

Quantum Mechanics II

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LECTURE 1: GROUP THEORY

Monday, January 13, 2020

0.1 Symmetries

What's so special about sines and cosines? We know that the equation

$$f'' + f = 0$$

has solutions

$$Ae^{it} = A \sin(t) + B \cos(t)$$

Let's generalize this. Let O be a differential operator. We can rewrite our equation as

$$O[f] = 0$$

where

$$O = \frac{d^2}{dt^2} + 1$$

If we transform to a new coordinate, $t \rightarrow t'$ or $t \rightarrow t + a$, $O \rightarrow O$, since

$$\frac{d}{dt} = \frac{d}{dt'} \frac{dt'}{dt} = \frac{d}{dt'}$$

Therefore, we say that O is invariant under time translations. If f is a solution to $O[f] = 0$, then performing a time translation leaves O invariant, but f is not invariant, so

$$O[f] \rightarrow O'[f(t+a)] = O[f(t+a)]$$

so we can conclude that $f(t + a)$ must also be a solution. Therefore, if Ae^{it} is a solution, so is $Ae^{ia}e^{it}$, so if we shift our coordinate t , our solutions are still sines and cosines. Why are Bessel functions and spherical harmonics special? Certain coordinate transformations (symmetry transformations) cause these functions to transform into versions of themselves. They are solutions to differential equations that allow you to generate other solutions through transformations. For instance, spherical harmonics transform to themselves under rotations. These invariances are symmetries.

0.1.1 Mathematical Formalism

There are two types of symmetries: continuous and discrete. These symmetries are defined by having invariants which are only invariant under continuous or discrete transformations.

We define transformations as a map $A \mapsto B$. A symmetry is a map which takes an object to itself: $A \mapsto A$. In physics, symmetries must leave the Hamiltonian invariant: $H \mapsto H$.

Example. Let

$$H = \frac{\vec{P}^2}{2m} \quad (\text{Free Particle})$$

This Hamiltonian is invariant under rotations. If we take a rotation matrix $R(\theta, \varphi)$ and operate it on \vec{P} , the Hamiltonian will not change. \diamond

In QM, we have restrictions on allowed symmetry transformations. We define the state of the system as $|\psi\rangle$, a ray in a Hilbert space, a vector space where $\langle\psi|\psi\rangle > 0$. It's technically not a vector, since there is no physical difference between $|\psi\rangle$ and $e^{i\lambda}|\psi\rangle$.

Call our symmetry transformation operator T , and let $T|\psi\rangle = |\psi'\rangle$ be our transformed state. We require that such a transformation preserves the inner product:

$$\langle\psi|\psi\rangle = 1 \implies \langle\psi'|\psi'\rangle = 1$$

If we transform the inner product,

$$\langle\psi|\psi\rangle \mapsto \langle\psi|T^\dagger T|\psi\rangle = 1$$

so

$$T^\dagger T = 1$$

This makes T unitary by definition.

Any symmetry operator in QM **must be unitary** (although they can also be anti-unitary, but that's not important for now).

The next constraint is that a symmetry transformation should form a group.

Definition 0.1.1 (Group). A group is a collection of elements $\{A_i\} = G$ and an operation \cdot which maps two group elements to another ($A_i \cdot A_j = A_k, A_{i,j,k} \in G$). In other words, the group (G, \cdot) must be closed. Additionally,

- There is an identity element A_0 such that $A_0 \cdot A_i = A_i \forall A_i$
- For each A_i , there exists an inverse element A_i^{-1} such that $A_i \cdot A_i^{-1} = A_0$
- The operation \cdot is associative: $(A_i \cdot A_j) \cdot A_k = A_i \cdot (A_j \cdot A_k)$

Example. The integers form a group under addition: $(\mathbb{Z}, +)$ \diamond

Example. The integers do not form a group under division, since, for example, $\frac{1}{2} \notin \mathbb{Z}$ \diamond

Example. The real numbers form a group under division if zero is not included, since $\frac{a}{0}$ is undefined \diamond

Given some Hermitian operator X ($X = X^\dagger$), we can form a unitary operator by exponentiation:

$$U = e^{iX}$$

since $U^\dagger = e^{-iX^\dagger} = e^{-iX}$, so $U^\dagger U = 1$.

What do we mean by an exponential of an operator? If we are in a finite-dimensional Hilbert space, our operator would be a matrix. We can write exponentiation as a Taylor series:

$$e^{iX} = \sum_{n=0}^{\infty} \frac{(-iX)^n}{n!}$$

These X operators are called the “generator” of the group. In general, a group has more than one generator. If we call these generators X_i , the elements of the group can be enumerated

$$U(\lambda_i) = e^{i\lambda_i X_i} = e^{i\vec{\lambda} \cdot \vec{X}}$$

We call $\vec{\lambda}$ the “group parameter”.

Example. We can define an arbitrary rotation by an axis of rotation \hat{n} and the magnitude of the rotation θ . We require $\hat{n} \cdot \hat{n} = 1$, so the entire rotation is defined by three parameters (two independent parts of the unit vector and the magnitude). Therefore

$$U = e^{i\hat{n} \cdot \vec{T}\theta} a \in G$$

where $\vec{X} = \vec{T}$ is the group generator for rotations.

Since these are elements of a group,

$$e^{i\hat{n}_1 \cdot \vec{T}\theta_1} e^{i\hat{n}_2 \cdot \vec{T}\theta_2} = e^{i\hat{n}_3 \cdot \vec{T}\theta_3}$$

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LECTURE 2: SYMMETRIES, CONTINUED

Wednesday, January 15, 2020

Last time, we showed that symmetries are groups. For example, rotations and translations are groups. Quantum mechanically, the group action is implemented by a unitary operator, U :

$$|\psi\rangle \mapsto U|\psi\rangle \quad U^\dagger U = 1 \quad U = e^{i\lambda_a X_a}$$

where X_a are the generators of the group and λ_a are the parameters which specify the particular element of the group.

The *group manifold* is the space of the group elements. For example, in the group $(\mathbb{R}, +)$, the group manifold is \mathbb{R} .

Consider 2-D rotations in a plane. You don’t need the whole real line to define the rotations, just the interval $[0, 2\pi)$. We parameterize this like a 1-D sphere, S^1 . As a point of clarity, we refer to spheres as the boundary of a disk, which is the closure of a ball.

In the last lecture, we also discussed discrete and continuous symmetries. In continuous symmetries, the group manifold contains an infinite number of elements and is smooth. The group manifolds of discrete symmetries have a finite number of elements and/or they are not smooth.

0.1.2 Action of a Group on an Operator

$$O \rightarrow UOU^\dagger \quad \text{when} \quad |\psi\rangle \rightarrow U|\psi\rangle$$

since

$$\langle\psi|O|\psi\rangle = \langle\psi|U^\dagger UOU^\dagger U|\psi\rangle = \langle\psi|O|\psi\rangle$$

0.1.3 Abelian Groups

In Abelian group, every element commutes. A classic example of a non-Abelian group is rotations.

For Abelian groups,

$$U(\vec{\lambda}_1)U(\vec{\lambda}_2) = e^{i\vec{\lambda}_1 \cdot \vec{X}} e^{i\vec{\lambda}_2 \cdot \vec{X}} = e^{i(\vec{\lambda}_1 + \vec{\lambda}_2) \cdot \vec{X}}$$

or

$$[\vec{\lambda}_1 \cdot \vec{X}, \vec{\lambda}_2 \cdot \vec{X}] = 0$$

For non-Abelian groups, $e^A e^B \neq e^{A+B}$, so the group generators do not commute. However, we know that the product must be a group element:

$$e^{i\vec{\lambda}_1 \cdot \vec{Y}} e^{i\vec{\lambda}_2 \cdot \vec{Y}} = e^{i\vec{\lambda}_3 \cdot \vec{Y}}$$

We can determine this element using the commutator:

$$[Y^a, Y^b] = i f^{abc} Y^c \quad (\text{Lie Algebra})$$

The value of $\vec{\lambda}_3$ only depends on the commutator of the \vec{Y} s, since if the commutator was zero, we would know exactly what it was.

f^{abc} are called *structure constants*. Notice that the left-hand side is antisymmetric, so the right-hand side must be:

$$f^{abc} = -f^{bac}$$

It can be shown that f^{abc} can be taken to be totally anti-symmetric.

Given f^{abc} , we can almost uniquely determine the group. Two different groups can have the same Lie Algebra.

0.1.4 Representations of the Rotation Group

There is a one-to-one map between the groups $(\{a, b\}, +)$ and $(\{e^a, e^b\}, \cdot)$. These are called representations—They form the same group. The rotation group can have an infinite number of representations.

