Chem. 540
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## Symmetries, Commutators and Conservation Laws

In class we proved a theorem that relates the time derivative of an observable to the commutator between the corresponding operator and the system's Hamiltonian. Thus, if an operator (which is not explicitly time-dependent) commutes with the Hamiltonian, the corresponding observable is a conserved quantity.

The classical version of this involves the classical analogue of the commutator, which is called Poisson bracket. If a dynamical variable Poisson commutes with the Hamiltonian, the dynamical variable is a constant of the motion.

Noether's theorem relates this to symmetries. It states that any differentiable symmetry of the action integral in a physical system has a corresponding conservation law. For example, the Lagrangian (and thus the action) of a system with orientational symmetry is rotationally invariant. This symmetry leads to conservation of the total angular momentum.

Perhaps the simplest way to understand this is through Hamilton's equations of motion: A symmetry manifests itself as the absence of dependence of the system's Lagrangian (by extension, the Hamiltonian) on a particular coordinate (in a judiciously chosen coordinate system of course!) If the Hamiltonian does not contain explicitly a particular coordinate, the corresponding canonical momentum is conserved. Hamilton-Jacobi theory takes advantage of this in the most elegant (yet formal, often impractical) way.

I note in passing that a classical system of $N$ degrees of freedom can have up to $N$ (independent) constants of the motion. Most systems in the real world have between 1 and $N$ constants of the motion (e.g., the energy, often the angular momentum, and sometimes some non-obvious quantities, which may be related to hidden symmetries).

We also proved that when two operators commute, they share common eigenstates. We should be a bit careful here: if there are degeneracies, not every eigenstate of either operator will be an eigenstate of the other. What we proved is that if $[\hat{A}, \hat{B}]=0$ and if $\Phi$ is the only eigenstate of $\hat{A}$ with the particular eigenvalue, then $\Phi$ must also be an eigenstate of $\hat{B}$. If there are other eigenstates of $\hat{A}$ that are degenerate to $\Phi$, we have no guarantee that the chosen state will be an eigenstate of $\hat{B}$. Consider, for example, $\hat{A}=\hat{p}, \hat{B}=\hat{p}^{2} / 2 m$, the Hamiltonian for a free particle. Any eigenstate of momentum, i.e. any function of the type $\exp (i k x)$, is an simultaneous eigenstate of both operators. However, not every eigenstate of the free particle Hamiltonian is an eigenstate of momentum, because we can form such states by taking linear combinations of states corresponding to momenta $\pm \hbar k$ (i.e., states that describe particles moving in opposite directions.)

Similarly, if $[\hat{A}, \hat{B}]=0$ and $[\hat{B}, \hat{C}]=0$, we can say that the operators in each pair share common eigenstates. If there are no degeneracies, then each eigenstate of $\hat{B}$ will also be an eigenstate of $\hat{A}$ and of $\hat{C}$, such that $\hat{A}$ and $\hat{C}$ have the same eigenstates, thus they must commute. But if there are degeneracies the common eigenstates of $\hat{A}$ and $\hat{B}$ may be different from the common eigenstates of $\hat{B}$ and $\hat{C}$, meaning that $\hat{A}$ and $\hat{C}$ may not have common eigenstates and may not commute. As an illustration consider the angular momentum operators $\hat{A}=\hat{L}_{z}, \hat{B}=\hat{L}^{2}, \hat{C}=\hat{L}_{x}$. Even though two pairs commute, the operators in the third pair do not commute, because there are degeneracies in the spectrum of $\hat{L}^{2}$.

Another subtle implication of the above note on degeneracies is that if two operators act in different spaces (e.g., if they depend on different coordinates), one has to be extra careful to avoid arriving at the wrong conclusion. For example, let's choose $\hat{A}=\hat{x}, \hat{B}=\hat{p}_{y}, \hat{C}=\hat{p}_{x}$. Again $[\hat{A}, \hat{B}]=[\hat{B}, \hat{C}]=0$, and now none of these operators have degenerate states. Should we conclude that $[\hat{x}, \hat{p}]=0$ ? The resolution of this apparent paradox is that the operators operate in different spaces, so that the common eigenstates of pairs are states in two dimensions. So even though $\hat{A}=\hat{x}$ does not have degeneracies within its own space, there are an infinity of states of the type $|x\rangle\left|\varphi_{y}\right\rangle$ which satisfy the eigenvalue equation for this operator. Clearly, the vast majority of those are not eigenstates of $\hat{B}=\hat{p}_{y}$. Once we recognize this massive degeneracy we realize there is no contradiction.

Combining the theorems on simultaneous eigenstates and conservation laws, we see that if an operator commutes with the Hamiltonian, then not only will the expectation value of the observable be conserved, but also know (for non-degenerate states) we can determine with arbitrary precision both the given observable and the energy of the system.

Below I discuss a few examples.

## Momentum conservation

In the absence of external forces the Hamiltonian of a system is translationally invariant. Thus the momentum commutes with the Hamiltonian, and this implies conservation of momentum (both classically and quantum mechanically). If we prepare the system in a momentum eigenstate, thus we know its momentum with arbitrary precision, we are also able to determine its energy with arbitrary precision. (Note again the converse is not always true, according to the above discussion on degeneracies.) This statement applies to any dimension (i.e., in 3d space we are able to determine all three components of the momentum vector simultaneously, and all are conserved). How many constants of the motion do we have? For a particle in 3d that is not subject to external forces, there are three momentum components, and also the energy is conserved. However, the energy is a function of the three momentum components in this case (no potential field), so this is not independent, leaving us with three constants of the motion.

If we place a particle in an external potential field, we destroy translational symmetry. The Hamiltonian now includes a potential function, thus it no longer commutes with the momentum. Thus, the momentum is no longer a conserved quantity.

## Angular momentum conservation

If the Hamiltonian is invariant under rotations, as in spherically symmetric problems, the angular momentum commutes (classically and quantum mechanically) with the Hamiltonian. This leads to conservation of the angular momentum vector. Typical examples are a rigid body that is not subject to torques, a particle confined on a sphere, and the central force problem (a single planet orbiting a sun or an electron interacting with a nucleus, as in the hydrogen atom).

Just as in the previous example, all three components of the angular momentum vector $\mathbf{L}$ commute with $|\mathbf{L}|^{2}$, and (as mentioned in the context of Noether's theorem) also commute with the Hamiltonian. Thus we have several conserved quantities: $L_{x}, L_{y}, L_{z},|\mathbf{L}|^{2}$, and the energy. Once again, though, only three of these are independent.

What about simultaneous eigenstates? Although the three components of the angular momentum vector commute with the Hamiltonian, they don't commute with each other. Thus we have to pick: we can place the system in a simultaneous eigenstate of the energy, $|\mathbf{L}|^{2}$, and only one of the three components of $\mathbf{L}$. The choice is rather arbitrary (as is the choice of a coordinate system in the absence of symmetry breaking fields), but traditionally people prefer to work with the $z$ component. We may place the system in an eigenstate of $|\mathbf{L}|^{2}$ and $L_{z}$. Then we will be able to know the exact value of the energy, angular momentum magnitude, and the $z$ component of the angular momentum vector. However, we do not have precise information about the other two components of $\mathbf{L}$; if we measure those we will get a distribution of eigenvalues according to the measurement postulate.

For those who may want to learn more...
We will study the free particle very soon, also motion in various models including potential fields. Angular momentum will be discussed next month.

More on Poisson brackets, Lagrangian/Hamiltonian mechanics, action integral, Hamilton-Jacobi theory, time dependence, etc. will be presented in Chem. 550.

