note that I have used the fact that the set of all eigenvectors of a Hermitean operators is complete in the above. Ie, any vector can always be written as a linear combination of the eigenvectors. I have not proven this in this course. You will have to accept it on faith, or wait until it is proven in your Linear algebra course.)