A rotation is any transformation on a vector that preserves the length of the vector:

$$R\vec{x} = \vec{x}' \quad \|\vec{x}\| = \|\vec{x}'\|$$

By this definition,

$$\begin{aligned} \vec{x}^T \cdot \vec{x} &= \vec{x}'^T \cdot \vec{x}' \\ &= \vec{x}^T R^T R \vec{x} = 1 \end{aligned}$$

so

$$R^T = R^{-1}$$

This is the definition of orthogonality. We call the group of 3-D rotations $SO(3)$, which stands for *special orthogonal transformations in 3-D*. The S means that the group elements must have unit determinants. This preserves the “handedness” of the coordinate system under the transformation. 3-by-3 matrices are the defining representation of this group, although they are not the only representation. Let’s call \vec{L} the generators of $SO(3)$. There must be three generators since there are three parameters needed to specify a rotation. Recall that each group element is defined by $e^{i\vec{\lambda}\vec{L}}$ so \vec{L} and $\vec{\lambda}$ must have the same dimensionality.

The Lie Algebra of $SO(3)$ is

$$[L_a, L_b] = i\epsilon_{abc} L_c$$

Here, the structure constants are the Levi-Civita symbol.

Now, let us introduce another, seemingly unrelated group, $SU(2)$, or *special unitary 2x2 matrices*. Unitary implies complex values, otherwise it would be orthogonal. If $g_1, g_2 \in SU(2)$, we should find that $g_1 g_2 = g_3 \in SU(2)$:

$$\begin{aligned}(g_1 g_2)^\dagger &= g_2^\dagger g_1^\dagger \\ (g_1 g_2)(g_1 g_2)^\dagger &= g_1 g_2 g_2^\dagger g_1^\dagger \\ &= g_1 g_1^\dagger = 1\end{aligned}$$

If $g \in SU(2)$, we can write

$$g = e^{i\vec{\lambda} \cdot \vec{T}}$$

Recall that all generators are Hermitian: $T^\dagger = T$. We also know, by definition of the group (special) that

$$\det(e^{i\vec{\lambda} \cdot \vec{T}}) = 1$$

In general,

$$\det(A) = e^{\text{Tr} \ln A}$$

If

$$A = \begin{pmatrix} \alpha_1 & & \\ & \ddots & \\ & & \alpha_n \end{pmatrix}$$

then

$$\ln A = \begin{pmatrix} \ln \alpha_1 & & \\ & \ddots & \\ & & \ln \alpha_n \end{pmatrix}$$

If we are in such a basis,

$$e^{\text{Tr} \ln e^{i\vec{\lambda} \cdot \vec{T}}} = e^{\text{Tr}[i\vec{\lambda} \cdot \vec{T}]} = 1$$

so

$$\text{Tr}[\vec{T}] = 0$$

We now know that \vec{T} are 2-by-2, traceless, Hermitian matrices. A general 2-by-2 complex matrix has eight parameters, but because it's Hermitian, the diagonal elements must be real and the off-diagonals must be complex conjugates, so we have four independent parameters. Next, if we require the trace to be zero, we require the off-diagonals to be additive inverses, so there are only three defining parameters for each group element.

Therefore, $SU(2)$ has three parameters (the generators are parameterized by three real numbers) and the generators are Hermitian ($T = T^\dagger$) and traceless ($\text{Tr}(T) = 0$). There are many (infinite) choices of generators. Let's choose the Pauli matrices:

$$\begin{aligned}T_1 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ T_2 &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ T_3 &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\end{aligned}$$

From this choice, we can see that $[T_a, T_b] = i\epsilon_{abc}T_c$, which is the same Lie Algebra as $SO(3)$.

LECTURE 3: SYMMETRIES, CONTINUED
Friday, January 17, 2020

Recall that we said there exist representations of groups which are quantum mechanically written as

$$U = e^{i\vec{\lambda} \cdot \vec{X}}$$

where \vec{X} are called generators. The generators of continuous groups obey a Lie Algebra:

$$[X_i, X_j] = if_{ijk}X_k$$

Definition 0.1.2 (Representation). If we consider an abstract group space G and everything in that space is a group element, we know that if we pick out two elements g_1 and g_2 from that space and multiply them together, we will get an element $g_3 \in G$. This is a bilinear map because it takes two elements of one space and maps to a third element. This map happens to be a mapping $G \mapsto G$.

If we consider matrix representations, there is a mapping from the group elements to a matrix, and the product of those matrices must map to the representation of the third group element as above.

Suppose we have some operator \hat{O} acting on an eigenstate:

$$\hat{O}|\psi\rangle = \lambda\psi$$

Suppose that G is a symmetry that leaves \hat{O} invariant.

$$\hat{O} \rightarrow U\hat{O}U^\dagger = \hat{O}$$

Recall $U^\dagger U = 1$:

$$\hat{O}U^\dagger U|\psi\rangle = \lambda|\psi\rangle$$

Multiply both sides by U :

$$(U\hat{O}U^\dagger)U|\psi\rangle = \lambda U|\psi\rangle$$

However, since the symmetry leaves \hat{O} invariant, this is equivalent to

$$\hat{O}(U|\psi\rangle) = \lambda(U|\psi\rangle)$$

so we find that $U|\psi\rangle$ is also an eigenvector. Essentially, we've found an additional solution by examining the symmetries of the system.

0.2 Conservation Laws

Symmetries imply conservation laws. Suppose we are given a Lagrangian:

$$L(x, \dot{x})$$

Suppose the Lagrangian is invariant under some group transformation $\vec{x} \rightarrow \vec{x}'$. There is an action

$$S = \int dt L(x, \dot{x})$$

Minimizing this action gives us the equations of motion for the system:

$$x(t) \rightarrow x(t) + \delta x(t)$$

We are going to look for x 's that minimize the action:

$$\begin{aligned}\delta S &= \int \left[\frac{\delta L}{\delta x} \delta x + \frac{\delta L}{\delta \dot{x}} \delta \dot{x} \right] dt \\ &= \int \left[\frac{\delta L}{\delta x} \delta x + \frac{d}{dt} \left(\frac{\delta L}{\delta \dot{x}} \delta x \right) - \delta x \frac{d}{dt} \frac{\delta L}{\delta x} \right] \\ &= \int_{t_i}^{t_f} dt \delta x \left[\frac{\delta L}{\delta x} - \frac{d}{dt} \frac{\delta L}{\delta \dot{x}} \right] + \underbrace{\frac{\delta L}{\delta \dot{x}} \delta x}_{0} \Big|_{t_i}^{t_f}\end{aligned}$$

Therefore, to minimize δS , we require

$$\frac{\delta L}{\delta x} = \frac{d}{dt} \frac{\delta L}{\delta \dot{x}}$$

which are the Euler-Lagrange equations.

If we have a transformation that keeps the Lagrangian invariant, we can take a total derivative of the Lagrangian:

$$\delta L = \frac{\delta L}{\delta x} \delta x + \frac{\delta L}{\delta \dot{x}} \delta \dot{x}$$

so

$$\int \left[\frac{\delta L}{\delta x} - \frac{d}{dt} \frac{\delta L}{\delta \dot{x}} \right] \delta x + \frac{d}{dt} \left[\frac{\delta L}{\delta \dot{x}} \delta x \right] = 0$$

If we assume the Euler-Lagrange equations hold and we no longer take the end points to be fixed,

$$\frac{d}{dt} \left[\frac{\delta L}{\delta \dot{x}} \delta x \right] = 0 \quad (\text{Noether's Theorem})$$

Therefore, $\frac{\delta L}{\delta \dot{x}} \delta x$ is a constant along a classical trajectory.

Example. Suppose L is invariant under translations. Under translations, $\vec{x} \rightarrow \vec{x} + \vec{\epsilon}$ so $\delta \vec{x} = \vec{\epsilon}$. Therefore, the corresponding conserved quantity is

$$\frac{\delta L}{\delta \dot{\vec{x}}} \vec{\epsilon}$$

If $\vec{\epsilon}$ does not change with time (fixed velocity), $\frac{\delta L}{\delta \dot{\vec{x}}} = \vec{p}$ is conserved (momentum conservation). \diamond

Example. Now consider a Lagrangian invariant rotations. $\delta L = 0$ and $\vec{x} \rightarrow R\vec{x}$. Recall we can represent a rotation by a unit vector and a magnitude:

$$R(\hat{n}, \theta) = e^{i\vec{L} \cdot \hat{n}\theta}$$

Recall that $R^T R = 1$, so if we consider infinitesimal rotations, we find that

$$R^T R = 1 = (1 + i\vec{L}^T \cdot \hat{n}\theta)(1 + i\vec{L} \cdot \hat{n}\theta)$$

so

$$1 + i\vec{L}^T \cdot \hat{n}\theta + i\vec{L} \cdot \hat{n}\theta + \mathcal{O}(\theta^2) = 1$$

so

$$\vec{L}^T \cdot \hat{n}\theta + \vec{L} \cdot \hat{n}\theta = 0$$

so

$$\vec{L}^T = -\vec{L}$$

so the generators are anti-symmetric.

$$\delta \vec{x} = \vec{x}' - \vec{x} = e^{i\vec{L} \cdot \hat{n}\theta} \vec{x} - \vec{x} = (\vec{x} + i\vec{L} \cdot \hat{n}\theta \vec{x} - \vec{x})$$

so

$$\delta \vec{x} = i\vec{L} \cdot \hat{n}\theta \vec{x}$$

Our conservation law is now

$$\frac{d}{dt} \left[\frac{\delta L}{\delta \dot{\vec{x}}} \left(\dot{\vec{L}} \cdot \hat{n} \theta \vec{x} \right) \right] = 0$$

There are three generators, and we will denote them using an upper index for now (a, b, c) . The lower indices will be the matrix element.

$$(\vec{L}) = (L)_{ij}^a$$

Recall the Lie algebra of the rotation group:

$$[L^a, L^b] = \epsilon^{abc} L^c$$

The 3-by-3 representation of the L can be written

$$\iota L_{ij}^a = \epsilon_{ij}^a$$

Don't confuse this with the structure constants, although it is the same Levi-Civita tensor. This tells us that

$$\iota^2 \epsilon_{ij}^a \epsilon_{jk}^b - \iota^2 \epsilon_{ij}^b \epsilon_{jk}^a = \iota^2 \epsilon^{abc} \epsilon_{ik}^b$$

The Levi-Civita Symbol

$$\epsilon_{ijk} \epsilon_{ijk} = 6$$

$$[\epsilon_{ija} \epsilon_{ijb} = \delta_{ab} A] \delta_{ab}$$

now

$$\epsilon_{ija} \epsilon_{ija} = A \delta_{aa}$$

or $6 = 3A$, or $A = 2$, so

$$\epsilon_{ija} \epsilon_{ijb} = 2 \delta_{ab}$$

Finally,

$$\epsilon_{ija} \epsilon_{kla} = A \delta_{ik} \delta_{jl} + B \delta_{il} \delta_{jk} + C \delta_{ij} \delta_{kl}$$

If we interchange i and j , the right side must be antisymmetric. Therefore C is zero, since that term is symmetric in i and j . We can also conclude that $B = -A$ so

$$\epsilon_{ija} \epsilon_{kla} = A [\delta_{ik} \delta_{jl} - \delta_{il} \delta_{jk}]$$

Contract both sides with $\delta_{ik} \delta_{jl}$, and we find

$$6 = A [\delta_{ii} \delta_{jj} - \delta_{ij} \delta_{ji}] = A[9 - 3] = 6$$

so $A = 1$:

$$\epsilon_{ija} \epsilon_{kla} = \delta_{ik} \delta_{jl} - \delta_{il} \delta_{jk}$$

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LECTURE 4: CONSERVED CHARGE OF ROTATIONAL INVARIANCE

Wednesday, January 22, 2020

Recall Noether's theorem from the previous lecture:

$$\frac{d}{dt} \left[\frac{\delta L}{\delta \dot{\vec{x}}} \delta \vec{x} \right] = 0$$

If the action is rotationally invariant,

$$\vec{x} \rightarrow R(\hat{n}, \theta) \vec{x}$$

where

$$R(\hat{\mathbf{n}}, \theta) = e^{i\vec{\mathbf{L}} \cdot \hat{\mathbf{n}}\theta}$$

In the previous lecture, we found that

$$\imath(L^a)_{ij} = \epsilon_{ij}^a \equiv \epsilon_{aij}$$

If we expand the exponential to a few terms, we find

$$e^{i\vec{\mathbf{L}} \cdot \hat{\mathbf{n}}\theta} \rightarrow 1 + i\vec{\mathbf{L}} \cdot \hat{\mathbf{n}}\theta + \mathcal{O}(\theta^2)$$

as $\theta \rightarrow 0$. We find $\delta\vec{\mathbf{x}}$ to be

$$\begin{aligned}\delta\vec{\mathbf{x}} &= \left[(i\vec{\mathbf{L}} \cdot \hat{\mathbf{n}})_{ij} \theta \right] x_j \\ &= (\imath(L^a)_{ij} n^a x_j) \theta \\ &= (\epsilon_{aij} n_a x_j) \theta\end{aligned}$$

If our Lagrangian has the form

$$L = \frac{1}{2} m \dot{x}^2 - V(x)$$

we find that Noether's theorem gives us

$$\begin{aligned}\frac{d}{dt} [m\dot{x}_i \delta x_i] &= 0 \\ &= \frac{d}{dt} m [\dot{x}_i (n_a \theta \epsilon_{aij} x_j)] \\ &= \frac{d}{dt} [m\dot{x}_i \epsilon_{aij} x_j n_a \theta]\end{aligned}$$

Because $\hat{\mathbf{n}}$ and θ are arbitrary and this equation must be true for all $\hat{\mathbf{n}}$ and θ ,

$$\frac{d}{dt} \left[\underbrace{m\dot{x}_i}_{p_i} \epsilon_{aij} x_j \right] = 0$$

so

$$p_i x_j \epsilon_{aij} = \vec{\mathbf{x}} \times \vec{\mathbf{p}} = \vec{\mathbf{L}} \quad \longrightarrow \quad \text{invariant}$$

0.3 Conservation Laws in Quantum Mechanics

The fundamental time-evolution equation in QM is the Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = H |\psi\rangle$$

The Schrödinger picture is a formulation where we make the operators independent of time, but allow the wave functions to be time-dependent.

The Heisenberg picture is a formulation where all of the operators are time-dependent whereas the wave functions are time-independent.

There is a simple way to transform between the two using a time-evolution operator:

$$U(t', t) = e^{-iH(t'-t)/\hbar}$$

If we work in the Schrödinger picture, we know that $|\psi(t')\rangle = U(t', t) |\psi(t)\rangle$. If we consider the expectation value of some operator:

$$\langle \psi(t') |_S O_S |\psi(t)\rangle_S = \langle \psi(t') | U^\dagger(t', t) O U(t', t) |\psi(t)\rangle$$

We could equivalently define

$$O_H(t') = U^\dagger(t', t) O_S U(t', t)$$

such that

$$\langle \psi(t') |_S O_S |\psi(t)\rangle_S = \langle \psi |_H O_H(t') |\psi\rangle_H$$

where

$$|\psi\rangle_H \equiv U(t', t) |\psi(t)\rangle_S$$

We can use the Schrödinger equation on the Heisenberg picture operator:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} O_H(t) &= \\ i\hbar \frac{\partial}{\partial t} \langle \psi |_S O_S |\psi\rangle_S &= \left[i\hbar \frac{\partial}{\partial t} \langle \psi |_S \right] O |\psi\rangle_S + \langle \psi |_S O \left[i\hbar \frac{\partial}{\partial t} |\psi\rangle_S \right] \\ &= -\langle HO |\psi\rangle_H O + \langle OH |\psi\rangle_H O \\ &= \langle [O, H] |\psi\rangle_H \\ &= i\hbar \langle \psi |_H \frac{d}{dt} O_H(t) |\psi\rangle_H \end{aligned}$$

so

$$i\hbar \frac{d}{dt} O_H(t) = [O, H]$$

What does this have to do with conserved quantities? If $[O, H] = 0$, O is time independent. In quantum mechanics, a symmetry is always expressible in terms of a unitary transformation

$$U = e^{i\vec{X} \cdot \vec{\lambda}}$$

where $\vec{X}^\dagger = \vec{X}$ are the generators of the symmetry which obey a Lie algebra $[X_a, X_b] = if_{abc} X_c$.

The difference between classical and quantum mechanics is that everything is an operator, and operators transform under symmetries:

$$O \rightarrow U^\dagger(\vec{\lambda}) O U(\vec{\lambda})$$

where $\vec{\lambda}$ is the set of parameters which determine the group element. Now consider some of the typical operators and how they transform. Under rotations, the position operator transforms as

$$\vec{x} \rightarrow U(\hat{n}, \theta) \vec{x} U(\hat{n}, \theta)$$

or

$$\vec{x}' = e^{-i\vec{L} \cdot \hat{n}\theta/\hbar} \vec{x} e^{i\vec{L} \cdot \hat{n}\theta/\hbar}$$

Consider an infinitesimal rotation ($\theta \rightarrow 0$):

$$\vec{x}' = (1 - i\frac{\vec{L}}{\hbar} \cdot \hat{n}\theta) \vec{x} (1 + i\frac{\vec{L}}{\hbar} \cdot \hat{n}\theta) + \mathcal{O}(\theta^2)$$

or

$$\vec{x}' = \vec{x} - (i\frac{\vec{L}}{\hbar} \cdot \hat{n}\theta) \vec{x} + \vec{x} (i\frac{\vec{L}}{\hbar} \cdot \hat{n}\theta)$$

so

$$\delta \vec{x} = \vec{x} (i\frac{\vec{L}}{\hbar} \cdot \hat{n}\theta) - (i\frac{\vec{L}}{\hbar} \cdot \hat{n}\theta) \vec{x}$$

so

$$\delta x_a = [(x_a (iL_b)/\hbar) - (iL_b X_a)/\hbar] \hat{n}_b \theta$$

We define the angular momentum operator as

$$\vec{L} \equiv \vec{x} \times \vec{p} = \vec{x} \times \left(i\hbar \frac{\partial}{\partial \vec{x}} \right)$$

We can also write this in index notation:

$$L_b = -i\hbar x_i \partial_j \epsilon_{ijb}$$

Let's now apply this to our δx_a formula:

$$\delta x_a = (i\hat{\mathbf{n}}_b\theta) \left[x_a, i\frac{L_b}{\hbar} \right]$$

Now we just need to figure out what the commutator is.

$$\left[x_a, i\frac{L_b}{\hbar} \right] = [x_a, x_c p_d \epsilon_{cdb}]$$

ϵ_{cdb} is just a constant, we can take it out, and we are left with

$$[x_a, i x_c p_d] = i[x_a, x_c] p_d + x_c i[x_a, p_d]$$

since

$$[A, BC] = [A, B]C + B[A, C]$$

Position commutes with itself and $[x_a, p_d] = i\hbar\delta_{ad}$ so

$$[x_a, x_c p_d] = -x_c(\delta_{ad})$$

Finally

$$\begin{aligned} \delta x_a &= i\hat{\mathbf{n}}_b\theta\epsilon_{cdb}(i\hbar x_c\delta_{ad}) \\ &= -\hat{\mathbf{n}}_b\theta x_c\epsilon_{cab} \\ &= -\hat{\mathbf{n}}_b\theta x_c\epsilon_{abc} \end{aligned}$$

This is very similar to the classical case where

$$\delta x_a = \hat{\mathbf{n}}_b\theta x_c\epsilon_{abc}$$

Whereas in the quantum case we have

$$\delta x_a = -\hat{\mathbf{n}}_b\theta x_c\epsilon_{abc}$$

We have shown that the operator $\vec{\mathbf{x}}$ transforms just like a vector under rotation. If you did the same thing with $\vec{\mathbf{p}}$, you would find the exact same result (and a similar result with any vector operator).

LECTURE 5: SYMMETRIES AND CONSERVATION LAWS

Friday, January 24, 2020

From last lecture, $[H, O] = 0$, then O is a constant of motion as long as O has no explicit time dependence. If U implements a symmetry group G , under the action of G , $H \rightarrow U^\dagger H U$. We can write this as

$$e^{-i\vec{\lambda} \cdot \vec{\mathbf{X}}} H e^{i\vec{\lambda} \cdot \vec{\mathbf{X}}}$$

As a consequence, if $[H, \vec{\mathbf{X}}] = 0$, then H is invariant under G , since we pull H through the exponentials and they will cancel out. Therefore, if H is invariant under G , X is conserved.

If L is invariant, then maybe (usually) H is invariant, so this is a similar result to Noether's theorem in classical mechanics. The simplest counterexample is boosts. Take

$$L = \frac{1}{2}m\dot{x}^2$$

A boost transformation is $x \rightarrow x + \delta vt$, so

$$L \rightarrow \frac{1}{2}m\dot{x}^2 + m x \delta v$$

The action is still invariant, since

$$\delta S = \int dt \delta L = \int m \delta v x dt = \left[\frac{d}{dt} (m \delta v x) \right] dt = 0$$

Total derivatives have no effect on the equations of motion, since they don't change the Euler-Lagrange equations. A symmetry which takes $L \rightarrow L + \frac{d}{dt}f(x, \dot{x}, t)$ is still a symmetry. However, the Hamiltonian, which leads to quantum conservation laws, is not invariant under boosts, and there is no time integral to get rid of the consequences.

0.4 Degeneracy

Symmetries imply degeneracies. If G is a symmetry with generators \vec{X} , then $[H, \vec{X}] = 0$ implies

$$H|\lambda\rangle = E(\lambda)|\lambda\rangle \implies H\vec{X}|\lambda\rangle = E(\lambda)\vec{X}|\lambda\rangle$$

so if $\vec{X}|\lambda\rangle \neq |\lambda\rangle$, there exists a degeneracy.

Let's first look at a case which is not degenerate: rotations. On the homework, we saw that the group defined by 3D rotations (SO(3)) has the same Lie algebra as SU(2). We are going to call the generators of SO(3) $J_i \in \mathfrak{so}(3)$ such that

$$[J_i, J_j] = i\hbar\epsilon_{ijk}J_k$$

In QM, there are two ways of forming a group representation. The first are matrices, and the second are differential operators acting on an infinite dimensional space of square integrable functions L^2 ($L^2 = \{f(x) \mid \int |f(x)|^2 dx < \infty\}$). In other words, we can write

$$\vec{L} = i\vec{r} \times \vec{p}$$

but we can also write

$$\vec{p} = -i\hbar \frac{\partial}{\partial \vec{x}}$$

such that

$$\left[-i\hbar r_a \frac{\partial}{\partial r_b} \epsilon_{abi}, -i\hbar r_c \frac{\partial}{\partial r_d} \epsilon_{cdj} \right] = -i\hbar^2 \epsilon_{ijk} r_f \frac{\partial}{\partial r_g} \epsilon_{fgk}$$

Let's now find the matrix representations. First, find operators which commute with all elements of the Lie algebra:

$$[O, \vec{J}] = 0$$

These are called Casimir operators. For rotations, these operators happen to be \vec{J}^2 (for both SO(3) and SU(2)). As it turns out, this works for all vector operators:

$$U^\dagger(\hat{n}, \theta) \{P_i, X_i, L_i\} U(\hat{n}, \theta) = R(\hat{n}, \theta)_{ij} \{P_j, X_j, L_j\}$$

$$\begin{aligned} [\vec{J}^2, J_i] &= [J^a J^a, J^i] \\ &= J^a [J^a, J^i] - [J^i, J^a] J^a \\ &= J^a (i\hbar\epsilon^{aik} J^k) - (i\hbar\epsilon^{iak} J^k) J^a \\ &= i\hbar [e^{aik} J^a J^k - \epsilon^{iak} J^k J^a] \\ &= i\hbar [\epsilon^{kia} J^k J^a - \epsilon^{iak} J^k J^a] \\ &= [\epsilon^{kia} - \epsilon^{iak}] J^k J^a = 0 \end{aligned}$$

Or you could just say \vec{J}^2 is a scalar under rotations so it is invariant under rotations.

Every representation is labelled by eigenvalues of the Casimir operator.

Lemma 0.4.1 (Schur's Lemma). *Any group element which commutes with all other group elements is proportional to I (the identity).*

The eigenvalues of \vec{J}^2 are the total angular momentum:

$$\vec{J}^2 |a\rangle = a |a\rangle$$

The next step is to choose a generator to diagonalize (in $SO(3)$ you can only diagonalize one of them at a time since they don't commute with each other). We will arbitrarily choose J_z such that

$$J_z |a, b\rangle = b |a, b\rangle$$

We are working in a basis which are eigenvectors of J_z . There is nothing else we can diagonalize simultaneously, since the J 's don't individually commute. These a 's and b 's label the states of the representation. a will not change if we operate on this state with J_x or J_y , but b will change. What are the possible values of b ?

Define raising and lowering operators

$$J_{\pm} = \frac{(J_x \pm iJ_y)}{\sqrt{2}}$$

such that

$$[J_z, J_{\pm}] = \pm \hbar J_{\pm}$$

$$J_z J_{\pm} |a, b\rangle = (b \pm \hbar) J_{\pm} |a, b\rangle$$

Call $b = \hbar \hat{b}$:

$$J_z J_{\pm} |a, b\rangle = \hbar (\hat{b} \pm 1) J_{\pm} |a, b\rangle$$

so the action of the raising and lowering operators is to raise and lower b .

LECTURE 6: ANGULAR MOMENTUM

Monday, January 27, 2020

Last time we were talking about representations of rotations, either the $SO(3)$ or $SU(2)$ groups. We decided to label our representations using a Casimir operator (for vector operators, we use J^2), and we chose our basis to diagonalize J_z . We then defined raising and lowering operators

$$J_{\pm} = J_x \pm iJ_y$$

such that

$$J^2 |ab\rangle = a\hbar^2 |ab\rangle$$

$$J_z |ab\rangle = b\hbar |ab\rangle$$

and

$$J_{\pm} |ab\rangle \propto |a, \pm b\rangle$$

Now we want to determine the allowed values of b . Consider $J^2 - J_z^2 = J_x^2 + J_y^2$:

$$J^2 - J_z^2 = \frac{1}{2} [J_+ J_- + J_- J_+]$$

Recall that $J_{\pm}^{\dagger} = J_{\mp}$, so

$$J^2 - J_z^2 = \frac{1}{2} [J_+ J_+^{\dagger} + J_- J_-^{\dagger}]$$

Since $\langle \psi | O O^{\dagger} | \psi \rangle \geq 0$ (because $\|O|\psi\rangle\|^2 \geq 0$),

$$(J^2 - J_z^2) \geq 0 \implies (a - b^2) \geq 0 \implies |b| \leq |a|$$

Next, we will solve for b_{\max} and b_{\min} :

$$J_- J_+ |b_{\max}\rangle = 0$$

since $J_+ |b_{\max}\rangle = J_- |b_{\min}\rangle = 0$.

$$J_- J_+ = J_x^2 + J_y^2 + i[J_x, J_y] = J_x^2 + J_y^2 - \hbar J_z$$

Therefore, we can rewrite this as

$$J_- J_+ = J^2 - J_z^2 - \hbar J_z$$

Let's now operate this on the b_{\max} state:

$$0 = (J^2 - J_z^2 - \hbar J_z) |ab_{\max}\rangle = (\hbar^2) [a - b_{\max}^2 - b_{\max}] |ab_{\max}\rangle \implies a = b_{\max}(b_{\max} + 1)$$

We can do a similar calculation for b_{\min} with J_+J_- to show that $a = b_{\min}(b_{\min} - 1)$. Finally, we can equate the a terms to show that

$$b_{\max}(b_{\max} + 1) = b_{\min}(b_{\min} - 1) \implies b_{\max} = -b_{\min}$$

The only way for this to be true is for $b_{\max} \in \frac{\mathbb{Z}}{2}$. Therefore, the number of states in a representation is $d = (2b_{\max} + 1)$. If b_{\max} is a half-integer, this corresponds to representations of $\text{SU}(2)$, whereas integer b_{\max} give representations of $\text{SO}(3)$. $d = 2$ are not "faithful" (one-to-one) representations of $\text{SO}(3)$, but they are faithful representations of $\text{SU}(2)$.

0.4.1 Matrix Representation

If we consider

$$\langle j'm' | J^2 | jm \rangle = \langle j'm' | jm \rangle \hbar^2 j(j+1) = \delta_{jj'} \delta_{mm'} \hbar^2 j(j+1)$$

so

$$J^2 = \mathbb{I} \cdot \hbar^2 j(j+1)$$

Next, consider

$$\langle j'm' | J_z | jm \rangle = \delta_{jj'} \delta_{mm'} m \hbar$$

so J_z is also diagonal:

$$J_z = \begin{bmatrix} m & & & & \\ & m-1 & & & \\ & & m-2 & & \\ & & & \ddots & \\ & & & & -m \end{bmatrix}$$

Finally, consider the ladder operators:

$$|J_{\pm} | jm \rangle = c_{\pm} |j, m \pm 1\rangle^2$$

so

$$|c_{\pm}|^2 = \langle jm | J_{\mp} J_{\pm} | jm \rangle$$

For the c_+ case,

$$|c_+|^2 = \langle jm | \underbrace{J_x^2 + J_y^2}_{J^2 - J_z^2} - \hbar J_z | jm \rangle = \hbar^2 \left[j(j+1) - \underbrace{m(m+1)}_{m^2 - m} \right]$$

In general, we often write this constant with a phase:

$$|c_{\pm}|^2 = \hbar e^{i\varphi} [(j \mp m)(j \pm m + 1)]^{\frac{1}{2}}$$

so

$$\langle j'm' | J_{\pm} | jm \rangle = \hbar \delta_{jj'} \delta_{m', m \pm 1} [(j \mp 1)(j \pm m + 1)]^{\frac{1}{2}}$$

0.4.2 Representations of Rotation Matrices

$$U(\hat{\mathbf{n}}, \theta) = e^{-i\hat{\mathbf{n}} \cdot \vec{\mathbf{J}}\theta}$$

We can write the general matrix elements as

$$\langle j'm' | e^{-i\hat{\mathbf{n}} \cdot \vec{\mathbf{J}}\theta} | jm \rangle = D_{mm'}^{(j)}(\hat{\mathbf{n}}, \theta)$$

These are known as the Wigner functions. The representations are labeled by j , so j' doesn't really matter here, it just specifies the dimensionality of the matrix.

0.4.3 Irreducible Representations

There are two types of representations, reducible and irreducible. An irreducible representation has no invariant subspaces. This means that there is no way to write it in block-diagonal form:

$$\begin{bmatrix} A_{n \times n} & & & \\ & B_{m \times m} & & \\ & & \ddots & \\ & & & Z_{l \times l} \end{bmatrix}$$

LECTURE 7: REPRESENTATIONS OF SU(2)

Wednesday, January 29, 2020

From last lecture, we were examining the (irreducible) representations of SU(2). We found that $-(2j+1) \leq m \leq (2j+1)$ and that the dimensionality of any representation of this form is

$$\dim(R) = 2j+1 \quad j \in \frac{\mathbb{Z}}{2}$$

$$J^2 |jm\rangle = \hbar^2 j(j+1) |jm\rangle$$

$$J_z |jm\rangle = \hbar m |jm\rangle$$

and

$$J_{\pm} |m\rangle = c_{\pm} |m \pm 1\rangle$$

where

$$c_{\pm} = \hbar \sqrt{(j \pm m)(j \pm m + 1)}$$

Consider the 3-dimensional representation ($j = 1$). We can write down the matrix elements of any given group element:

$$\langle m' | J_x | m \rangle = \langle m' | \frac{1}{2} (J_+ + J_-) | m \rangle = c \delta_{m', m+1} + c' \delta_{m', m-1}$$

We also discussed the unitary operator which comes from exponentiating the group elements and defined these as the Wigner matrices:

$$U(\hat{\mathbf{n}}, \theta) = e^{-i \frac{\hat{\mathbf{n}} \cdot \hat{\mathbf{J}}}{\hbar} \theta}$$

$$\langle jm | U(\hat{\mathbf{n}}, \theta) | jm' \rangle = D_{mm'}^{(j)}(\hat{\mathbf{n}}, \theta)$$

We also showed that

$$D_{m'm}^{(j)} | jm \rangle = | jm' \rangle$$

so

$$J^2 | jm' \rangle = J^2 D_{m'm}^{(j)} | jm \rangle = D_{m'm}^{(j)} \hbar^2 j(j+1) | jm \rangle = \hbar^2 j(j+1) D_{m'm}^{(j)} | jm \rangle = \hbar^2 j(j+1) | jm' \rangle$$

The Wigner matrices form an irreducible representation of SU(2):

$$D_{mm'}^{(j)}(R_1) D_{m'm''}^{(j)}(R_2) = D_{mm''}^{(j)}(R_1 R_2)$$

0.4.4 Euler Angles

Any rotation can be written as a sum of rotations about three axes. By convention, we call the magnitudes of the rotations (α, β, γ) , where the rotations are over the axes $\hat{\mathbf{z}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ again in that order. We can write the Wigner matrices in terms of Euler angles:

$$D_{m'm}^{(j)}(\alpha, \beta, \gamma) = \langle m' | e^{-i\alpha J_z/\hbar} e^{-i\beta J_y/\hbar} e^{-i\gamma J_z/\hbar} | m \rangle = e^{-i(\alpha m' + \gamma m)} \underbrace{\langle m' | e^{-i\beta J_y/\hbar} | m \rangle}_{d_{m'm}^{(j)}(\beta)}$$

0.5 Orbital Angular Momentum

Let's now look at the observable \vec{L} . We can carry some similar terms over from the discussion of \vec{J} . Eigenstates will be written as

$$|lm\rangle \quad -(2l+1) \leq m \leq 2l+1$$

$$\hat{\mathbf{n}} \equiv \hat{\mathbf{n}}(\theta, \varphi)$$

We want to write our eigenvectors in terms of the axis of rotation $\hat{\mathbf{n}}$:

$$\langle \hat{\mathbf{n}} | L_z | lm \rangle = \hbar m \langle \hat{\mathbf{n}} | lm \rangle$$

Define

$$F_{l,m}(\theta, \varphi) = \langle \hat{\mathbf{n}} | lm \rangle$$

Consider

$$\begin{aligned} \langle \hat{\mathbf{n}} | R_z(\delta\varphi) | lm \rangle &\xrightarrow{\varphi \rightarrow 0} \langle \hat{\mathbf{n}} | \left(I - i \frac{L_z}{\hbar} \delta\varphi \right) | lm \rangle \\ &= \langle \hat{\mathbf{n}} | lm \rangle - i \frac{\delta\varphi L}{\hbar} \langle \hat{\mathbf{n}} | L_z | lm \rangle \\ \langle \theta, \varphi | R_z(\delta\varphi) | lm \rangle &= \\ \langle \theta, \varphi + \delta\varphi | &\approx \langle \theta, \varphi | - \frac{\partial}{\partial \varphi} \langle \theta, \varphi | \delta\varphi = \end{aligned}$$

Therefore

$$\begin{aligned} \langle \hat{\mathbf{n}} | lm \rangle - i \frac{\delta\varphi}{\hbar} \langle \hat{\mathbf{n}} | L_z | lm \rangle &= \langle \hat{\mathbf{n}} | lm \rangle - \delta\varphi \frac{\partial}{\partial \varphi} \langle \hat{\mathbf{n}} | lm \rangle \\ \langle \hat{\mathbf{n}} | L_z | lm \rangle &= \hbar m \langle \hat{\mathbf{n}} | lm \rangle = -i\hbar \frac{\partial}{\partial \varphi} \langle \hat{\mathbf{n}} | lm \rangle \end{aligned}$$

The solutions to this differential equation are the spherical harmonics:

$$F_{lm} \rightarrow Y_{lm}(\theta, \varphi) \implies -i\hbar \frac{\partial}{\partial \varphi} Y_{lm}(\theta, \varphi) = \hbar m Y_{lm}(\theta, \varphi)$$

However, this only clears up the φ dependence. Now we need to figure out how θ works:

$$L^2 Y_{lm} = \hbar^2 l(l+1) Y_{lm}$$

We can write

$$L_x = -i\hbar \left[-\sin(\varphi) \frac{\partial}{\partial \theta} - \cot(\theta) \cos(\varphi) \frac{\partial}{\partial \varphi} \right]$$

and

$$L_y = -i\hbar \left[\cos(\varphi) \frac{\partial}{\partial \theta} - \cot(\theta) \sin(\varphi) \frac{\partial}{\partial \varphi} \right]$$

so

$$L^2 = \left[-\frac{1}{\sin(\theta)} \frac{\partial}{\partial \theta} \left(\sin(\theta) \frac{\partial}{\partial \theta} \right) - \frac{1}{\sin^2(\theta)} \frac{\partial^2}{\partial \varphi^2} \right]$$

In certain cases, the Wigner matrices are actually equivalent to the spherical harmonics. Consider $|\hat{\mathbf{n}}\rangle = D(R) |\hat{\mathbf{z}}\rangle$. If we use our Euler rotation convention, the γ rotation is about $\hat{\mathbf{z}}$, but we are acting on $|\hat{\mathbf{z}}\rangle$, so this rotation does nothing:

$$D(R) |\hat{\mathbf{z}}\rangle = D(\alpha = \varphi, \beta = \theta, 0) |\hat{\mathbf{z}}\rangle$$

Let's insert the identity:

$$|\hat{\mathbf{n}}\rangle = \sum_{lm} D(R) |lm\rangle \langle lm | \hat{\mathbf{z}} \rangle$$

Next, project onto $|l'm'\rangle$:

$$\langle l'm'|\hat{\mathbf{n}}\rangle = \sum_{lm} \langle l'm'|D(R)|lm\rangle \langle lm|\hat{\mathbf{z}}\rangle$$

Rotation matrices don't change the length of the vector, so

$$\begin{aligned} \langle l'm'|\hat{\mathbf{n}}\rangle &= \sum_m \langle l'm'|D(R)|lm\rangle \langle lm|\hat{\mathbf{z}}\rangle \\ &= \sum_m D_{m'm}^{(l)}(R) \underbrace{\langle lm|\hat{\mathbf{z}}\rangle}_{Y_{lm}^*(\theta=0,\varphi)} \end{aligned}$$

Note

$$e^{iL_z\varphi}|\hat{\mathbf{z}}\rangle = |\hat{\mathbf{z}}\rangle \implies L_z|\hat{\mathbf{z}}\rangle = 0 \quad \text{and} \quad L_z|m=0\rangle = 0$$

Therefore

$$\langle l'm'|\hat{\mathbf{n}}\rangle = D_{m'0}^{(l)}(R)Y_{l0}^*(\theta=0,\varphi) = Y_{lm'}^*(\theta,\varphi)$$

We already know the φ -dependence:

Aside

The professor is not implying anything by raising the l -index (no Condon-Shortley phase)

$$L_z Y_m^l = \hbar m Y_m^l = -i\hbar \frac{\partial}{\partial \varphi} Y_m^l \implies Y_m^l \sim e^{im\varphi} F(\theta)$$

Therefore

$$Y_{l0}^*(\theta=0,\varphi) = Y_{l0}^*(\theta=0,\varphi=0) = \text{const.}$$

since all the φ -dependence only happens when $m \neq 0$.

For homework, we will show that

$$Y_0^l(0,0) = \sqrt{\frac{2l+1}{4\pi}}$$

Finally, this means that

$$Y_{lm'}^*(\theta,\varphi) = D_{m'0}(\alpha=\varphi,\beta=\theta,\gamma=0) \sqrt{\frac{2l+1}{4\pi}}$$

We have found that

$$D_{m'0}^{(l)}(\varphi,\theta,0) = \sqrt{\frac{4\pi}{2l+1}} Y_{lm'}^*(\theta,\varphi)$$

LECTURE 08: UTILIZING SYMMETRIES
Friday, January 31, 2020

0.6 The Hydrogen Atom

We've found that symmetries can tell us many things about our system, particularly degeneracies and conserved quantities. The Hamiltonian for the hydrogen atom can be written as

$$H = \sum_{i=1}^2 \frac{p_i^2}{2m_i} + V(|\vec{\mathbf{r}}_1 - \vec{\mathbf{r}}_2|)$$

This is a very general form of an interaction between two particles ($i = 1, 2$) where the potential just depends on the distance between the particles. Let's list the symmetries of this system

Symmetry	Invariant
SU(2) or SO(3)	\vec{L}
Time translation	H
Parity	? (discrete transformations don't have a conserved charge)
Translations	$\vec{p}_1 + \vec{p}_2 = \vec{p}_{\text{total}}$
Galilean Boosts ($\vec{r} \rightarrow \vec{r} - \vec{\beta}t$)	$\vec{R}_{\text{com}} = \frac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m_1 + m_2}$

The normalization on the center of mass position makes the math easier later and doesn't change the conserved property.

Galilean Boosts

$$L = \sum_{i=1}^2 \frac{1}{2} m_i \vec{v}_i^2 - V(|\vec{r}_1 - \vec{r}_2|)$$

$$L \rightarrow \sum_{i=1}^2 \frac{1}{2} m_i (\vec{v}_i - \vec{\beta})^2 - V(|\vec{r}_1 - \vec{r}_2|)$$

so

$$\delta L = - \sum_{i=1}^2 m_i \vec{v}_i \cdot \vec{\beta} = - \sum_{i=1}^2 m_i \vec{\beta} \cdot \frac{d}{dt}(\vec{r}_i)$$

This is just a total time derivative, which we showed on the homework leaves the action invariant:

$$\delta S = \int dt \left(- \sum_{i=1}^2 m_i \vec{\beta} \cdot \frac{d}{dt}(\vec{r}_i) \right)$$

Noether's theorem tells us that

$$\delta S = \int \sum \frac{d}{dt} \left(\frac{\delta L}{\delta \dot{\vec{r}}_i} \delta \vec{r}_i \right) = - \int \sum m_i \vec{\beta} \cdot \frac{d}{dt}(\vec{r}_i)$$

$$\frac{d}{dt} \left[\frac{\delta L}{\delta \dot{\vec{r}}_i} \delta \vec{r}_i + m_i (\vec{r}_i \cdot \vec{\beta}) \right] = 0$$

so the conserved quantity(s) are

$$0 = \frac{d}{dt} \left[m_i \dot{\vec{r}}_i (-\vec{\beta}t) + m_i (\vec{r}_i \cdot \vec{\beta}) \right] = \frac{d}{dt} \left[-m_i \dot{\vec{r}}_i t + m_i \vec{r}_i \right] \cdot \vec{\beta}$$

so we can define

$$\vec{k} = m_i \vec{r}_i - \vec{p}t$$

as the conserved constant of motion. Since \vec{p} is conserved, we can say that if $p_i = 0$, then $m_1 \vec{r}_1 + m_2 \vec{r}_2$ is a constant. This is the position of the center of mass, so invariance under Galilean boosts implies that the center of mass is conserved. In other words, we can boost to the center of mass frame of a hydrogen atom and the spectrum will remain the same.

Additionally, \vec{K} should generate boosts.

$$[\vec{\beta} \cdot \vec{K}, \vec{r}_i] = \vec{\beta} [(m_a \vec{r}_a - \vec{p}t), \vec{r}_i]$$

Write this with indices on everything. Raised indices refer to the vector ($\hat{x}, \hat{y}, \hat{z}$) while lowered indices refer to the particle number (1, 2). The $m_a \vec{r}_a$ term goes away because it commutes with \vec{r}_i , and we can reverse the commutator to reverse the sign on \vec{p} :

$$\begin{aligned} [\vec{\beta} \cdot \vec{K}, \vec{r}_i] &= \beta^A [r_i^A, (p_1^A + p_2^A)t] \\ &= \beta^A t ([r_1^A, p_1^A + p_2^A]) \\ \delta \vec{r}_i &= \vec{\beta} t (i\hbar \delta_{i1} + i\hbar \delta_{i2}) \end{aligned}$$

Recall that the infinitesimal transformation is

$$e^{i\vec{\beta} \cdot \vec{\mathbf{K}}/\hbar} \approx 1 + i\vec{\beta} \cdot \vec{\mathbf{K}}$$

so technically we should be computing

$$\left[\frac{i}{\hbar} \vec{\beta} \cdot \vec{\mathbf{K}}, \vec{\mathbf{r}}_i \right] = \delta \vec{\mathbf{r}}_i = -\beta t (\delta_{i1} + \delta_{i2})$$

This gives us the correct sign and form ($\vec{\mathbf{r}} = \vec{\mathbf{r}} - \vec{\beta}t$). When we change this to a quantum operator, we have

$$U(\vec{\beta}) = e^{i\vec{\beta} \cdot \vec{\mathbf{K}}/\hbar}$$

How does this act on the $\vec{\mathbf{r}}$ operator?

$$U^\dagger(\beta) \vec{\mathbf{r}} U(\beta) = \vec{\mathbf{r}} - \vec{\beta}t + \mathcal{O}(\beta^2) \approx \left(1 + \frac{i}{\hbar} \vec{\mathbf{K}} \cdot \vec{\beta}\right) \vec{\mathbf{r}} \left(1 - \frac{i}{\hbar} \vec{\mathbf{K}} \cdot \vec{\beta}\right) = \vec{\mathbf{r}} + \frac{i}{\hbar} [\vec{\mathbf{K}} \cdot \vec{\beta}, \vec{\mathbf{r}}]$$

Since the center of momentum position is invariant, it might be good to work in those coordinates. Let's also define $\vec{\mathbf{r}} = \vec{\mathbf{r}}_1 - \vec{\mathbf{r}}_2$:

$$\sum_{i=1}^2 \frac{1}{m_i} \dot{\vec{\mathbf{r}}}_i^2 = \frac{1}{2} M \dot{\vec{\mathbf{r}}}_{\text{com}}^2 + \frac{1}{2} \mu \dot{\vec{\mathbf{r}}}^2$$

where

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

and $M = m_1 + m_2$. Therefore, the Hamiltonian becomes

$$H = \frac{\vec{\mathbf{p}}_{\text{com}}^2}{2M} + \frac{\vec{\mathbf{p}}^2}{2\mu} - V(\vec{\mathbf{r}})$$

where $\vec{\mathbf{p}} = \mu \dot{\vec{\mathbf{r}}}$. We have changed a 2-body problem into a 1-body problem using this symmetry.

LECTURE 9: THE HYDROGEN ATOM, CONTINUED

Monday, February 03, 2020

Last time we used our knowledge of symmetries to reduce our two-body central force problem to a one-body problem in the center of mass frame:

$$H = \frac{\vec{\mathbf{p}}^2}{2\mu} + V(r) \left(+ \frac{\vec{\mathbf{p}}_{\text{com}}^2}{2M} \right)$$

The last term is not needed because it is conserved and has no effect on the equations of motion aside from offsetting the energy. In our discussion of symmetry, we found that things that commute with the Hamiltonian introduce degeneracies (since the symmetry operator acting on the state is an eigenstate with the same eigenvalue). In other words, if

$$[H, Q^a] = 0,$$

there may exist a degeneracy. If the representation of the group G (generated by Q^a) has dimension d , then there exists a d -fold degeneracy. Of course, a one-dimensional group representation would not introduce any degeneracy. We can move around states with raising and lowering operators, and those operators are made of things that commute with the Hamiltonian, so those raised and lowered states must be degenerate. So far, in our Hamiltonian, there are six conserved quantities in the vectors $\vec{\mathbf{K}}$ and $\vec{\mathbf{L}}$ corresponding to the center of mass momentum (boosts) and angular momentum (rotations). Of course, parity is also conserved, but recall that when we derived Noether's theorem, there are no conserved quantities arising from parity because it is a discrete symmetry. Boosts will not necessarily

create degeneracies because $[H, \vec{K}] \neq 0$, since $\vec{K} = M\vec{x} - \vec{p}t$ and $H_{\text{free}} = \frac{\vec{p}^2}{2\mu}$, so

$$[H_{\text{free}}, \vec{K}] = \left[\frac{\vec{p}^2}{2\mu}, M\vec{x} \right] = \frac{1}{2} [\vec{p}^2, \vec{x}] = -i\hbar\vec{p}$$

Note

$$[x, f(p)] = i\hbar f'(p)$$

However, \vec{L} does commute with the Hamiltonian, so we expect a $(2l+1)$ degeneracy for $\vec{L}^2 = \hbar^2 l(l+1)$. Since we have a central potential, it makes sense to work in spherical coordinates. In spherical coordinates, θ and φ are “cyclical” variables, so they won’t show up outside of derivatives in spherical coordinate formulation.

$$H = -\frac{\hbar^2 \nabla^2}{2\mu} + V(r) = f \left[\frac{\partial}{\partial r}, \frac{\partial}{\partial \theta}, \frac{\partial}{\partial \varphi}, r \right] = f \left[r, \frac{\partial}{\partial r}, \vec{L}^2 \right]$$

This means we can always write the energy eigenstates as

$$H\psi_E = E\psi_E$$

where

$$\psi_E = Y_l^m(\theta, \varphi) \tilde{\psi}_{l,m,E}(r)$$

Therefore, we can write

$$H = F \left[r, \frac{\partial}{\partial r}, l(l+1) \right]$$

when operating on wave functions of this form. In fact, if you work out the Laplacian in spherical coordinates,

$$H = -\frac{\hbar^2}{2\mu} \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{2mr^2} \vec{L}^2 + V(r)$$

If we operate this on energy eigenstates, the \vec{L} part will give

$$\frac{\hbar^2 l(l+1)}{2mr^2}$$

which is called the centrifugal barrier.

Notice that $H = H[l]$, but from undergraduate QM, we learn that the energy depends on n , not l . It turns out that hydrogen has more degeneracies than we expected. We have missed something in our analysis of the system.

If $V(r) \sim \frac{1}{r}$, there exist additional symmetries. In particular, there exists a conserved quantity resulting from the following operator:

$$\vec{A} = \frac{1}{2m} [\vec{p} \times \vec{L} - \vec{L} \times \vec{p}] - \frac{e^2 \vec{r}}{r}$$

We’ll come back to the units on this one, we haven’t really decided the units for charge yet. We claim that this vector commutes with H (this is on the homework this week). It has other interesting properties. In particular, it is Hermitian and orthogonal to \vec{L} ($\vec{A} \cdot \vec{L} = 0$). Additionally,

$$[L_i, A_j] = i\hbar \epsilon_{ijk} A_k \quad [A_i, A_j] = -\frac{2i\hbar H}{\mu} \epsilon_{ijk} L_k$$

Let’s now define a new vector by rescaling this one. This rescaling only makes sense for $E < 0$ bound states:

$$\tilde{\vec{A}} = \sqrt{\frac{-\mu}{E}} \vec{A}$$

and define

$$T_i = \frac{1}{2}(L_i + \tilde{A}_i) \quad S_i = \frac{1}{2}(L_i - \tilde{A}_i)$$

then

$$\begin{aligned} [T_i, T_j] &= \frac{1}{4} \left([L_i, L_j] + [\tilde{A}_i, L_j] + [L_i, \tilde{A}_j] + [\tilde{A}_i, \tilde{A}_j] \right) \\ &= \frac{1}{4} \left[i\hbar\epsilon_{ijk}L_k - i\hbar\epsilon_{jik}\tilde{A}_k + i\hbar\epsilon_{ijk}\tilde{A}_k - 2i\hbar\frac{H}{\mu}\epsilon_{ijk}L_k \left[\sqrt{-\frac{\mu}{E}} \right]^2 \right] \\ &= \frac{1}{4} \left[i\hbar\epsilon_{ijk}L_k + 2i\hbar\epsilon_{ijk}\tilde{A}_k + i\hbar\epsilon_{ijk}\tilde{A}_k + (2)i\hbar\epsilon_{ijk}L_k \right] \\ &= \frac{i\hbar}{2}\epsilon_{ijk}(L_k + \tilde{A}_k) = i\hbar\epsilon_{ijk}T_k \end{aligned}$$

so

$$[T_i, T_j] = i\hbar\epsilon_{ijk}T_k$$

In this derivation we are off by a factor of 2 for some reason, possibly in the scaling term. The professor is going to check this after class and send out an email, so I will hopefully incorporate it or you can just take my word for the final result. You should also find

$$[S_i, S_j] = i\hbar\epsilon_{ijk}S_k$$

and

$$[T_i, S_j] = 0$$

We've taken our conserved operators and reformed them into two operators which have a $\mathfrak{su}(2)$ Lie algebra. The symmetry group of this potential is actually $SU(2) \otimes SU(2)$. There is a $2l + 1$ degeneracy from each $SU(2)$ group, so there is a $(2l + 1)^2$ total degeneracy.

LECTURE 10: THE HYDROGEN ATOM, CONTINUED

Wednesday, February 05, 2020

Let's talk about units really quickly

$$H = \frac{\vec{p}^2}{2\mu} - \frac{e^2}{r}$$

where e^2 has units of length \cdot energy. Last time we showed that both angular momentum and the Runge-Lenz vector commute with the Hamiltonian, and from these vectors, we developed two new vectors, \vec{T} and \vec{S} and found they both have $SU(2)$ symmetry, so the symmetry group is $SU(2) \otimes SU(2)$. We would now expect the degeneracy to be $(2t + 1)(2s + 1)$, but we can show that $\vec{T}^2 = \vec{S}^2$ so $t = s$. Therefore, the true degeneracy is $(2t + 1)^2 = n^2$.

Notice that we haven't said anything about the Schrödinger equation yet, but we will be able to use these symmetries to determine the energy levels of hydrogen. We can do some clever rearranging to show that

$$4\vec{T}^2 = -\hbar^2 - \frac{me^4}{2E}$$

since

$$\vec{T}^2 = \frac{1}{4} [\vec{L}^2 + \tilde{\vec{A}}^2]$$

where

$$\begin{aligned} \tilde{\vec{A}} &= \sqrt{\frac{-m}{2E}} \vec{A} \\ \vec{A}^2 &= e^4 + \frac{2H}{m}(\vec{L}^2 + \hbar^2) \end{aligned}$$

The first equation can then be shown by expanding

$$\vec{T}^2 = \frac{1}{4} \left[\vec{L}^2 - \frac{m}{2E} \vec{A}^2 \right]$$

Then, using our knowledge of the degeneracies, we know that

$$\vec{T}^2 |t\rangle = t(t+1)\hbar^2 |t\rangle$$

or

$$\begin{aligned} \frac{me^4}{2E} &= (4t(t+1) + 1)\hbar^2 \\ \implies E &= \frac{me^4}{2\hbar^2 n^2} \quad n^2 = (2t+1)^2 \end{aligned}$$

0.7 The Hydrogen Wave Function

We know that the wave function should transform as a representation of $SU(2)$ so it has to be proportional to $Y_{lm}(\theta, \varphi)$. Therefore, just from group theory, we know that the wave function must take the form

$$\psi_{k,l} = Y_{lm}(\theta, \varphi) R_{kl}(r)$$

(recall that we showed the energy does not depend on m , but rather m introduces a degeneracy)

We can write the Hamiltonian in spherical coordinates as

$$H = -\frac{\hbar^2}{2\mu} \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{2\mu r^2} \vec{L}^2 + V(r)$$

Using the ansatz wave function, we know that

$$H R_{k,l}(r) = \left[-\frac{\hbar^2}{2\mu} \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r) \right]$$

Recall that

$$\mu = \frac{m_e m_p}{(m_e + m_p)}$$

but

$$m_p \sim 1\text{GeV} \quad m_e \sim 0.5\text{MeV}$$

so

$$\mu \sim m_p \equiv m$$

from here on out.

In principle, E does not depend on l —we showed that the Runge-Lenz vector conservation makes the energy only dependent on one quantum number. However, for the sake of the argument, let's pretend l still matters here:

$$H R_{kl} = E R_{kl}$$

Let's now define

$$R_{kl} = \frac{U_{kl}}{r}$$

such that

$$-\frac{\hbar^2}{2m} \frac{1}{r} U_{kl}'' + \frac{\hbar^2 l(l+1)}{2mr^3} U_{kl} - \frac{e^2}{r^2} U_{kl} = \frac{U_{kl}}{r}$$

we do this because $V = -\frac{e_e e_p}{r} = -\frac{e^2}{r}$. The reason these charges are the same has to do with quantum field theory and quark confinement. Let's divide out an $\frac{1}{r}$ everywhere to get

$$-\frac{\hbar^2}{2m} U'' + \left[\frac{\hbar^2 l(l+1)}{2mr^2} - \frac{e^2}{r} \right] U = E_{kl} U$$

At this point, it is useful to talk about dimensionful quantities:

$$[e^2] = \text{energy} \cdot \text{length}$$

$$[\hbar] = \text{energy} \cdot \text{time}$$

$$[m] = \frac{\text{energy} \cdot \text{time}^2}{\text{length}^2}$$

It might be useful to define a new length scale:

$$[a_0] \equiv \left[\frac{\hbar^2}{me^2} \right] = [\text{length}]$$

This is the only way to form length out of these variables, and we will find out that the average radius for the ground state orbits is exactly equal to this value. We will call this length scale the “Bohr radius”. We could have also known that e^2 had to be in the denominator, because as e^2 gets bigger, this radius should get smaller. We can also form a typical energy scale:

$$E_0 = \frac{e^4 m}{2\hbar^2}$$

Put a 2 in the denominator (we technically don’t know this is true from dimensional analysis, but we already know what the energy levels of Hydrogen are) and call this the “Rydberg constant”. Let’s work in our new scaled system with $\rho = \frac{r}{a_0}$

$$-\frac{\hbar^2}{2m} \frac{1}{a_0^2} \frac{d^2}{d\rho^2} U + \left[\frac{\hbar^2 l(l+1)}{2ma_0^2 \rho^2} - \frac{e^2}{a_0 \rho} \right] U = E_0 U$$

or

$$\left[\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + \frac{2}{\rho} - \lambda_{kl}^2 \right] U_{kl} = 0$$

where $\lambda_{kl} = \left[-\frac{E_{kl}}{E_0} \right]^{1/2}$. Solving this differential equation is hard, and we’re going to solve it by guessing. When $\rho \rightarrow \infty$,

$$(U'' - \lambda_{kl}^2 U) = 0$$

so

$$U \underset{\sim}{\overset{\rho \rightarrow \infty}{\sim}} e^{-\lambda_{kl} \rho}$$

This inspired guess is a series solution:

$$U = e^{-\lambda_{lm} \rho} \overbrace{\left(\sum_{q=0}^y C_q \rho^q \right)}^y \rho^S \quad (s > 0)$$

Now we plug this guess into our original differential equation. This gives a relationship between the C factors and a constraint that $S = l + 1$ and the series must terminate (since in theory if it didn’t, the power series could overcome the exponential and make the wave function non-normalizable):

$$C_q [q(q + 2l + 1)] = 2C_{q-1} [\lambda_{kl}(q + l) - 1]$$

$$\exists q \equiv \hat{k} \quad \text{such that} \quad \lambda_{kl}(\hat{k} + l) = 1$$

so

$$y_{kl} = \sum_{q=0}^{\hat{k}} [C_q \rho^q] \rho^{l+1}$$

and

$$\lambda_{k+l} = \frac{1}{\hat{k} + l} \in \mathbb{Z}$$

which we will define as $\lambda_n = \frac{1}{n}$.